Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2022 – 02:29 pm BST

PDB ID	:	7R0H
Title	:	STRUCTURAL BASIS OF ION UPTAKE IN COPPER-TRANSPORTING P1B-TYPE ATPASES
Authors	:	Salustros, N.; Groenberg, C.; Wang, K.; Gourdon, P.
Deposited on	:	2022-02-02
Resolution	:	3.31 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 (i) 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 (i)) were used in the production of this report:

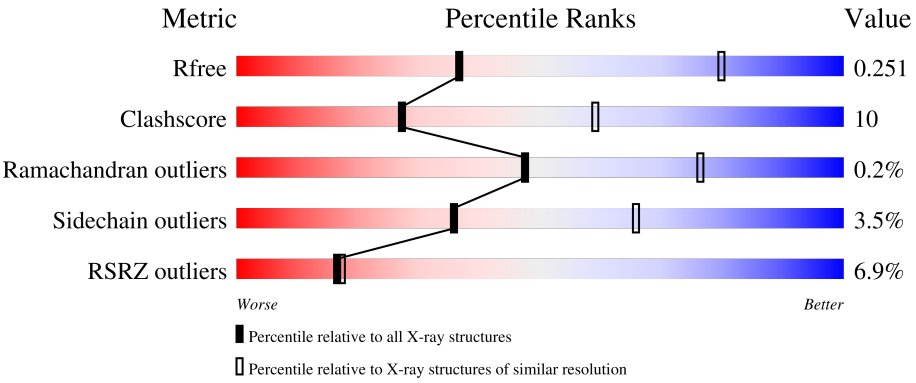
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 <=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	658	7% 73% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4928 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 Putative copper-exporting P-type ATPase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			4927	3174	829	909	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	-	expression tag	UNP A0A117KM49

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

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: Putative copper-exporting P-type ATPase A

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	130.12Å 151.12Å 219.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.93 – 3.31 49.30 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.93-3.31) 92.0 (49.30-3.31)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.214 , 0.251 0.211 , 0.251	Depositor DCC
R_{free} test set	1628 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	104.0	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4928	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.54	0/5001	0.78	1/6782 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	LEU	CB-CG-CD2	5.42	120.21	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	PHE	Peptide
1	A	361	ALA	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	4927	0	5164	102	0
2	A	1	0	0	0	0
All	All	4928	0	5164	102	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 10.

All (102) 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:181:LEU:HB3	1:A:365:LEU:HD11	1.62	0.82
1:A:189:GLU:OE1	1:A:703:ARG:NH1	2.26	0.68
1:A:731:PRO:HA	1:A:734:ARG:HG3	1.76	0.68
1:A:558:VAL:HG22	1:A:568:VAL:HG11	1.76	0.67
1:A:260:ASP:HB2	1:A:307:ARG:HB2	1.79	0.64
1:A:687:ILE:HG13	1:A:688:PRO:HD3	1.80	0.63
1:A:500:VAL:HG22	1:A:534:VAL:HG12	1.80	0.62
1:A:200:LEU:HD22	1:A:712:ALA:HB1	1.81	0.62
1:A:703:ARG:NE	1:A:705:GLU:OE2	2.34	0.61
1:A:371:THR:O	1:A:375:VAL:HG12	2.00	0.61
1:A:457:GLU:HB2	1:A:468:ILE:HD11	1.83	0.61
1:A:225:LYS:HG2	1:A:226:THR:HG22	1.82	0.60
1:A:431:LYS:HE2	1:A:551:LYS:HA	1.84	0.60
1:A:159:ASP:O	1:A:163:SER:OG	2.11	0.59
1:A:373:ILE:HA	1:A:376:LEU:HB2	1.84	0.59
1:A:524:LEU:HD13	1:A:545:ALA:HB2	1.85	0.59
1:A:320:LEU:HD22	1:A:405:LEU:HB3	1.85	0.59
1:A:452:LEU:HD22	1:A:498:ILE:HG12	1.83	0.59
1:A:163:SER:HA	1:A:166:VAL:HG12	1.83	0.58
1:A:204:LEU:HD11	1:A:716:VAL:HG12	1.85	0.58
1:A:421:VAL:HG22	1:A:614:ALA:HB3	1.86	0.58
1:A:223:GLN:HG2	1:A:314:LEU:HD23	1.86	0.57
1:A:492:GLY:HA3	1:A:505:LEU:HD22	1.87	0.56
1:A:190:THR:OG1	1:A:705:GLU:OE2	2.22	0.56
1:A:267:GLU:HG2	1:A:283:LEU:HD11	1.88	0.55
1:A:491:GLU:HB3	1:A:505:LEU:HD13	1.87	0.55
1:A:313:LEU:HD13	1:A:639:SER:HA	1.89	0.55
1:A:682:TYR:CE2	1:A:686:LEU:HD12	2.41	0.54
1:A:151:LEU:HD13	1:A:160:VAL:HG11	1.89	0.54
1:A:125:ASP:OD2	1:A:177:THR:HG22	2.08	0.53
1:A:477:ILE:HG22	1:A:479:LEU:HD23	1.89	0.53
1:A:95:LEU:HD22	1:A:206:ALA:HB1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:O	1:A:234:LYS:HG3	2.08	0.52
1:A:216:ILE:O	1:A:220:VAL:HG23	2.09	0.52
1:A:158:MET:HA	1:A:380:CYS:SG	2.49	0.52
1:A:159:ASP:OD2	1:A:202:ARG:NH2	2.43	0.52
1:A:207:ARG:HH11	1:A:211:ARG:NH2	2.08	0.51
1:A:121:LEU:HB3	1:A:122:PRO:HD3	1.93	0.50
1:A:388:THR:HG22	1:A:672:ILE:HG23	1.93	0.50
1:A:358:TYR:CE1	1:A:364:PRO:HD3	2.47	0.50
1:A:162:TYR:CZ	1:A:377:VAL:HG23	2.47	0.50
1:A:331:ILE:N	1:A:413:GLU:OE1	2.45	0.50
1:A:436:VAL:HG12	1:A:546:VAL:HG12	1.93	0.50
1:A:188:TYR:O	1:A:192:VAL:HG23	2.12	0.49
1:A:553:SER:C	1:A:556:PRO:HD2	2.33	0.49
1:A:614:ALA:HA	1:A:631:LEU:O	2.12	0.48
1:A:388:THR:HA	1:A:672:ILE:HG12	1.95	0.48
1:A:158:MET:HE1	1:A:201:GLY:HA3	1.96	0.47
1:A:185:TYR:CE2	1:A:365:LEU:HD22	2.49	0.47
1:A:640:ASP:O	1:A:644:GLU:HG2	2.15	0.47
1:A:373:ILE:HD11	1:A:704:PRO:HG3	1.95	0.47
1:A:412:LEU:HD22	1:A:665:SER:HA	1.96	0.47
1:A:364:PRO:HA	1:A:368:ALA:HB3	1.97	0.47
1:A:501:GLY:HA3	1:A:505:LEU:HD23	1.96	0.47
1:A:438:ASP:HB2	1:A:545:ALA:HB3	1.96	0.47
1:A:185:TYR:H	1:A:185:TYR:HD1	1.63	0.47
1:A:241:GLU:OE2	1:A:241:GLU:N	2.44	0.47
1:A:681:ILE:HA	1:A:684:VAL:HG22	1.96	0.46
1:A:424:ASP:O	1:A:428:THR:HB	2.16	0.46
1:A:415:ALA:HA	1:A:418:VAL:HG13	1.98	0.46
1:A:462:HIS:CG	1:A:463:PRO:HD2	2.50	0.45
1:A:378:VAL:HG23	1:A:707:ALA:HB1	1.97	0.45
1:A:321:VAL:O	1:A:325:MET:HG2	2.16	0.45
1:A:447:ARG:NH1	1:A:477:ILE:HA	2.32	0.45
1:A:336:ASP:HA	1:A:339:VAL:HG12	1.97	0.45
1:A:212:THR:HG22	1:A:393:THR:HG21	1.97	0.45
1:A:457:GLU:HB3	1:A:465:ALA:HB1	1.97	0.45
1:A:702:PHE:HE2	1:A:707:ALA:HB2	1.82	0.45
1:A:136:ILE:CD1	1:A:192:VAL:HG22	2.47	0.44
1:A:439:LEU:HD12	1:A:439:LEU:HA	1.71	0.44
1:A:107:PHE:HA	1:A:110:VAL:HG22	1.98	0.44
1:A:395:GLY:HA3	1:A:668:THR:HG21	2.00	0.43
1:A:175:LEU:HB3	1:A:180:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:HG23	1:A:239:PRO:O	2.19	0.43
1:A:586:LEU:HB2	1:A:588:LEU:HG	2.01	0.43
1:A:610:LYS:HG3	1:A:611:GLU:HG2	2.01	0.43
1:A:171:LEU:HA	1:A:174:VAL:HG22	2.01	0.42
1:A:561:LEU:HG	1:A:659:VAL:HG22	2.02	0.42
1:A:511:VAL:HG13	1:A:538:GLY:O	2.20	0.42
1:A:588:LEU:HD23	1:A:588:LEU:HA	1.73	0.42
1:A:375:VAL:HA	1:A:378:VAL:HB	2.01	0.42
1:A:337:LYS:HD3	1:A:337:LYS:HA	1.61	0.42
1:A:269:TYR:HA	1:A:282:VAL:O	2.20	0.41
1:A:392:LEU:O	1:A:396:MET:HG3	2.21	0.41
1:A:152:ARG:HD2	1:A:152:ARG:HA	1.71	0.41
1:A:682:TYR:CZ	1:A:686:LEU:HD11	2.55	0.41
1:A:133:LEU:HB3	1:A:134:PRO:HD3	2.01	0.41
1:A:484:LYS:H	1:A:484:LYS:HG2	1.59	0.41
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.82	0.41
1:A:668:THR:HA	1:A:725:LEU:HD11	2.02	0.41
1:A:445:ASP:OD2	1:A:448:GLU:N	2.34	0.41
1:A:682:TYR:CZ	1:A:686:LEU:CD1	3.04	0.41
1:A:729:VAL:O	1:A:734:ARG:NH2	2.53	0.41
1:A:181:LEU:HA	1:A:182:PRO:HD3	1.85	0.41
1:A:207:ARG:HD3	1:A:211:ARG:NH2	2.36	0.41
1:A:336:ASP:O	1:A:339:VAL:HG12	2.21	0.40
1:A:617:GLY:O	1:A:634:ALA:HA	2.20	0.40
1:A:225:LYS:HB3	1:A:225:LYS:HE3	1.90	0.40
1:A:267:GLU:HA	1:A:284:LYS:O	2.22	0.40
1:A:283:LEU:HD12	1:A:284:LYS:H	1.84	0.40
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.87	0.40
1:A:482:PRO:HB2	1:A:484:LYS:HG2	2.04	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	652/658 (99%)	605 (93%)	46 (7%)	1 (0%)	47 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	LEU

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	520/523 (99%)	502 (96%)	18 (4%)	36 66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	137	PHE
1	A	152	ARG
1	A	183	ARG
1	A	185	TYR
1	A	207	ARG
1	A	223	GLN
1	A	451	ARG
1	A	458	ARG
1	A	466	GLU
1	A	504	ARG
1	A	506	MET
1	A	518	GLU
1	A	526	ARG
1	A	560	GLU
1	A	563	ARG
1	A	621	ASN
1	A	695	TYR

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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^{th} 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	654/658 (99%)	0.24	45 (6%)	16	17	63, 106, 177, 223	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	736	GLY	4.6
1	A	464	ILE	4.4
1	A	490	GLY	4.3
1	A	461	GLU	4.0
1	A	122	PRO	4.0
1	A	442	LEU	3.8
1	A	489	ALA	3.3
1	A	118	PHE	3.3
1	A	531	ALA	3.3
1	A	232	ASP	3.2
1	A	539	ARG	3.2
1	A	499	LEU	3.2
1	A	439	LEU	3.1
1	A	493	VAL	3.1
1	A	234	LYS	3.1
1	A	434	PRO	3.1
1	A	435	GLU	3.1
1	A	492	GLY	3.1
1	A	546	VAL	3.0
1	A	547	SER	2.9
1	A	533	ILE	2.9
1	A	537	ASN	2.8
1	A	457	GLU	2.8
1	A	95	LEU	2.8
1	A	468	ILE	2.7
1	A	472	ALA	2.7
1	A	121	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	534	VAL	2.6
1	A	466	GLU	2.6
1	A	536	ARG	2.6
1	A	441	PRO	2.5
1	A	436	VAL	2.5
1	A	725	LEU	2.5
1	A	230	ILE	2.4
1	A	542	GLY	2.3
1	A	500	VAL	2.3
1	A	543	ILE	2.2
1	A	433	LYS	2.2
1	A	463	PRO	2.2
1	A	233	GLY	2.1
1	A	535	ALA	2.1
1	A	456	ALA	2.1
1	A	120	SER	2.1
1	A	498	ILE	2.0
1	A	444	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

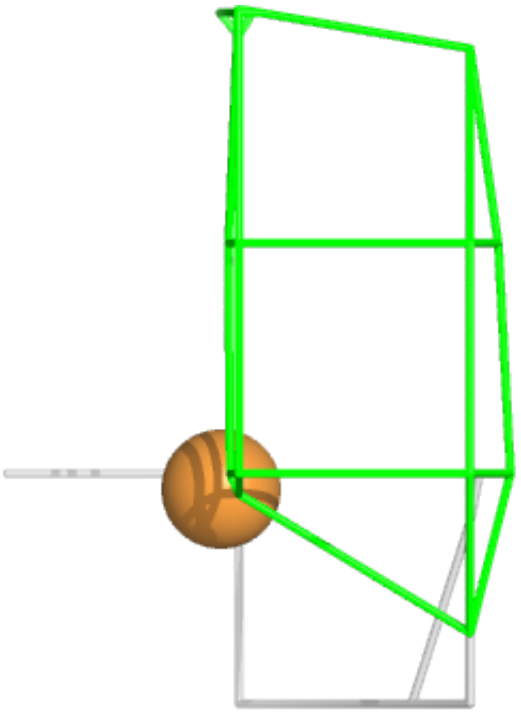
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

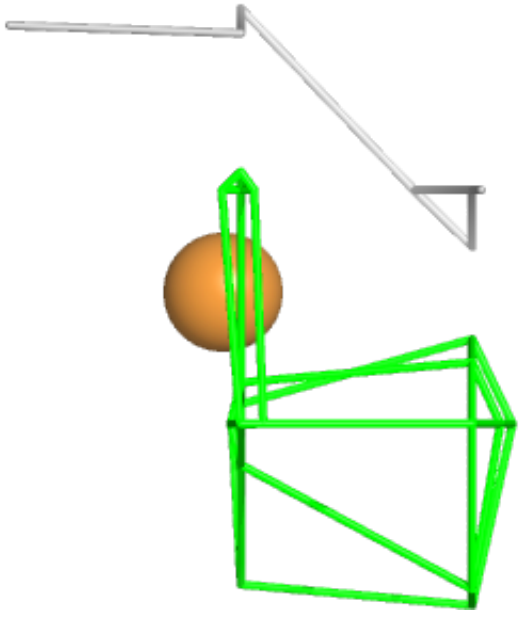
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	A	801	1/1	0.71	0.22	358,358,358,358	0

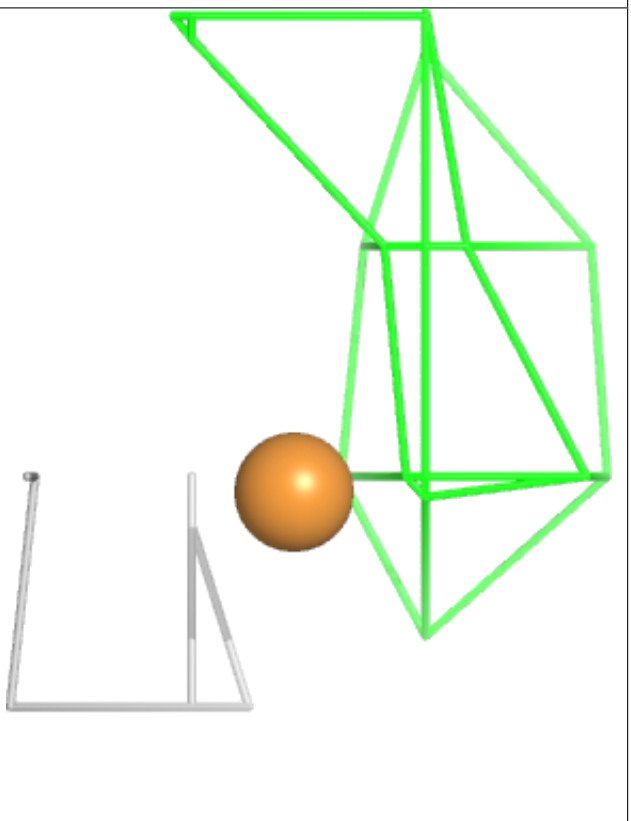
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CU A 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.