



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:57 AM GMT

PDB ID : 2YXW
Title : The deletion mutant of Multicopper Oxidase CueO
Authors : Higuchi, Y.; Komori, H.
Deposited on : 2007-04-27
Resolution : 1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

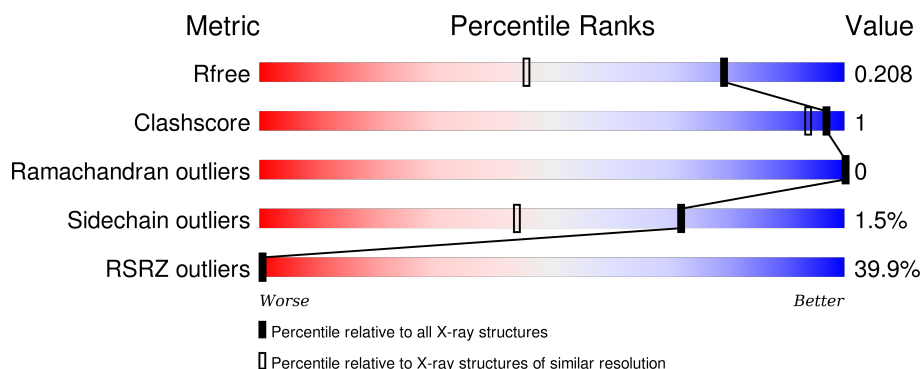
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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. 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	446	<div> <div>38%</div> <div>94%</div> <div>..</div> </div>
1	B	446	<div> <div>41%</div> <div>95%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	A	706	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7442 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 Blue copper oxidase cueO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3365	2139	591	617	18			
1	B	444	Total	C	N	O	S	0	0	0
			3406	2163	603	622	18			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	GLY	PRO	ENGINEERED	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	LEU	DELETION	UNP P36649
A	?	-	ASP	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	GLN	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	LEU	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	GLU	DELETION	UNP P36649
A	?	-	LYS	DELETION	UNP P36649
A	?	-	TYR	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	ASP	DELETION	UNP P36649
A	?	-	GLN	DELETION	UNP P36649
A	?	-	ALA	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	ALA	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	ASP	DELETION	UNP P36649
A	?	-	HIS	DELETION	UNP P36649

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP P36649
A	?	-	GLN	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	HIS	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	HIS	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	ASN	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	ASN	DELETION	UNP P36649
A	?	-	HIS	DELETION	UNP P36649
A	?	-	MET	DELETION	UNP P36649
A	?	-	ASN	DELETION	UNP P36649
A	?	-	HIS	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	GLY	DELETION	UNP P36649
A	?	-	LYS	DELETION	UNP P36649
A	?	-	PHE	DELETION	UNP P36649
A	?	-	ASP	DELETION	UNP P36649
A	?	-	PHE	DELETION	UNP P36649
A	?	-	HIS	DELETION	UNP P36649
A	406	GLY	HIS	ENGINEERED	UNP P36649
A	517	GLY	-	EXPRESSION TAG	UNP P36649
A	518	HIS	-	EXPRESSION TAG	UNP P36649
A	519	HIS	-	EXPRESSION TAG	UNP P36649
A	520	HIS	-	EXPRESSION TAG	UNP P36649
A	521	HIS	-	EXPRESSION TAG	UNP P36649
A	522	HIS	-	EXPRESSION TAG	UNP P36649
B	357	GLY	PRO	ENGINEERED	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	LEU	DELETION	UNP P36649
B	?	-	ASP	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	GLN	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	LEU	DELETION	UNP P36649

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	DELETION	UNP P36649
B	?	-	GLU	DELETION	UNP P36649
B	?	-	LYS	DELETION	UNP P36649
B	?	-	TYR	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	ASP	DELETION	UNP P36649
B	?	-	GLN	DELETION	UNP P36649
B	?	-	ALA	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	ALA	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	ASP	DELETION	UNP P36649
B	?	-	HIS	DELETION	UNP P36649
B	?	-	SER	DELETION	UNP P36649
B	?	-	GLN	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	HIS	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	HIS	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	ASN	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	ASN	DELETION	UNP P36649
B	?	-	HIS	DELETION	UNP P36649
B	?	-	MET	DELETION	UNP P36649
B	?	-	ASN	DELETION	UNP P36649
B	?	-	HIS	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	GLY	DELETION	UNP P36649
B	?	-	LYS	DELETION	UNP P36649
B	?	-	PHE	DELETION	UNP P36649
B	?	-	ASP	DELETION	UNP P36649
B	?	-	PHE	DELETION	UNP P36649
B	?	-	HIS	DELETION	UNP P36649
B	406	GLY	HIS	ENGINEERED	UNP P36649
B	517	GLY	-	EXPRESSION TAG	UNP P36649
B	518	HIS	-	EXPRESSION TAG	UNP P36649
B	519	HIS	-	EXPRESSION TAG	UNP P36649

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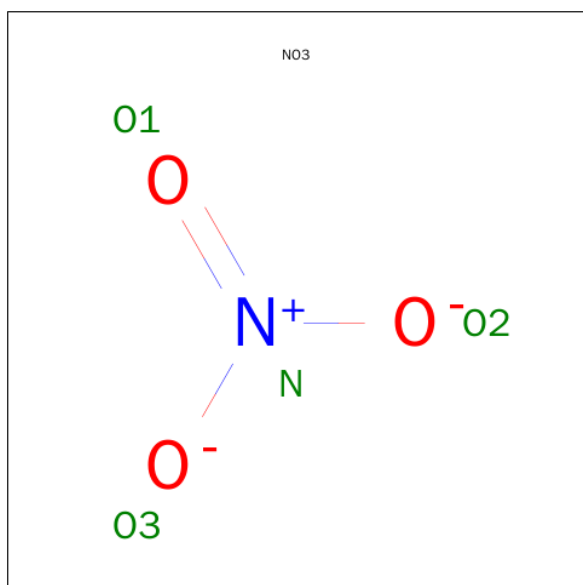
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Chain	Residue	Modelled	Actual	Comment	Reference
B	520	HIS	-	EXPRESSION TAG	UNP P36649
B	521	HIS	-	EXPRESSION TAG	UNP P36649
B	522	HIS	-	EXPRESSION TAG	UNP P36649

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

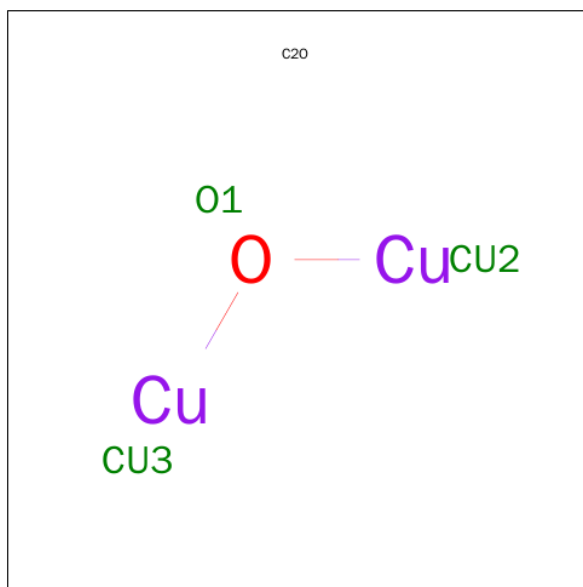
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cu	0	0
			3	3		
2	A	3	Total	Cu	0	0
			3	3		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		

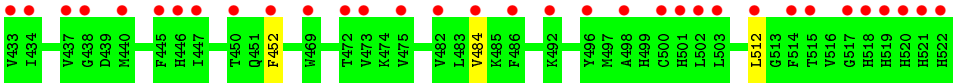
- Molecule 4 is CU-O-CU LINKAGE (three-letter code: C2O) (formula: Cu₂O).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	353	Total	O	0	0
			353	353		
5	B	302	Total	O	0	0
			302	302		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.33Å 51.57Å 86.70Å 83.77° 90.38° 67.14°	Depositor
Resolution (Å)	25.90 – 1.50 25.94 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.90-1.50) 91.4 (25.94-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.177 , 0.207 0.181 , 0.208	Depositor DCC
R_{free} test set	6113 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 121074 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7442	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: C2O, CU, NO3

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	0.55	1/3450 (0.0%)	0.69	0/4696
1	B	0.44	0/3495	0.63	0/4756
All	All	0.50	1/6945 (0.0%)	0.66	0/9452

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	ASN	CG-ND2	6.63	1.49	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ASN	Peptide

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	3365	0	3352	10	0
1	B	3406	0	3380	8	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	353	0	0	2	0
5	B	302	0	0	1	0
All	All	7442	0	6732	18	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.

The worst 5 of 18 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:431:ARG:HD2	1:A:481:GLU:OE2	2.04	0.58
1:B:181:VAL:HG13	1:B:233:LEU:HD23	1.87	0.57
1:B:343:LEU:HG	1:B:431:ARG:HD2	1.87	0.56
1:A:485:LYS:HE3	5:A:992:HOH:O	2.08	0.53
1:A:228:ARG:HD2	1:A:289:ASP:OD2	2.11	0.51

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	438/446 (98%)	421 (96%)	17 (4%)	0	100	100
1	B	442/446 (99%)	429 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	880/892 (99%)	850 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	360/365 (99%)	356 (99%)	4 (1%)	80	58
1	B	364/365 (100%)	357 (98%)	7 (2%)	65	31
All	All	724/730 (99%)	713 (98%)	11 (2%)	72	44

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	40	LEU
1	B	56	GLN
1	B	169	LYS
1	A	409	LYS
1	B	143	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	C2O	A	702	1	0,2,2	0.00	-	0,1,1	0.00	-
3	NO3	A	706	-	3,3,3	2.91	3 (100%)	3,3,3	0.46	0
4	C2O	B	702	1	0,2,2	0.00	-	0,1,1	0.00	-

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	C2O	A	702	1	-	0/0/0/0	0/0/0/0
3	NO3	A	706	-	-	0/0/0/0	0/0/0/0
4	C2O	B	702	1	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	NO3	O3-N	2.63	1.38	1.25
3	A	706	NO3	O2-N	2.64	1.39	1.25
3	A	706	NO3	O1-N	3.41	1.38	1.24

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](#)

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, 95th 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 ²)	Q<0.9
1	A	440/446 (98%)	1.91	170 (38%) 0 0	19, 23, 32, 38	1 (0%)
1	B	444/446 (99%)	1.94	183 (41%) 0 0	14, 20, 29, 32	1 (0%)
All	All	884/892 (99%)	1.92	353 (39%) 0 0	14, 22, 30, 38	2 (0%)

The worst 5 of 353 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	GLY	12.9
1	A	44	ALA	8.6
1	A	289	ASP	8.6
1	B	437	VAL	8.5
1	B	406	GLY	7.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NO3	A	706	4/4	0.94	0.15	-0.18	25,25,25,25	0
2	CU	A	701	1/1	1.00	0.12	-0.92	22,22,22,22	0
2	CU	B	701	1/1	0.97	0.10	-2.02	18,18,18,18	0
4	C2O	A	702	3/3	0.99	0.14	-2.50	25,25,29,36	0
4	C2O	B	702	3/3	0.98	0.10	-3.12	20,20,24,24	0
2	CU	B	703	1/1	0.98	0.05	-5.23	29,29,29,29	0
2	CU	A	703	1/1	0.99	0.07	-5.62	33,33,33,33	0
2	CU	B	705	1/1	0.99	0.26	-	30,30,30,30	0
2	CU	A	704	1/1	0.99	0.22	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.