



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:45 pm BST

PDB ID : 2CUA  
Title : THE CUA DOMAIN OF CYTOCHROME BA3 FROM THERMUS THERMOPHILUS  
Authors : Williams, P.A.; Blackburn, N.J.; Sanders, D.; Bellamy, H.; Stura, E.A.; Fee, J.A.; Mccree, D.E.  
Deposited on : 1999-02-18  
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

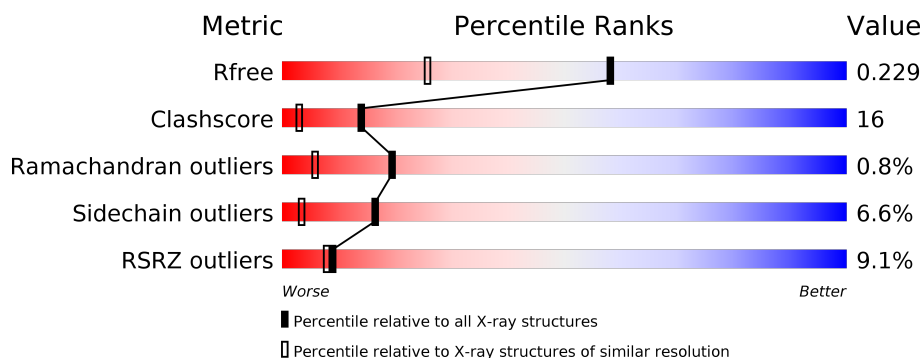
# 1 Overall quality at a glance

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	135	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	135	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>...</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2170 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.

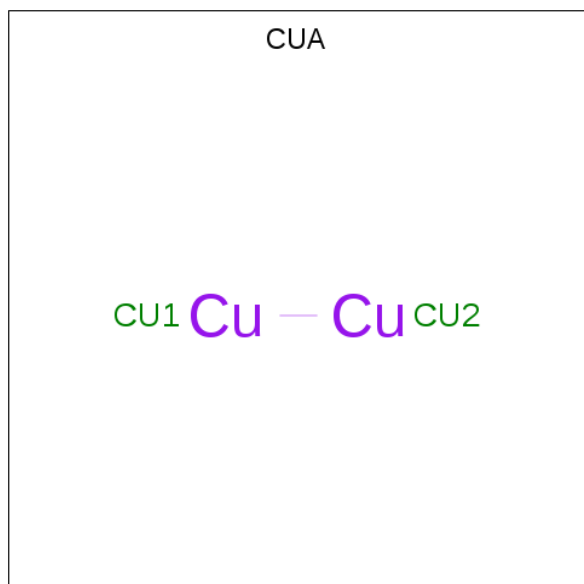
- Molecule 1 is a protein called PROTEIN (CUA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			955	612	162	178	3			
1	B	132	Total	C	N	O	S	0	0	0
			1023	655	174	191	3			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 2 2	0	0
3	B	1	Total Cu 2 2	0	0

- Molecule 4 is water.

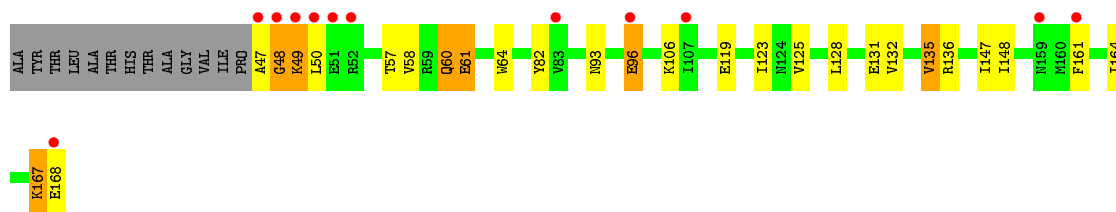
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	94	Total O 94 94	0	0
4	B	92	Total O 92 92	0	0

### 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.

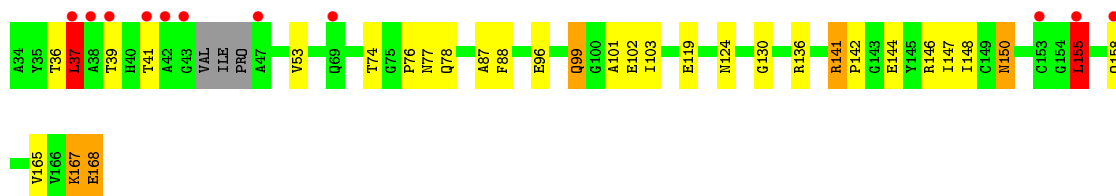
#### • Molecule 1: PROTEIN (CUA)

Chain A: 



#### • Molecule 1: PROTEIN (CUA)

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	34.90 Å   70.60 Å   53.50 Å 90.00°   98.12°   90.00°	Depositor
Resolution (Å)	50.00 – 1.60 24.79 – 1.50	Depositor EDS
% Data completeness (in resolution range)	88.7 (50.00-1.60) 69.2 (24.79-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	SHELXL-97, XTALVIEW	Depositor
R, $R_{free}$	0.226   ,   0.296 0.198   ,   0.229	Depositor DCC
$R_{free}$ test set	1490 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 67.7	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

<sup>1</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: ZN, CUA

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	2.57	2/980 (0.2%)	1.00	1/1336 (0.1%)
1	B	1.95	2/1050 (0.2%)	1.16	1/1433 (0.1%)
All	All	2.27	4/2030 (0.2%)	1.09	2/2769 (0.1%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	C-OXT	79.20	2.73	1.23
1	B	168	GLU	C-OXT	61.12	2.39	1.23
1	A	119	GLU	CD-OE2	7.90	1.34	1.25
1	B	119	GLU	CD-OE2	6.96	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	37	LEU	C-N-CA	11.13	149.52	121.70
1	A	48	GLY	CA-C-O	8.60	136.09	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	144	GLU	Sidechain

## 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	955	0	927	25	0
1	B	1023	0	987	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	94	0	0	1	0
4	B	92	0	0	4	0
All	All	2170	0	1914	60	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 16.

All (60) 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:168:GLU:OXT	1:B:168:GLU:HA	1.35	1.23
1:B:168:GLU:CA	1:B:168:GLU:OXT	2.07	1.02
1:A:48:GLY:C	1:A:49:LYS:N	2.16	0.98
1:A:50:LEU:HD12	1:A:106:LYS:HE3	1.60	0.84
1:B:36:THR:HG22	1:B:37:LEU:HB2	1.60	0.83
1:B:77:ASN:ND2	1:B:101:ALA:HA	2.03	0.74
1:A:128:LEU:HD12	1:A:131:GLU:OE1	1.88	0.74
1:A:57:THR:HB	1:A:61:GLU:HG3	1.71	0.72
1:A:50:LEU:HD11	1:A:82:TYR:HE1	1.53	0.71
1:B:102:GLU:OE2	1:B:136:ARG:HB3	1.93	0.69
1:B:37:LEU:HG	1:B:39:THR:N	2.08	0.67
1:A:96:GLU:HB3	1:A:167:LYS:HE3	1.80	0.63
1:B:148:ILE:HG23	4:B:6132:HOH:O	1.99	0.62
1:A:57:THR:HA	1:A:60:GLN:NE2	2.16	0.60
1:B:168:GLU:C	1:B:168:GLU:OXT	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLU:HG3	1:B:167:LYS:HD3	1.82	0.60
1:A:49:LYS:HZ1	1:A:136:ARG:NH2	2.00	0.60
1:A:58:VAL:HA	4:A:6135:HOH:O	2.04	0.57
1:B:99:GLN:OE1	1:B:168:GLU:HG2	2.04	0.57
1:B:96:GLU:CG	1:B:167:LYS:HZ3	2.18	0.56
1:B:96:GLU:CB	1:B:167:LYS:HZ3	2.19	0.56
1:B:146:ARG:HG2	1:B:148:ILE:HD11	1.87	0.55
1:B:99:GLN:NE2	1:B:142:PRO:HD3	2.22	0.54
1:A:148:ILE:HG22	1:A:161:PHE:CD1	2.42	0.53
1:A:50:LEU:HD12	1:A:106:LYS:CE	2.36	0.53
1:B:96:GLU:HG3	1:B:167:LYS:HZ3	1.73	0.53
1:B:76:PRO:HD2	1:B:78:GLN:NE2	2.23	0.52
1:A:136:ARG:HG3	1:A:136:ARG:HH11	1.74	0.52
1:B:147:ILE:O	1:B:148:ILE:HD13	2.08	0.52
1:B:155:LEU:H	1:B:155:LEU:HD23	1.73	0.51
1:A:50:LEU:HB3	1:A:132:VAL:HG21	1.93	0.51
1:B:96:GLU:O	1:B:96:GLU:HG2	2.11	0.50
1:A:50:LEU:HD22	1:A:64:TRP:HH2	1.76	0.50
1:B:96:GLU:HB2	1:B:167:LYS:HZ3	1.76	0.50
1:B:77:ASN:HD21	1:B:101:ALA:HA	1.77	0.49
1:B:102:GLU:HG3	4:B:6045:HOH:O	2.11	0.49
1:B:74:THR:O	1:B:74:THR:HG22	2.13	0.49
1:A:50:LEU:HB3	1:A:132:VAL:HG11	1.95	0.49
1:A:47:ALA:N	1:A:48:GLY:HA2	2.26	0.49
1:B:53:VAL:O	1:B:130:GLY:HA2	2.13	0.48
1:A:147:ILE:HD11	1:A:164:ILE:HG13	1.96	0.48
1:A:50:LEU:CB	1:A:132:VAL:HG11	2.43	0.48
1:A:48:GLY:O	1:A:49:LYS:N	2.47	0.47
1:A:57:THR:HA	1:A:60:GLN:HE21	1.77	0.47
1:A:125:VAL:HG11	1:A:135:VAL:HG12	1.98	0.45
1:B:146:ARG:HG2	1:B:148:ILE:CD1	2.47	0.45
1:B:167:LYS:HE3	1:B:167:LYS:HB3	1.55	0.45
1:B:141:ARG:HA	1:B:142:PRO:HD3	1.70	0.44
1:B:124:ASN:ND2	4:B:6002:HOH:O	2.50	0.44
1:B:74:THR:HB	4:B:6130:HOH:O	2.17	0.44
1:B:124:ASN:ND2	1:B:150:ASN:OD1	2.50	0.44
1:A:50:LEU:HD11	1:A:82:TYR:CE1	2.43	0.43
1:A:50:LEU:HD22	1:A:64:TRP:CH2	2.52	0.42
1:B:96:GLU:HG3	1:B:167:LYS:CD	2.47	0.42
1:A:123:ILE:HG23	1:A:135:VAL:HG21	2.02	0.42
1:B:165:VAL:CG1	1:B:167:LYS:HZ1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG11	1:A:135:VAL:CG1	2.50	0.41
1:B:102:GLU:OE1	1:B:103:ILE:N	2.53	0.41
1:B:87:ALA:HB1	1:B:88:PHE:CZ	2.56	0.41
1:B:87:ALA:HA	1:B:88:PHE:HA	1.90	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	118/135 (87%)	115 (98%)	3 (2%)	0	100	100
1	B	128/135 (95%)	120 (94%)	6 (5%)	2 (2%)	9	1
All	All	246/270 (91%)	235 (96%)	9 (4%)	2 (1%)	19	6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155	LEU
1	B	41	THR

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/112 (92%)	96 (93%)	7 (7%)	16	3
1	B	108/112 (96%)	101 (94%)	7 (6%)	17	3
All	All	211/224 (94%)	197 (93%)	14 (7%)	16	3

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	60	GLN
1	A	61	GLU
1	A	93	ASN
1	A	96	GLU
1	A	135	VAL
1	A	167	LYS
1	B	37	LEU
1	B	99	GLN
1	B	141	ARG
1	B	150	ASN
1	B	155	LEU
1	B	158	GLN
1	B	167	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	93	ASN
1	B	60	GLN
1	B	77	ASN
1	B	78	GLN
1	B	124	ASN
1	B	151	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
3	CUA	A	169	1	0,1,1	0.00	-	-		
3	CUA	B	170	1	0,1,1	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	48:GLY	C	49:LYS	N	2.16

## 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	122/135 (90%)	0.85	12 (9%) <b>7</b> <b>6</b>	12, 21, 48, 158	0
1	B	132/135 (97%)	0.50	11 (8%) <b>11</b> <b>10</b>	10, 20, 47, 97	0
All	All	254/270 (94%)	0.67	23 (9%) <b>9</b> <b>8</b>	10, 20, 49, 158	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	ALA	15.8
1	A	50	LEU	12.1
1	B	41	THR	9.3
1	A	48	GLY	9.2
1	A	49	LYS	8.3
1	B	43	GLY	7.1
1	B	155	LEU	6.5
1	B	37	LEU	6.3
1	B	39	THR	5.6
1	A	168	GLU	4.0
1	A	159	ASN	3.3
1	B	42	ALA	3.2
1	A	52	ARG	3.0
1	A	51	GLU	2.8
1	B	153	CYS	2.6
1	A	83	VAL	2.5
1	A	107	ILE	2.4
1	A	96	GLU	2.4
1	B	69	GLN	2.4
1	B	158	GLN	2.1
1	A	161	PHE	2.1
1	B	47	ALA	2.0
1	B	38	ALA	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( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	171	1/1	0.97	0.08	29,29,29,29	0
3	CUA	A	169	2/2	0.99	0.06	18,18,18,18	0
3	CUA	B	170	2/2	0.99	0.04	18,18,18,20	0
2	ZN	B	172	1/1	0.99	0.04	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.