



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 09:22 PM BST

PDB ID : 5ZOU  
Title : Copper amine oxidase from *Arthrobacter globiformis* anaerobically reduced by ethylamine at pH6 at 288 K (1)  
Authors : Murakawa, T.; Baba, S.; Kawano, Y.; Hayashi, H.; Yano, T.; Tanizawa, K.; Kumasaka, T.; Yamamoto, M.; Okajima, T.  
Deposited on : 2018-04-16  
Resolution : 1.68 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.

---

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	:	2.13
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)	:	2.13

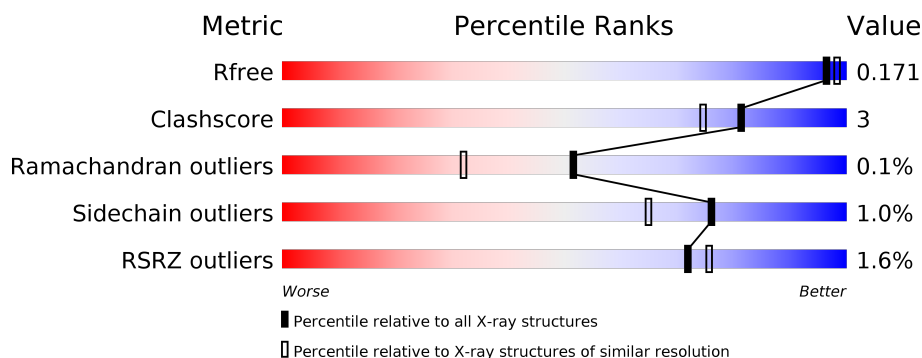
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	620	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>95%</span> <span>5%</span> </div> </div>
1	B	620	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>2%</span> <span>94%</span> <span>5%</span> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10903 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	9	0
			4916	3112	860	934	10			
1	B	620	Total	C	N	O	S	0	15	0
			4960	3142	868	940	10			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

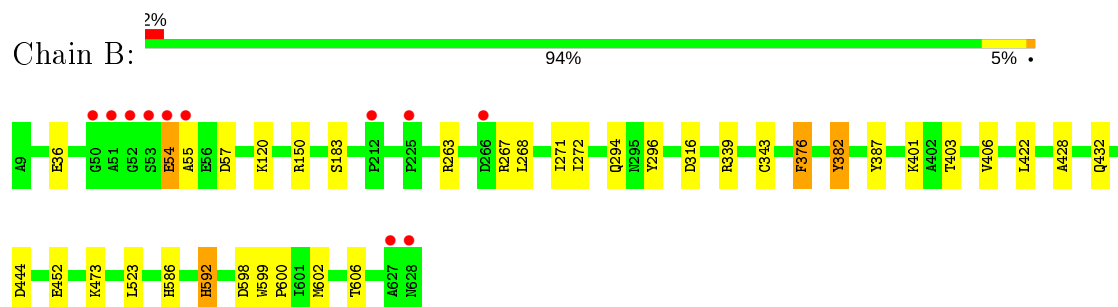
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	480	Total	O	0	3
			480	480		
4	B	544	Total	O	0	3
			544	544		



- Molecule 1: Phenylethylamine oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.44Å 64.24Å 158.81Å 90.00° 117.12° 90.00°	Depositor
Resolution (Å)	40.35 – 1.68 45.48 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.8 (40.35-1.68) 92.5 (45.48-1.68)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.154 , 0.172 0.153 , 0.171	Depositor DCC
$R_{free}$ test set	9579 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8517e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NA, TYQ, CU

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	0.34	0/5036	0.58	0/6858
1	B	0.34	0/5093	0.59	2/6933 (0.0%)
All	All	0.34	0/10129	0.59	2/13791 (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	B	343[A]	CYS	CA-CB-SG	5.57	124.03	114.00
1	B	343[B]	CYS	CA-CB-SG	5.57	124.03	114.00

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	4916	0	4766	23	0
1	B	4960	0	4817	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	1	0	0	0	0
4	A	480	0	0	4	0
4	B	544	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10903	0	9583	50	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 (50) 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:452:GLU:O	4:B:801:HOH:O	1.92	0.85
1:B:473:LYS:NZ	4:B:801:HOH:O	1.93	0.83
1:A:532:ARG:HG3	1:A:563:GLY:HA3	1.73	0.70
1:A:532:ARG:NH2	4:A:1101:HOH:O	2.24	0.69
1:B:150[A]:ARG:NH1	4:B:802:HOH:O	2.27	0.66
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.61	0.66
1:A:490:ARG:NH1	4:A:1102:HOH:O	2.27	0.65
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.34	0.62
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.35	0.61
1:B:54:GLU:OE2	1:B:57:ASP:HB3	2.04	0.58
1:B:150[A]:ARG:NH1	4:B:804:HOH:O	2.38	0.56
1:B:422:LEU:HD11	1:B:428:ALA:HB2	1.90	0.54
1:A:263:ARG:HG2	1:A:263:ARG:NH1	2.19	0.53
1:B:54:GLU:CD	1:B:57:ASP:HB3	2.28	0.53
1:B:592:HIS:NE2	1:B:602:MET:HE1	2.23	0.53
1:A:237:HIS:HE1	1:A:239:GLU:OE1	1.91	0.53
1:B:54:GLU:OE1	1:B:57:ASP:N	2.42	0.52
1:B:263[A]:ARG:HG2	1:B:268:LEU:HD13	1.91	0.52
1:A:106:GLU:OE1	1:A:106:GLU:N	2.22	0.52
1:A:263:ARG:NH2	4:A:1108:HOH:O	2.41	0.52
1:B:267:ARG:NH2	4:B:809:HOH:O	2.44	0.51
1:B:271:ILE:HG22	1:B:272:ILE:HG13	1.94	0.50
1:A:271:ILE:HG22	1:A:272:ILE:HG13	1.94	0.49
1:A:145:ALA:O	1:A:148:ARG:HD3	2.13	0.48
1:A:36:GLU:CD	1:A:36:GLU:H	2.17	0.48
1:B:406[B]:VAL:HG22	1:B:602:MET:HE3	1.96	0.48
1:B:150[A]:ARG:HH22	1:B:183:SER:HB3	1.78	0.48
1:A:351[A]:ILE:HD11	1:B:316:ASP:HA	1.96	0.48
1:B:406[B]:VAL:HG23	4:B:953:HOH:O	2.14	0.47
1:B:382[B]:TYQ:HD2	1:B:403:THR:O	2.15	0.47
1:A:280:MET:HG3	1:A:298:ASP:HB2	1.95	0.47
1:B:592:HIS:HE1	1:B:598:ASP:OD2	1.97	0.47
1:A:532:ARG:HG2	1:A:532:ARG:HH11	1.80	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:NH1	4:A:1116:HOH:O	2.48	0.46
1:A:13:ARG:NH1	1:A:56:GLU:OE2	2.40	0.46
1:B:432:GLN:HE22	1:B:523:LEU:H	1.64	0.45
1:B:586:HIS:HE1	4:B:978:HOH:O	1.99	0.45
1:A:106:GLU:CD	1:A:106:GLU:H	2.10	0.45
1:A:146:GLU:O	1:A:150:ARG:HD3	2.17	0.45
1:A:422:LEU:HD11	1:A:428:ALA:HB2	1.98	0.44
1:A:237:HIS:HD2	1:A:246:ASP:OD1	1.99	0.44
1:B:376:PHE:HE1	1:B:387:TYR:OH	2.00	0.43
1:A:296:TYR:CE2	1:A:382[A]:TYQ:N5	2.87	0.42
1:B:36:GLU:OE2	1:B:36:GLU:N	2.39	0.42
1:B:401:LYS:HG2	1:B:606:THR:HG22	2.02	0.42
1:A:154:ARG:HD3	1:A:178:TYR:CE1	2.55	0.41
1:B:296[A]:TYR:CE2	1:B:382[A]:TYQ:N5	2.88	0.41
1:B:296[A]:TYR:CZ	1:B:382[A]:TYQ:N5	2.84	0.41
1:B:294:GLN:OE1	1:B:296[B]:TYR:OH	2.19	0.40

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	625/620 (101%)	605 (97%)	20 (3%)	0	100	100
1	B	631/620 (102%)	608 (96%)	22 (4%)	1 (0%)	47	29
All	All	1256/1240 (101%)	1213 (97%)	42 (3%)	1 (0%)	51	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	55	ALA



### 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	521/513 (102%)	517 (99%)	4 (1%)	81	72
1	B	526/513 (102%)	520 (99%)	6 (1%)	73	61
All	All	1047/1026 (102%)	1037 (99%)	10 (1%)	76	65

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	184	LYS
1	A	376	PHE
1	A	444	ASP
1	B	54	GLU
1	B	120	LYS
1	B	339	ARG
1	B	376	PHE
1	B	444	ASP
1	B	592	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	237	HIS
1	A	259	ASN
1	B	24	GLN
1	B	259	ASN
1	B	431	HIS
1	B	432	GLN
1	B	586	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	TYQ	B	382[A]	-	13,14,15	1.13	1 (7%)	15,19,21	2.02	4 (26%)
1	TYQ	A	382[A]	-	13,14,15	1.17	1 (7%)	15,19,21	2.07	3 (20%)
1	TYQ	A	382[B]	2	13,14,15	1.12	1 (7%)	15,19,21	1.55	3 (20%)
1	TYQ	B	382[B]	2	13,14,15	0.95	0	15,19,21	1.72	3 (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
1	TYQ	B	382[A]	-	-	2/5/6/8	0/1/1/1
1	TYQ	A	382[A]	-	-	2/5/6/8	0/1/1/1
1	TYQ	A	382[B]	2	-	3/5/6/8	0/1/1/1
1	TYQ	B	382[B]	2	-	3/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382[A]	TYQ	CB-CG	-3.05	1.47	1.51
1	B	382[A]	TYQ	CB-CG	-2.71	1.48	1.51
1	A	382[B]	TYQ	CB-CG	-2.19	1.48	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382[A]	TYQ	CB-CA-C	-5.25	101.63	111.47
1	B	382[A]	TYQ	CB-CA-C	-4.63	102.78	111.47
1	B	382[B]	TYQ	CG-CB-CA	-3.51	109.10	114.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382[B]	TYQ	OH-CZ-CE2	3.36	121.88	116.25
1	A	382[A]	TYQ	OH-CZ-CE2	3.34	121.83	116.25
1	B	382[A]	TYQ	OH-CZ-CE2	3.32	121.81	116.25
1	B	382[A]	TYQ	CZ-CE2-N5	3.01	123.56	118.77
1	A	382[B]	TYQ	CG-CB-CA	-2.74	110.29	114.53
1	A	382[A]	TYQ	CZ-CE2-N5	2.67	123.01	118.77
1	A	382[B]	TYQ	OH-CZ-CE2	2.54	120.50	116.25
1	A	382[B]	TYQ	CB-CA-C	-2.38	107.00	111.47
1	B	382[A]	TYQ	CB-CG-CD1	2.26	123.31	120.95
1	B	382[B]	TYQ	CB-CA-C	-2.14	107.45	111.47

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	382[A]	TYQ	N-CA-CB-CG
1	A	382[A]	TYQ	N-CA-CB-CG
1	A	382[A]	TYQ	C-CA-CB-CG
1	A	382[B]	TYQ	C-CA-CB-CG
1	B	382[B]	TYQ	C-CA-CB-CG
1	A	382[B]	TYQ	N-CA-CB-CG
1	B	382[B]	TYQ	N-CA-CB-CG
1	A	382[B]	TYQ	CA-CB-CG-CD2
1	B	382[A]	TYQ	C-CA-CB-CG
1	B	382[B]	TYQ	CA-CB-CG-CD2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	382[A]	TYQ	3	0
1	A	382[A]	TYQ	1	0
1	B	382[B]	TYQ	1	0

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	619/620 (99%)	-0.23	9 (1%) 73 77	12, 24, 49, 156	0
1	B	619/620 (99%)	-0.33	11 (1%) 68 72	11, 21, 41, 161	0
All	All	1238/1240 (99%)	-0.28	20 (1%) 72 75	11, 22, 45, 161	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	ALA	19.0
1	B	51	ALA	18.9
1	A	52	GLY	12.2
1	B	52	GLY	10.7
1	B	54	GLU	8.9
1	B	53	SER	7.5
1	A	50	GLY	7.0
1	B	55	ALA	6.8
1	A	54	GLU	5.9
1	A	55	ALA	4.4
1	A	53	SER	4.2
1	B	628	ASN	4.0
1	A	628	ASN	4.0
1	B	50	GLY	3.5
1	B	627	ALA	3.2
1	A	145	ALA	3.0
1	B	266	ASP	2.2
1	A	462	PRO	2.2
1	B	212	PRO	2.1
1	B	225	PRO	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<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
1	TYQ	A	382[A]	14/15	0.94	0.14	17,35,40,42	11
1	TYQ	A	382[B]	14/15	0.94	0.14	17,30,39,48	11
1	TYQ	B	382[A]	14/15	0.97	0.12	15,30,32,34	11
1	TYQ	B	382[B]	14/15	0.97	0.12	15,26,39,51	11

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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	CU	B	701	1/1	0.99	0.06	18,18,18,18	0
2	CU	A	1001	1/1	0.99	0.07	19,19,19,19	0
3	NA	B	702	1/1	1.00	0.06	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.