

# Full wwPDB X-ray Structure Validation Report (i)

### May 17, 2020 – 09:13 pm BST

PDB ID : 4RE0

Title: Crystal structure of VmoLac in P622 space group

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Deposited on : 2014-09-20

Resolution : 2.35 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

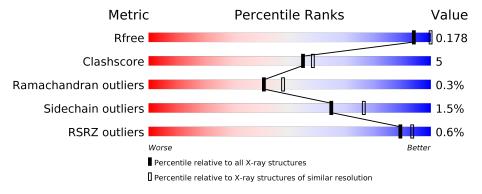
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.35 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 >=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 <=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	Α	316	89%	8%	•••



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2876 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	314	Total	С	N	О	S	0	6	0
1	A	314	2536	1629	437	462	8	0	0	0

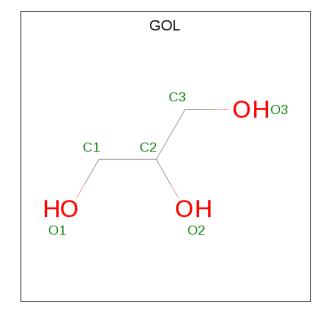
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Α	0	GLY	-	EXPRESSION TAG	UNP F0QXN6

• Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Co 2 2	0	0

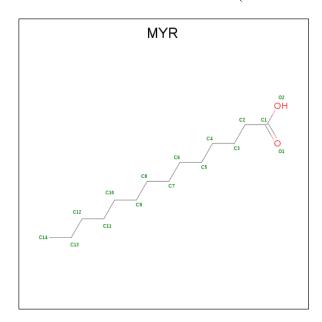
• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





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

 $\bullet$  Molecule 4 is MYRISTIC ACID (three-letter code: MYR) (formula:  $\mathrm{C}_{14}\mathrm{H}_{28}\mathrm{O}_2).$ 



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total C 0 16 14	O 2	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





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

• Molecule 6 is water.

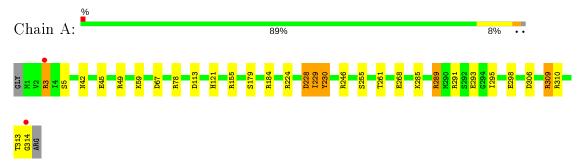
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	288	Total O 288 288	0	0



# 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: Parathion hydrolase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	134.67Å 134.67Å 126.40Å	Danagitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	46.08 - 2.35	Depositor
Resolution (A)	46.08 - 2.35	EDS
% Data completeness	100.0 (46.08-2.35)	Depositor
(in resolution range)	100.0 (46.08-2.35)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.60 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
D D.	0.140 , 0.170	Depositor
$R, R_{free}$	0.149 , 0.178	DCC
$R_{free}$ test set	1435 reflections $(4.99\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36, 40.5	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2876	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: GOL, MYR, CO, SO4, KCX

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).

Mal	Chain	Boı	nd lengths	Bond angles	
Mol   Chain		RMSZ	# Z  > 5	RMSZ	# Z >5
1	A	1.18	$4/2592 \ (0.2\%)$	1.18	$16/3510 \ (0.5\%)$

#### All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	A	268	GLU	CD-OE1	8.37	1.34	1.25
1	A	298	GLU	CD-OE1	6.69	1.33	1.25
1	A	309	ARG	CZ-NH1	-5.68	1.25	1.33
1	A	5	SER	CB-OG	-5.23	1.35	1.42

#### All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	228	ASP	CB-CG-OD1	-9.12	110.09	118.30
1	A	289[A]	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	289[B]	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	306	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	113	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	309	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	246	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	155	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	78	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	310	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	A	155	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	229	ILE	N-CA-C	-5.39	96.43	111.00
1	A	67	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	309	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	306	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	3	ARG	NE-CZ-NH2	5.23	122.92	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	2536	0	2589	24	0
2	A	2	0	0	0	0
3	A	24	0	32	0	0
4	A	16	0	27	4	0
5	A	10	0	0	0	0
6	A	288	0	0	14	3
All	All	2876	0	2648	27	3

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 5.

All (27) 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:179:SER:HB2	6:A:774:HOH:O	1.28	1.28
1:A:229:ILE:O	1:A:230:TYR:HB2	1.70	0.91
4:A:407:MYR:H21	6:A:772:HOH:O	1.72	0.87
1:A:229:ILE:O	1:A:230:TYR:CB	2.25	0.82
1:A:289[A]:ARG:NH1	6:A:709:HOH:O	2.15	0.78
1:A:42:ASN:CG	1:A:45[A]:GLU:HG3	2.06	0.76
1:A:49:ARG:NH2	1:A:261:THR:OG1	2.19	0.74
4:A:407:MYR:C2	6:A:772:HOH:O	2.30	0.73
1:A:121:HIS:HD2	6:A:624:HOH:O	1.76	0.68
1:A:184[A]:ARG:NH2	6:A:700:HOH:O	1.97	0.62
1:A:314:GLY:C	6:A:706:HOH:O	2.40	0.58
1:A:309:ARG:NH1	6:A:771:HOH:O	2.11	0.57
1:A:228:ASP:O	1:A:229:ILE:C	2.45	0.55
1:A:179:SER:CB	6:A:774:HOH:O	2.09	0.54
1:A:309:ARG:O	1:A:313:THR:HG23	2.09	0.53
1:A:224:ARG:HH21	4:A:407:MYR:H32	1.76	0.51
1:A:229:ILE:O	1:A:230:TYR:CG	2.64	0.51

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Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	Clash overlap (Å)
1:A:291[A]:ARG:HD2	1:A:295:ILE:O	2.12	0.49
1:A:184[A]:ARG:NE	6:A:700:HOH:O	2.46	0.49
1:A:228:ASP:C	1:A:229:ILE:O	2.47	0.49
1:A:42:ASN:ND2	1:A:45[A]:GLU:HG3	2.28	0.48
1:A:285:LYS:HE3	1:A:289[A]:ARG:HH21	1.78	0.47
1:A:289[A]:ARG:HD3	6:A:709:HOH:O	2.15	0.47
1:A:229:ILE:HD12	1:A:230:TYR:CD1	2.51	0.45
4:A:407:MYR:H22	6:A:772:HOH:O	2.09	0.44
1:A:314:GLY:HA3	6:A:580:HOH:O	2.17	0.44
1:A:228:ASP:OD1	6:A:780:HOH:O	2.21	0.42

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{aligned} &  ext{Interatomic} \ &  ext{distance} \ &  ext{(Å)} \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
6:A:755:HOH:O	6:A:773:HOH:O[12_545]	2.06	0.14
6:A:676:HOH:O	6:A:770:HOH:O[12_545]	2.07	0.13
6:A:570:HOH:O	6:A:726:HOH:O[8_555]	2.17	0.03

## 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	317/316 (100%)	306 (96%)	10 (3%)	1 (0%)	41 47	

#### All (1) Ramachandran outliers are listed below:

$\mathbf{Mol}$	Chain	Res	Type
1	A	230	TYR



### 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	275/270 (102%)	271 (98%)	4 (2%)	65 76	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	59	LYS
1	A	255	SER
1	A	293	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	90	ASN
1	A	251	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)

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 Re		Res	Link	Bond lengths			В	ond ang	gles	
MIOI	туре	Chain	nes Link		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	A	138	1,2	7,11,12	0.57	0	4,12,14	1.34	1 (25%)

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	$\mathbf{Type}$	Chain	${ m Res}$	Link	Chirals	Torsions	Rings
1	KCX	A	138	1,2	_	0/7/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	Α	138	KCX	CE-NZ-CX	-2.23	119.17	122.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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).

$ _{\mathbf{Mo}}$	Iol Type Chain Res Lin		Link	Bond lengths			Bond angles			
1010	l Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	409	-	4,4,4	0.97	0	6,6,6	1.40	1 (16%)



Mol	Т	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	403	-	5,5,5	1.44	1 (20%)	5,5,5	1.12	0
3	GOL	A	404	-	5,5,5	0.75	0	5,5,5	1.29	0
5	SO4	A	408	-	4,4,4	0.56	0	6,6,6	0.50	0
4	MYR	A	407	2	12,15,15	0.17	0	11,15,15	0.88	0
3	GOL	A	406	-	5,5,5	0.53	0	5,5,5	1.00	0
3	GOL	A	405	_	5,5,5	0.70	0	5,5,5	1.18	1 (20%)

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	MYR	A	407	2	-	11/11/13/13	_
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	A	406	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	A	404	-	-	1/4/4/4	-

#### All (1) bond length outliers are listed below:

$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$[Ideal(\AA)]$
3	A	403	GOL	O2-C2	2.34	1.50	1.43

#### All (2) bond angle outliers are listed below:

$\mathbf{Mol}$	Chain	${f Res}$	Type	${f Atoms}$	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^o)$
3	A	405	GOL	O3-C3-C2	2.16	120.54	110.20
5	A	409	SO4	O3-S-O2	2.07	120.09	109.31

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	407	MYR	C1-C2-C3-C4
3	A	406	GOL	C1-C2-C3-O3
3	A	405	GOL	C1-C2-C3-O3
4	A	407	MYR	C3-C4-C5-C6
4	A	407	MYR	C6-C7-C8-C9
3	A	404	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	407	MYR	C4-C5-C6-C7
3	A	406	GOL	O2-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
4	A	407	MYR	C11-C12-C13-C14
3	A	403	GOL	O1-C1-C2-O2
4	A	407	MYR	C11-C10-C9-C8
4	A	407	MYR	C7-C8-C9-C10
3	A	403	GOL	O2-C2-C3-O3
4	A	407	MYR	C9-C10-C11-C12
4	A	407	MYR	C10-C11-C12-C13
4	A	407	MYR	C5-C6-C7-C8
4	A	407	MYR	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407	MYR	4	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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	#RS	$\mathrm{SRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	313/316 (99%)	-0.55	2 (0%)	89 93	21, 30, 49, 87	0

#### All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ARG	2.1
1	A	314	GLY	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,  $95^{th}$  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	${f B-factors}({f A}^2)$	Q<0.9
1	KCX	A	138	12/13	0.97	0.10	21,24,26,27	0

## 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
3	GOL	A	406	6/6	0.77	0.35	74,85,92,93	0
3	GOL	A	405	6/6	0.79	0.20	68,76,98,110	0
3	GOL	A	403	6/6	0.83	0.27	51,60,66,71	0
5	SO4	A	408	5/5	0.84	0.45	81,105,120,127	0
3	GOL	A	404	6/6	0.93	0.28	53,67,71,86	0
4	MYR	A	407	16/16	0.94	0.22	31,58,68,81	0
5	SO4	A	409	5/5	0.98	0.27	30,32,37,38	5
2	CO	A	401	1/1	0.99	0.05	29,29,29,29	0
2	CO	Α	402	1/1	1.00	0.07	31,31,31,31	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

