



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2018 – 11:10 AM EDT

PDB ID : 4C13  
Title : x-ray crystal structure of Staphylococcus aureus MurE with UDP-MurNAc-Ala-Glu-Lys  
Authors : Ruane, K.M.; Roper, D.I.; Fulop, V.; Barreteau, H.; Boniface, A.; Dementin, S.; Blanot, D.; Mengin-Lecreulx, D.; Gobec, S.; Dessen, A.; Dowson, C.G.; Lloyd, A.J.  
Deposited on : 2013-08-09  
Resolution : 1.90 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
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-20031172

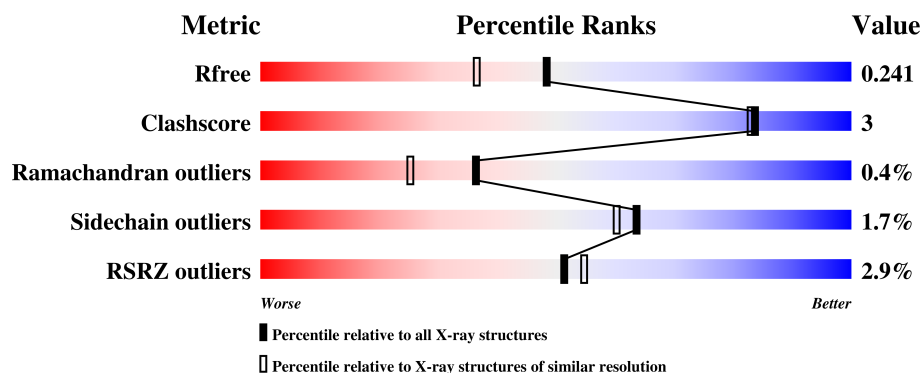
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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	501	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4075 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 UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--L-LYSINE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	2	0
			3786	2400	634	737	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	ARG	-	expression tag	UNP D4U2M7
A	495	SER	-	expression tag	UNP D4U2M7
A	496	HIS	-	expression tag	UNP D4U2M7
A	497	HIS	-	expression tag	UNP D4U2M7
A	498	HIS	-	expression tag	UNP D4U2M7
A	499	HIS	-	expression tag	UNP D4U2M7
A	500	HIS	-	expression tag	UNP D4U2M7
A	501	HIS	-	expression tag	UNP D4U2M7

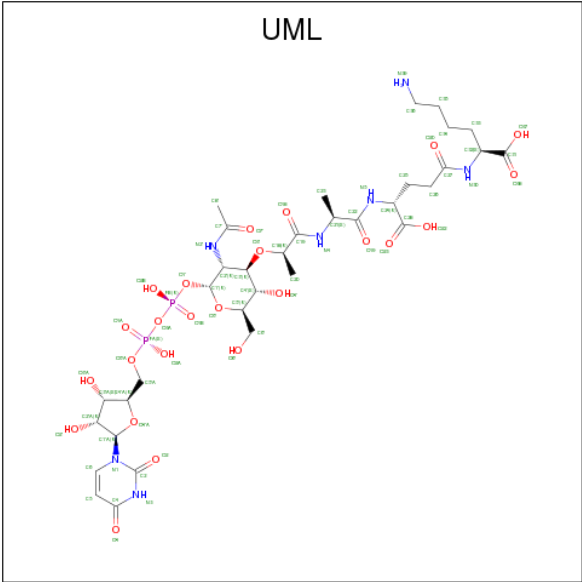
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

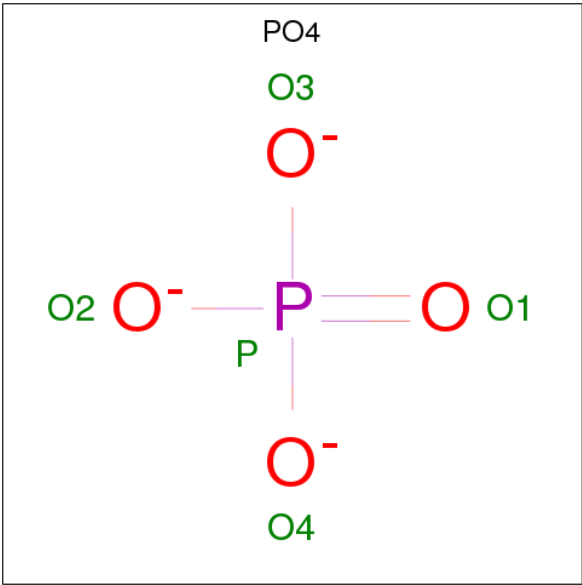
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is Uridine 5'Diphospho N-acetyl muramoyl-L-Alanyl-D-Glutamyl-L-Lysine (three-letter code: UML) (formula: C<sub>34</sub>H<sub>55</sub>N<sub>7</sub>O<sub>24</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			67	34	7	24	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	K 1	0	0

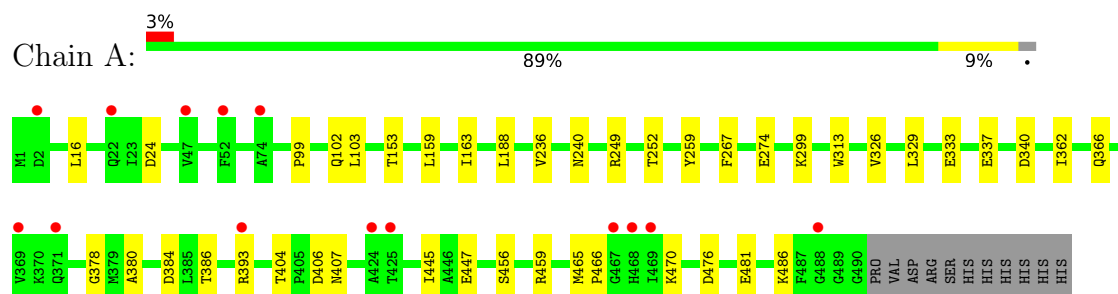
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	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: UDP-N-ACETYL-MURAMOYL-L-ALANYL-D-GLUTAMATE--L-LYSINE LIGASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.82Å 54.03Å 70.97Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	78.86 – 1.90 39.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.4 (78.86-1.90) 94.4 (39.43-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.196 , 0.241 0.195 , 0.241	Depositor DCC
$R_{free}$ test set	2271 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.9	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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: MG, CL, PO4, K, UML, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.77	1/3844 (0.0%)	0.81	1/5211 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	TRP	CD2-CE2	5.07	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ASP	CB-CG-OD1	5.42	123.18	118.30

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	3786	0	3758	20	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	67	0	51	0	0
5	A	5	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	213	0	0	1	0
All	All	4075	0	3809	20	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 3.

All (20) 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:384:ASP:OD1	1:A:386:THR:HG23	1.96	0.64
1:A:393:ARG:HH11	1:A:393:ARG:HG2	1.66	0.60
1:A:99:PRO:HB2	1:A:163:ILE:HG22	1.85	0.58
1:A:447:GLU:HG3	7:A:2205:HOH:O	2.05	0.55
1:A:236:VAL:HG21	1:A:252:THR:HG21	1.89	0.55
1:A:378:GLY:HA2	1:A:404:THR:O	2.08	0.53
1:A:362:ILE:O	1:A:366:GLN:HB2	2.10	0.52
1:A:326:VAL:HA	1:A:329:LEU:HG	1.93	0.50
1:A:259:TYR:HA	1:A:267:PHE:O	2.12	0.49
1:A:380:ALA:HA	1:A:406:ASP:O	2.13	0.49
1:A:333:GLU:HG3	1:A:459:ARG:HD2	1.94	0.49
1:A:337:GLU:CD	1:A:459:ARG:HH21	2.16	0.48
1:A:465:MET:HB3	1:A:466:PRO:HD2	1.93	0.48
1:A:153:THR:HG21	1:A:188:LEU:HD11	1.96	0.46
1:A:240:ASN:OD1	1:A:249[B]:ARG:NH2	2.48	0.46
1:A:159:LEU:HD23	1:A:159:LEU:C	2.39	0.43
1:A:274:GLU:OE2	1:A:299:LYS:NZ	2.44	0.43
1:A:459:ARG:NH1	1:A:476:ASP:OD2	2.48	0.42
1:A:406:ASP:O	1:A:407:ASN:C	2.58	0.42
1:A:465:MET:HB3	1:A:466:PRO:CD	2.50	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	489/501 (98%)	477 (98%)	10 (2%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	SER
1	A	340	ASP

### 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	411/426 (96%)	404 (98%)	7 (2%)	63	60

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

Mol	Chain	Res	Type
1	A	16	LEU
1	A	102	GLN
1	A	103	LEU
1	A	445	ILE
1	A	470	LYS
1	A	481	GLU
1	A	486	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	217	HIS

### 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	KCX	A	219	1,3	8,11,12	0.78	0	6,12,14	1.40	2 (33%)

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	KCX	A	219	1,3	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	KCX	O-C-CA	-2.30	118.66	124.96
1	A	219	KCX	CB-CA-C	-2.16	107.74	111.85

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 6 ligands modelled in this entry, 4 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
4	UML	A	598	-	55,69,69	1.28	5 (9%)	71,99,99	1.68	11 (15%)
5	PO4	A	601	3	4,4,4	1.90	1 (25%)	6,6,6	0.64	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	UML	A	598	-	-	0/56/105/105	0/3/3/3
5	PO4	A	601	3	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	598	UML	C25-C24	2.11	1.56	1.53
4	A	598	UML	PB-O1'	2.23	1.66	1.60
4	A	598	UML	C4-N3	2.76	1.38	1.33
5	A	601	PO4	P-O1	3.19	1.58	1.50
4	A	598	UML	O4-C4	4.35	1.35	1.24
4	A	598	UML	C32-N30	4.57	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	598	UML	PA-O3A-PB	-4.43	117.75	132.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	598	UML	C33-C32-C31	-4.26	105.78	112.11
4	A	598	UML	C23-C21-C22	-2.68	105.01	110.14
4	A	598	UML	C33-C32-N30	-2.68	106.27	110.19
4	A	598	UML	C1'-C2'-N2'	-2.62	106.32	111.00
4	A	598	UML	O20-C27-C26	-2.40	117.55	122.00
4	A	598	UML	C25-C24-C28	-2.29	108.72	112.11
4	A	598	UML	O3A-PB-O1'	2.07	106.75	102.53
4	A	598	UML	C26-C27-N30	2.31	119.82	115.83
4	A	598	UML	C23-C21-N4	3.30	116.49	110.36
4	A	598	UML	C4-N3-C2	6.88	120.06	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	489/501 (97%)	0.11	14 (2%) 51 55	10, 21, 36, 48	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	GLY	3.2
1	A	424	ALA	2.9
1	A	488	GLY	2.6
1	A	371	GLN	2.4
1	A	47	VAL	2.4
1	A	52	PHE	2.4
1	A	468	HIS	2.4
1	A	369	VAL	2.3
1	A	74	ALA	2.3
1	A	22	GLN	2.3
1	A	469	ILE	2.3
1	A	2	ASP	2.2
1	A	425	THR	2.1
1	A	393	ARG	2.0

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

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	KCX	A	219	12/13	0.98	0.12	9,11,12,12	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<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	CL	A	502	1/1	0.94	0.17	46,46,46,46	0
4	UML	A	598	67/67	0.95	0.10	12,19,29,30	0
5	PO4	A	601	5/5	0.96	0.10	21,22,26,28	0
6	K	A	605	1/1	0.97	0.08	32,32,32,32	0
3	MG	A	503	1/1	0.98	0.08	26,26,26,26	0
3	MG	A	504	1/1	0.98	0.08	26,26,26,26	0

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

There are no such residues in this entry.