



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:24 AM EDT

PDB ID : 2YXW / pdb_00002yxw
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 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

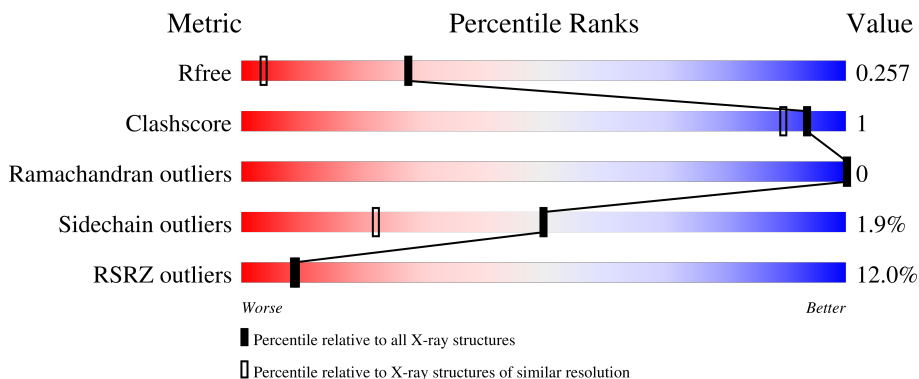
1 Overall quality at a glance

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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 of 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 $\leq 5\%$. 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	10% 94% 5%
1	B	446	13% 95% .

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 mutation	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 mutation	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 mutation	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 mutation	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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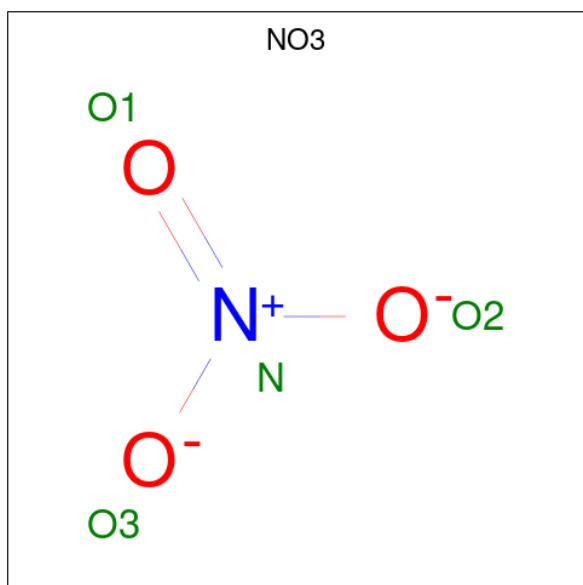
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Chain	Residue	Modelled	Actual	Comment	Reference
B	520	HIS	-	expression tag	UNP P36649
B	521	HIS	-	expression tag	UNP P36649
B	522	HIS	-	expression tag	UNP P36649

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

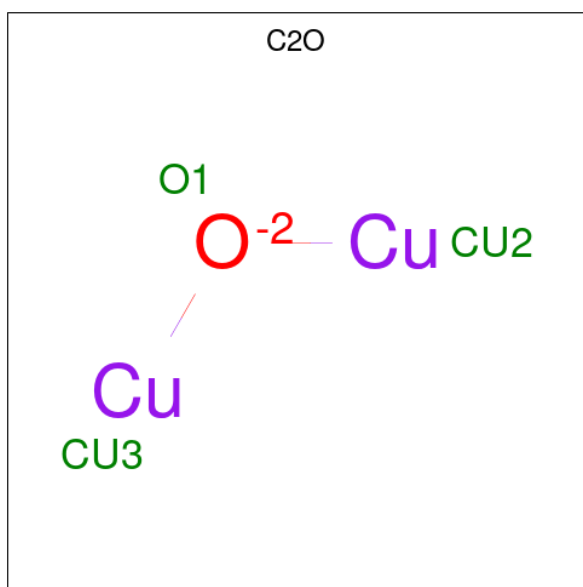
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cu	0	0
			3	3		
2	B	3	Total	Cu	0	0
			3	3		

- Molecule 3 is NITRATE ION (CCD ID: 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 (CCD ID: 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		

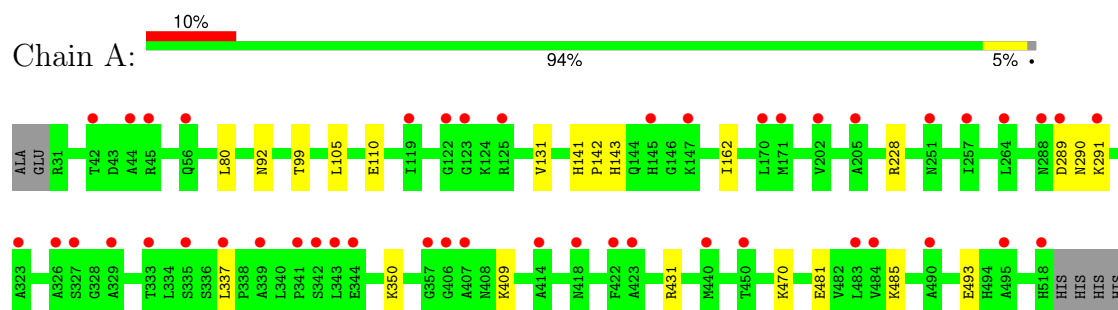
- Molecule 5 is water.

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

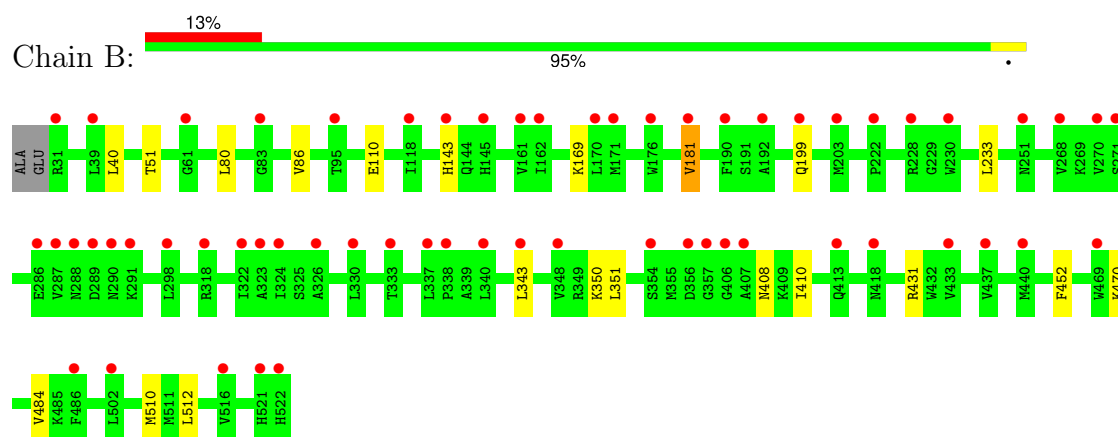
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Blue copper oxidase cueO



- Molecule 1: Blue copper oxidase cueO



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 25.90 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.90-1.50) 95.1 (25.90-1.50)	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 0.233 , 0.257	Depositor DCC
R_{free} test set	6112 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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, 0.333 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: CU, NO3, C2O

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	0.69	1/3450 (0.0%)	0.77	0/4696
1	B	0.55	0/3495	0.72	0/4756
All	All	0.63	1/6945 (0.0%)	0.74	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	7.71	1.49	1.33

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

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	9	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	19	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.

All (19) 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
1:A:337:LEU:HD13	5:A:1014:HOH:O	2.11	0.50
1:A:141:HIS:HB2	1:A:142:PRO:HD2	1.93	0.50
1:A:228:ARG:HG2	1:A:289:ASP:HA	1.95	0.49
1:B:350:LYS:C	1:B:351:LEU:HD12	2.38	0.49
1:A:105:LEU:CD2	1:A:162:ILE:HD11	2.45	0.47
1:A:431:ARG:CD	1:A:481:GLU:OE2	2.64	0.46
1:A:80:LEU:HD13	1:A:131:VAL:HG21	1.98	0.45
1:B:80:LEU:CD2	1:B:86:VAL:HG21	2.48	0.43
1:B:452:PHE:HB3	1:B:484:VAL:HG12	2.01	0.42
1:B:181:VAL:CG1	1:B:233:LEU:HD23	2.49	0.42
1:B:51:THR:HG23	5:B:839:HOH:O	2.19	0.42
1:B:410:ILE:HG21	1:B:512:LEU:HD23	2.03	0.41
1:B:408:ASN:HB3	1:B:510:MET:HE3	2.02	0.41
1:A:99:THR:O	1:A:142:PRO:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
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%)	353 (98%)	7 (2%)	50	22
1	B	364/365 (100%)	357 (98%)	7 (2%)	50	22
All	All	724/730 (99%)	710 (98%)	14 (2%)	50	22

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

Mol	Chain	Res	Type
1	A	110	GLU
1	A	143	HIS
1	A	291	LYS
1	A	350	LYS
1	A	409	LYS
1	A	470	LYS
1	A	493	GLU
1	B	40	LEU

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Mol	Chain	Res	Type
1	B	110	GLU
1	B	143	HIS
1	B	169	LYS
1	B	181	VAL
1	B	199	GLN
1	B	470	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	408	ASN
1	B	49	GLN
1	B	175	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NO3	A	706	-	1,3,3	2.85	1 (100%)	0,3,3	-	-
4	C2O	B	702	1	0,2,2	-	-	-		
4	C2O	A	702	1	0,2,2	-	-	-		

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	NO3	O1-N	2.85	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 ⓘ

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, 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%)	1.24	46 (10%)	11 12	17, 23, 32, 38	1 (0%)
1	B	444/446 (99%)	1.22	60 (13%)	7 7	12, 20, 29, 32	1 (0%)
All	All	884/892 (99%)	1.23	106 (11%)	9 9	12, 22, 30, 38	2 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	GLY	6.9
1	A	288	ASN	4.8
1	B	407	ALA	4.6
1	A	289	ASP	4.4
1	B	437	VAL	4.3
1	B	230	TRP	4.2
1	B	322	ILE	4.1
1	A	406	GLY	3.7
1	B	406	GLY	3.7
1	B	323	ALA	3.6
1	A	518	HIS	3.5
1	B	288	ASN	3.5
1	B	181	VAL	3.5
1	B	118	ILE	3.2
1	B	418	ASN	3.2
1	B	522	HIS	3.2
1	A	326	ALA	3.2
1	B	287	VAL	3.2
1	B	170	LEU	3.1
1	B	203	MET	3.0
1	B	521	HIS	3.0
1	A	147	LYS	3.0
1	A	171	MET	3.0
1	A	119	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	414	ALA	2.9
1	B	31	ARG	2.9
1	A	122	GLY	2.9
1	B	357	GLY	2.9
1	B	176	TRP	2.8
1	A	344	GLU	2.8
1	B	356	ASP	2.8
1	A	343	LEU	2.8
1	B	324	ILE	2.7
1	B	343	LEU	2.7
1	B	199	GLN	2.7
1	B	440	MET	2.7
1	B	290	ASN	2.7
1	B	251	ASN	2.6
1	A	202	VAL	2.6
1	A	333	THR	2.6
1	B	190	PHE	2.6
1	A	145	HIS	2.6
1	B	326	ALA	2.5
1	A	123	GLY	2.5
1	A	335	SER	2.5
1	B	145	HIS	2.5
1	B	289	ASP	2.5
1	A	45	ARG	2.5
1	A	407	ALA	2.5
1	A	170	LEU	2.5
1	A	484	VAL	2.5
1	A	339	ALA	2.4
1	A	337	LEU	2.4
1	A	341	PRO	2.4
1	A	44	ALA	2.4
1	B	171	MET	2.4
1	A	418	ASN	2.4
1	A	264	LEU	2.4
1	A	483	LEU	2.4
1	A	291	LYS	2.4
1	B	228	ARG	2.4
1	A	440	MET	2.4
1	B	516	VAL	2.4
1	A	342	SER	2.4
1	B	271	SER	2.4
1	B	318	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	340	LEU	2.4
1	B	192	ALA	2.3
1	B	469	TRP	2.3
1	A	450	THR	2.3
1	B	333	THR	2.3
1	A	56	GLN	2.3
1	A	323	ALA	2.3
1	A	422	PHE	2.3
1	B	143	HIS	2.3
1	B	338	PRO	2.3
1	A	251	ASN	2.3
1	B	348	VAL	2.3
1	B	433	VAL	2.3
1	B	61	GLY	2.3
1	B	291	LYS	2.3
1	A	327	SER	2.3
1	B	354	SER	2.3
1	B	95	THR	2.2
1	B	39	LEU	2.2
1	A	329	ALA	2.2
1	B	413	GLN	2.2
1	B	502	LEU	2.2
1	B	162	ILE	2.2
1	A	490	ALA	2.2
1	B	270	VAL	2.2
1	B	337	LEU	2.1
1	A	423	ALA	2.1
1	B	161	VAL	2.1
1	A	42	THR	2.1
1	B	83	GLY	2.1
1	B	486	PHE	2.1
1	B	268	VAL	2.1
1	A	257	ILE	2.1
1	B	286	GLU	2.1
1	A	495	ALA	2.0
1	A	125	ARG	2.0
1	B	330	LEU	2.0
1	B	222	PRO	2.0
1	A	205	ALA	2.0
1	B	298	LEU	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NO3	A	706	4/4	0.91	0.11	25,25,25,25	0
2	CU	B	701	1/1	0.94	0.05	18,18,18,18	0
2	CU	B	705	1/1	0.97	0.24	30,30,30,30	0
2	CU	B	703	1/1	0.97	0.10	29,29,29,29	0
2	CU	A	703	1/1	0.98	0.16	33,33,33,33	0
2	CU	A	704	1/1	0.98	0.24	21,21,21,21	0
4	C2O	B	702	3/3	0.98	0.06	20,20,24,24	0
4	C2O	A	702	3/3	0.99	0.08	25,25,29,36	0
2	CU	A	701	1/1	0.99	0.06	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.