

Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2022 – 12:10 pm GMT

PDB ID	:	7BDN
Title	:	Structure of the Streptomyces coelicolor small laccase - cubic crystal form
Authors	:	Zovo, K.; Majumdar, S.; Lukk, T.
Deposited on		
Resolution	:	2.70 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 following versions of software and data (see references (1)) were used in the production of this report:

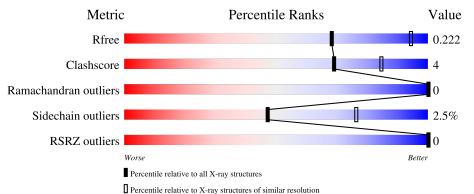
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.70 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	А	343	72%	9%	19%		
1	В	343	71%	9%	19%		



7BDN

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4645 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 oxidase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	277	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	211	2142	1338	391	402	11	0	0	0
1	В	277	Total	С	Ν	0	S	0	0	0
	D	211	2142	1338	391	402	11	0	U	0

• 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	А	3	Total Cu 3 3	0	0
2	В	3	Total Cu 3 3	0	0

• Molecule 3 is water.

N	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	А	176	Total O 176 176	0	0
	3	В	179	Total O 179 179	0	0



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.

Chain A:	72%		9%	19%	
MET ASP ARG ARG GLY PHE ASN	ARG VAL LEU LEU LEU CLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	LATA LYS GLY TLL TLL T38 NG3 Y63 K67	Y65 179 189	G105 L106 M153 Y155	G175 K182
G183 D184 V194 P205 H206	1223 1232 1232 1232 8239 8246 8246 8246 8246 8246 8246 8295 8295 8295 8295 8295 8295 8295 8295	GLU PRO GLU GLV GLY GLY ALA ALA ALA	LYS SER GLY SER SER GLY	GLU PRO GLY GLY ALA ALA ALA	HIS GLU SIH
BIH					
• Molecule	1: Putative copper oxidase				
Chain B:	71%	9	9%	19%	
MET ASP ARG GLY PHE ASN	ARG LEU LEU LEU CLEU CLY CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	ALA LYS GLY TLE T138 T38 T41 T41 K52 M53	Y54 K57 Y65	R98 6105 1106 H135 P147	W153 H154
Y155 E163 R170 G175	D184 P205 P205 M223 E228 E228 F228 P229 P229 R229 R229 R229 R229 R229 R229	M296 C297 1311 Y314 FLU PRO HIS GLU	HIS GLY GLY ALA ALA ALA	LYS SER GLY GLU SER GLU PRO	THR GLY GLY
ALA ALA ALA ALA HIS GLU GLU GLU HIS					

• Molecule 1: Putative copper oxidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
$\begin{array}{c} \text{Cell constants} \\ \text{a, b, c, } \alpha, \beta, \gamma \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness	99.8(29.50-2.70)	Depositor
(in resolution range)	99.9(29.50-2.70)	EDS
R _{merge}	0.17	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.13 (at 2.72 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D.	0.200 , 0.222	Depositor
R, R_{free}	0.200 , 0.222	DCC
R_{free} test set	2570 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.57, < L^2>=0.41$	Xtriage
Estimated twinning fraction	0.477 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4645	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: 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		lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.44	0/2204	0.62	0/2991	
1	В	0.44	0/2204	0.62	0/2991	
All	All	0.44	0/4408	0.62	0/5982	

There are no bond length outliers.

There are no bond angle outliers.

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	А	2142	0	2024	15	0
1	В	2142	0	2024	17	0
2	А	3	0	0	0	0
2	В	3	0	0	0	0
3	А	176	0	0	1	0
3	В	179	0	0	4	0
All	All	4645	0	4048	31	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 4.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:184:ASP:HB2	3:A:626:HOH:O	1.88	0.73
1:B:38:THR:N	3:B:501:HOH:O	2.23	0.70
1:A:53:MET:HE1	1:A:79:ILE:HD11	1.86	0.58
1:A:53:MET:HE3	1:A:89:ILE:HG21	1.87	0.54
1:B:232:THR:O	1:B:288:CYS:HA	2.09	0.53
1:A:53:MET:HE3	1:A:89:ILE:CG2	2.41	0.50
1:A:241:ALA:O	1:A:246:GLY:HA2	2.13	0.48
1:A:232:THR:O	1:A:288:CYS:HA	2.13	0.48
1:B:163:GLU:H	1:B:163:GLU:CD	2.16	0.48
1:B:206:HIS:CD2	1:B:297:GLY:HA2	2.49	0.48
1:A:308:ASP:O	1:B:57:LYS:HE2	2.16	0.46
1:B:228:GLU:HG2	3:B:521:HOH:O	2.16	0.45
1:A:206:HIS:CD2	1:A:297:GLY:HA2	2.50	0.45
1:B:155:TYR:CZ	1:B:175:GLY:HA3	2.51	0.45
1:A:155:TYR:CZ	1:A:175:GLY:HA3	2.52	0.45
1:A:205:PRO:HB3	1:A:296:MET:O	2.16	0.45
1:B:170:ARG:NH2	3:B:503:HOH:O	2.46	0.44
1:B:241:ALA:O	1:B:246:GLY:HA2	2.17	0.44
1:B:105:GLY:HA3	1:B:153:TRP:CD2	2.52	0.44
1:B:205:PRO:HB3	1:B:296:MET:O	2.18	0.44
1:A:105:GLY:HA3	1:A:153:TRP:CD2	2.53	0.44
1:B:311:ILE:HB	1:B:314:TYR:HB3	2.00	0.44
1:B:41:THR:HA	1:B:184:ASP:O	2.18	0.43
1:A:311:ILE:HB	1:A:314:TYR:HB3	1.99	0.43
1:B:98:ARG:NH1	3:B:502:HOH:O	2.35	0.42
1:B:54:TYR:O	1:B:65:TYR:HA	2.20	0.42
1:A:274:ILE:HB	1:A:277:GLU:HB2	2.02	0.41
1:A:54:TYR:O	1:A:65:TYR:HA	2.20	0.41
1:B:135:HIS:NE2	1:B:147:PRO:O	2.48	0.41
1:B:274:ILE:HB	1:B:277:GLU:HB2	2.03	0.41
1:A:194:VAL:HA	1:A:224:ILE:O	2.21	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	А	275/343~(80%)	266~(97%)	9~(3%)	0	100	100
1	В	275/343~(80%)	266~(97%)	9~(3%)	0	100	100
All	All	550/686~(80%)	532~(97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	А	222/262~(85%)	217~(98%)	5(2%)	50 78		
1	В	222/262~(85%)	216~(97%)	6 (3%)	44 74		
All	All	444/524~(85%)	433 (98%)	11 (2%)	47 76		

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	57	LYS
1	А	106	LEU
1	А	182	LYS
1	А	223	MET
1	А	239	ARG
1	В	38	THR
1	В	52	LYS
1	В	106	LEU
1	В	223	MET
1	В	236	HIS
1	В	239	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.



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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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 (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, 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	$\langle RSRZ \rangle$	#RSRZ>2		Z>2	$OWAB(Å^2)$	Q<0.9
1	А	277/343~(80%)	-0.09	0	100	100	26, 34, 45, 55	2 (0%)
1	В	277/343~(80%)	-0.07	0	100	100	26, 34, 46, 55	3 (1%)
All	All	554/686~(80%)	-0.08	0	100	100	26, 34, 46, 55	5 (0%)

There are no RSRZ outliers to report.

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.

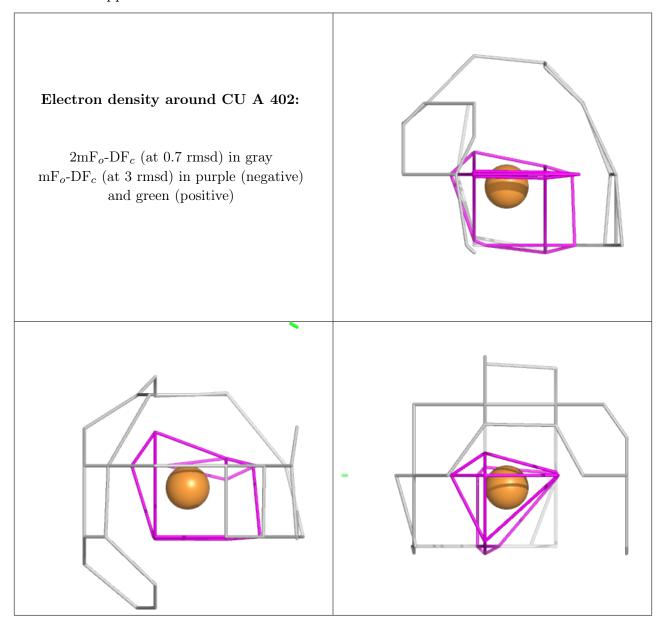
6.4 Ligands (i)

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.

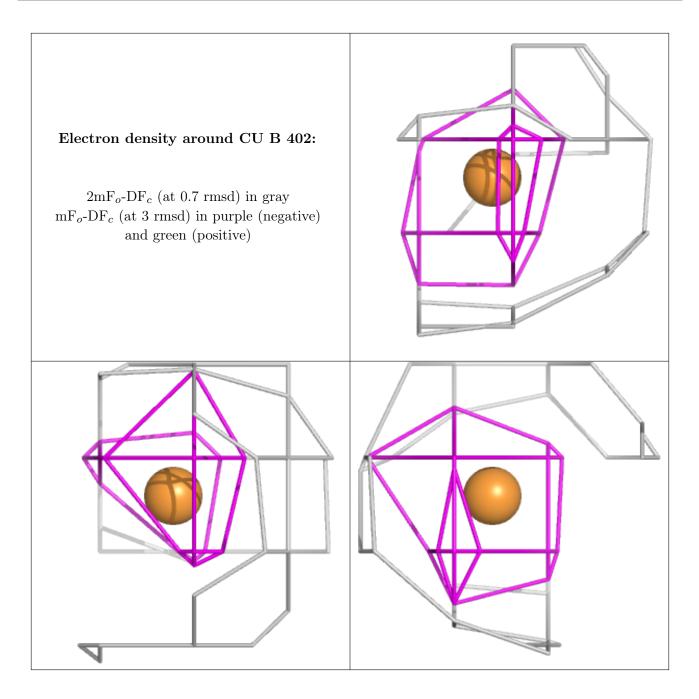
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	CU	А	402	1/1	0.98	0.09	75, 75, 75, 75, 75	0
2	CU	В	402	1/1	0.98	0.13	77,77,77,77	0
2	CU	В	401	1/1	0.99	0.16	$45,\!45,\!45,\!45$	0
2	CU	А	401	1/1	0.99	0.17	45,45,45,45	0
2	CU	А	403	1/1	1.00	0.17	34,34,34,34	0
2	CU	В	403	1/1	1.00	0.17	36,36,36,36	0



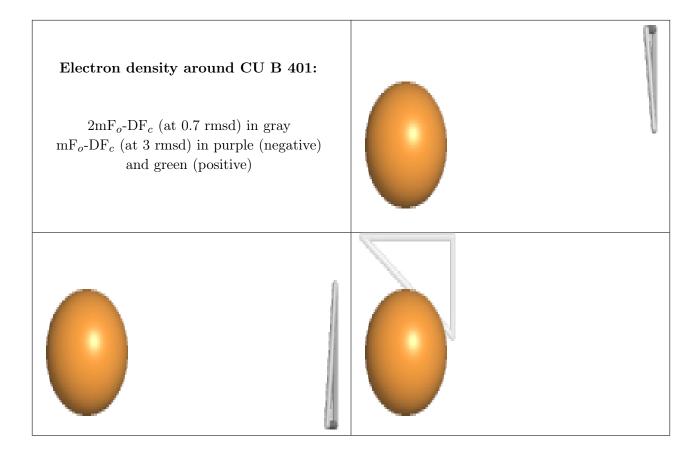
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



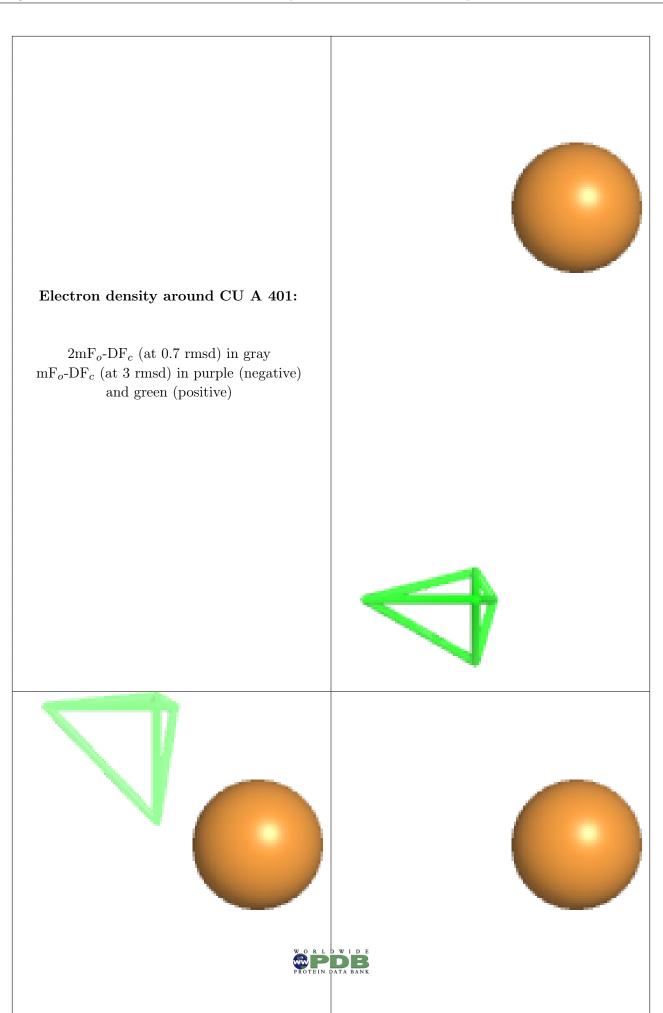


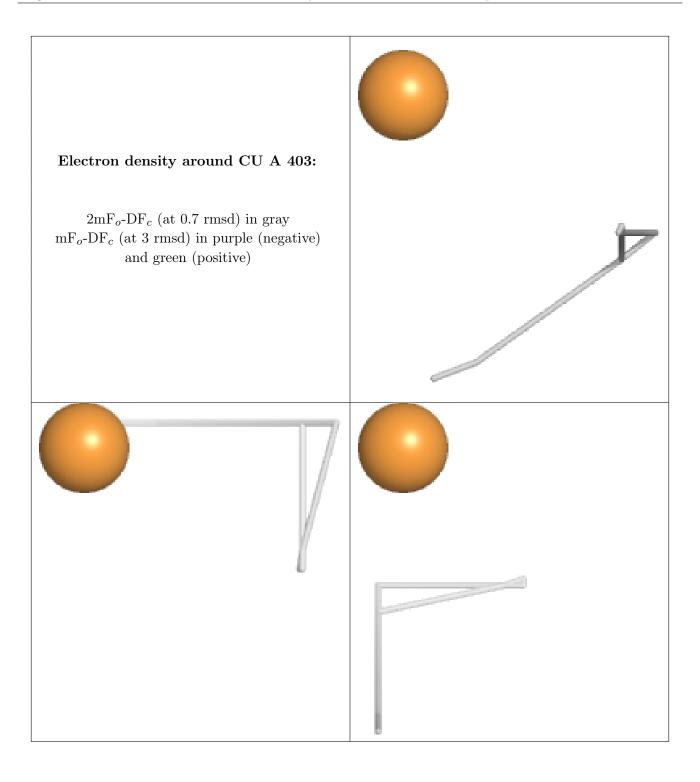




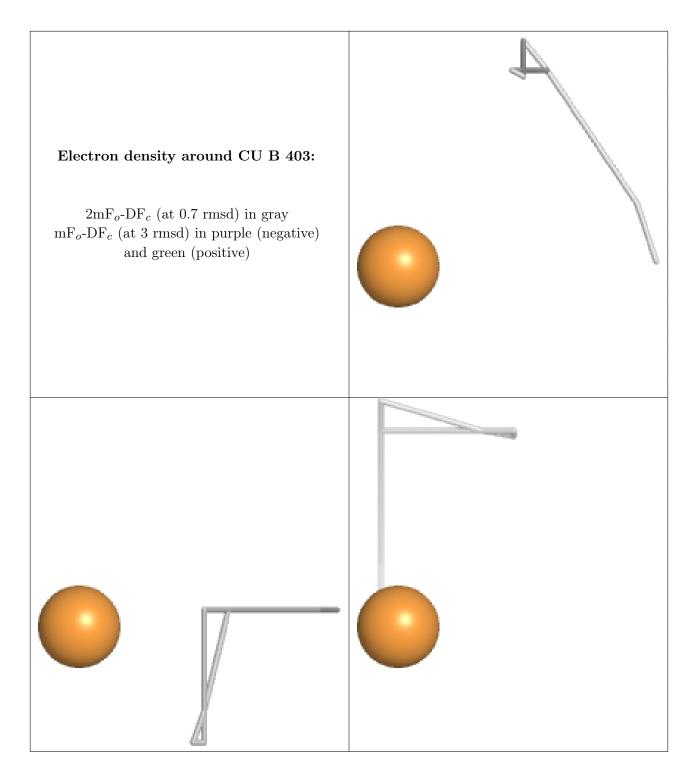












6.5 Other polymers (i)

There are no such residues in this entry.

