



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2022 – 02:26 pm BST

PDB ID : 7PXW
Title : LPMO, expressed in E.coli, in complex with Cellotetraose
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Deposited on : 2021-10-08
Resolution : 1.40 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

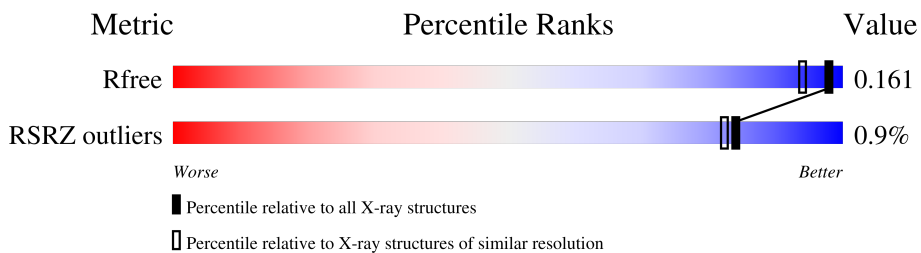
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2189 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 Auxiliary activity 9.

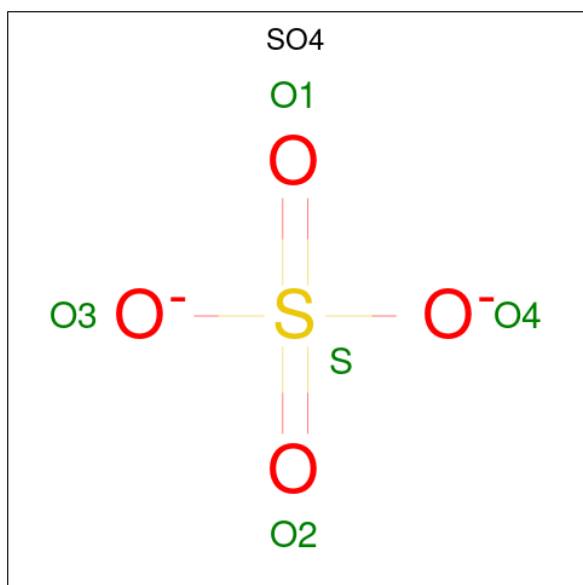
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	235	1812	1148	309	352	3	0	6	0

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	4	45	24	21	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total Cl 19 19	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	302	Total O 302 302	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	48.77Å 48.77Å 109.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.58 – 1.40 44.54 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.58-1.40) 99.6 (44.54-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.117 , 0.160 0.118 , 0.161	Depositor DCC
R_{free} test set	2492 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2189	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

4 monosaccharides 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
2	BGC	C	1	2	12,12,12	0.66	0	17,17,17	1.18	1 (5%)
2	BGC	C	2	2	11,11,12	1.31	3 (27%)	15,15,17	2.30	7 (46%)
2	BGC	C	3	2	11,11,12	1.16	1 (9%)	15,15,17	1.68	5 (33%)
2	BGC	C	4	2	11,11,12	0.76	0	15,15,17	1.63	2 (13%)

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
2	BGC	C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	C	2	2	-	1/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	BGC	O5-C1	-2.88	1.39	1.43
2	C	2	BGC	O2-C2	-2.32	1.38	1.43
2	C	2	BGC	O5-C1	-2.19	1.40	1.43
2	C	2	BGC	O3-C3	-2.09	1.38	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	BGC	O5-C5-C6	-4.51	100.14	107.20
2	C	4	BGC	C1-O5-C5	4.28	117.99	112.19
2	C	2	BGC	C1-C2-C3	3.79	114.33	109.67
2	C	2	BGC	O3-C3-C2	3.46	116.62	109.99
2	C	4	BGC	O5-C1-C2	-3.44	105.47	110.77
2	C	3	BGC	O2-C2-C1	3.06	115.41	109.15
2	C	2	BGC	O5-C5-C4	-2.89	103.79	110.83
2	C	3	BGC	O3-C3-C4	2.76	116.73	110.35
2	C	2	BGC	C1-O5-C5	-2.62	108.64	112.19
2	C	3	BGC	C6-C5-C4	-2.45	107.27	113.00
2	C	2	BGC	O6-C6-C5	-2.27	103.51	111.29
2	C	2	BGC	C6-C5-C4	2.11	117.94	113.00
2	C	1	BGC	O1-C1-O5	-2.07	104.15	110.38
2	C	3	BGC	O4-C4-C5	-2.07	104.17	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BGC	O6-C6-C5	-2.04	104.30	111.29

There are no chirality outliers.

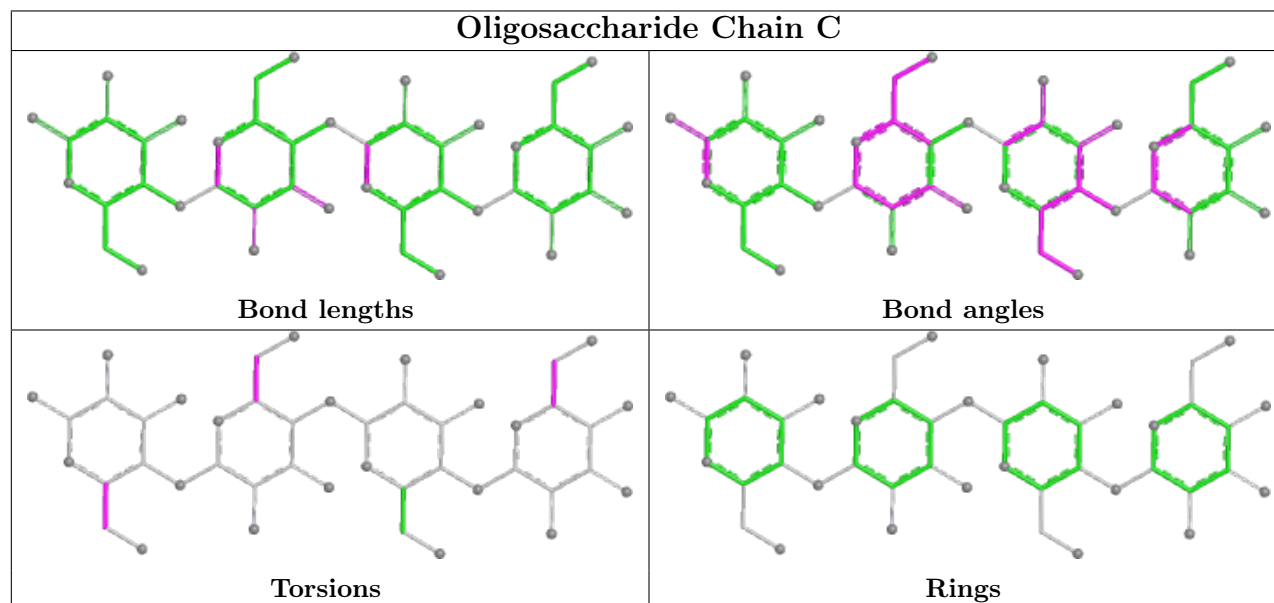
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	BGC	C4-C5-C6-O6
2	C	4	BGC	O5-C5-C6-O6
2	C	1	BGC	C4-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	C	2	BGC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



4.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 20 are monoatomic - leaving 2 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	SO4	A	402	-	4,4,4	0.39	0	6,6,6	0.29	0
3	SO4	A	401	-	4,4,4	0.32	0	6,6,6	0.41	0

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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	235/235 (100%)	-0.94	2 (0%) 84 82	16, 20, 27, 84	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	LEU	3.3
1	A	235	GLU	2.4

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

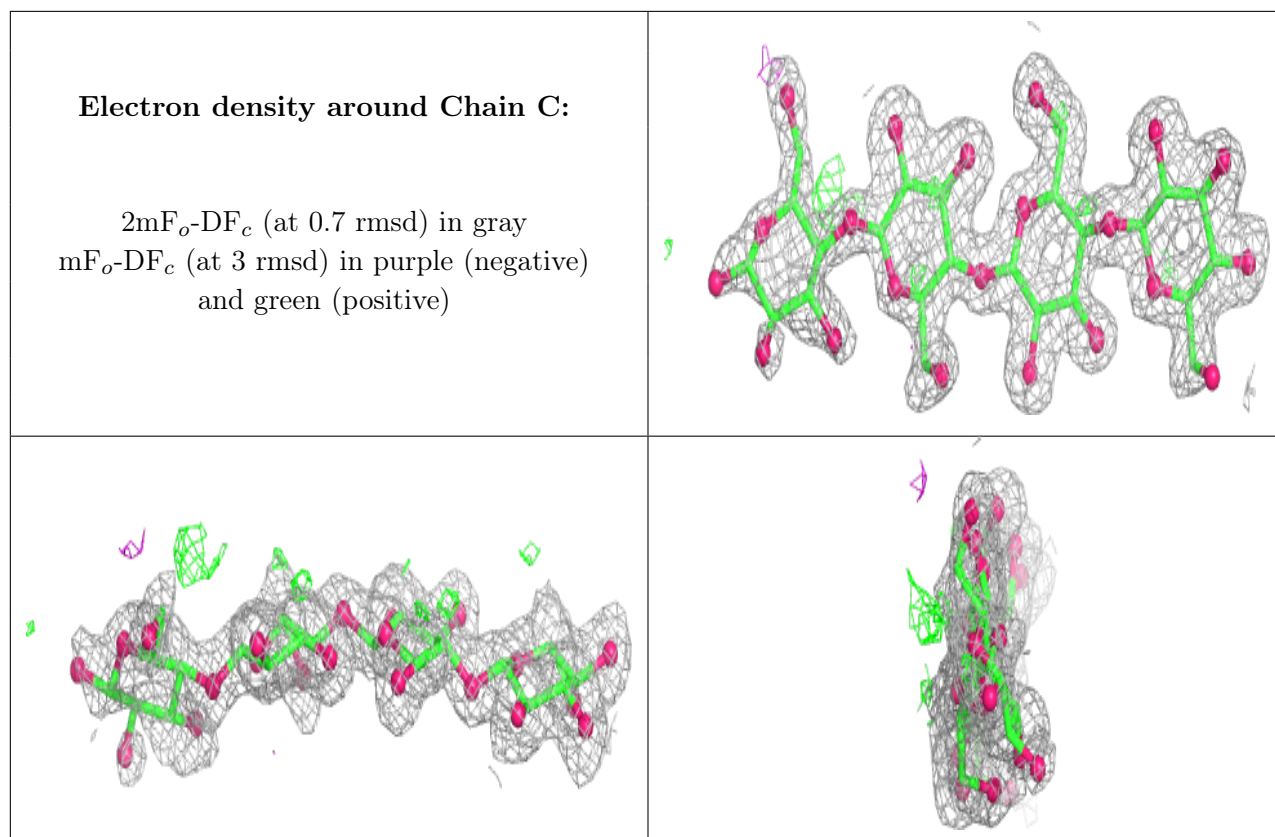
There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [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(Å ²)	Q<0.9
2	BGC	C	1	12/12	0.87	0.15	38,53,59,67	12
2	BGC	C	3	11/12	0.92	0.08	19,23,36,36	5
2	BGC	C	2	11/12	0.93	0.10	26,30,57,71	0
2	BGC	C	4	11/12	0.93	0.12	29,36,46,75	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



5.4 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.

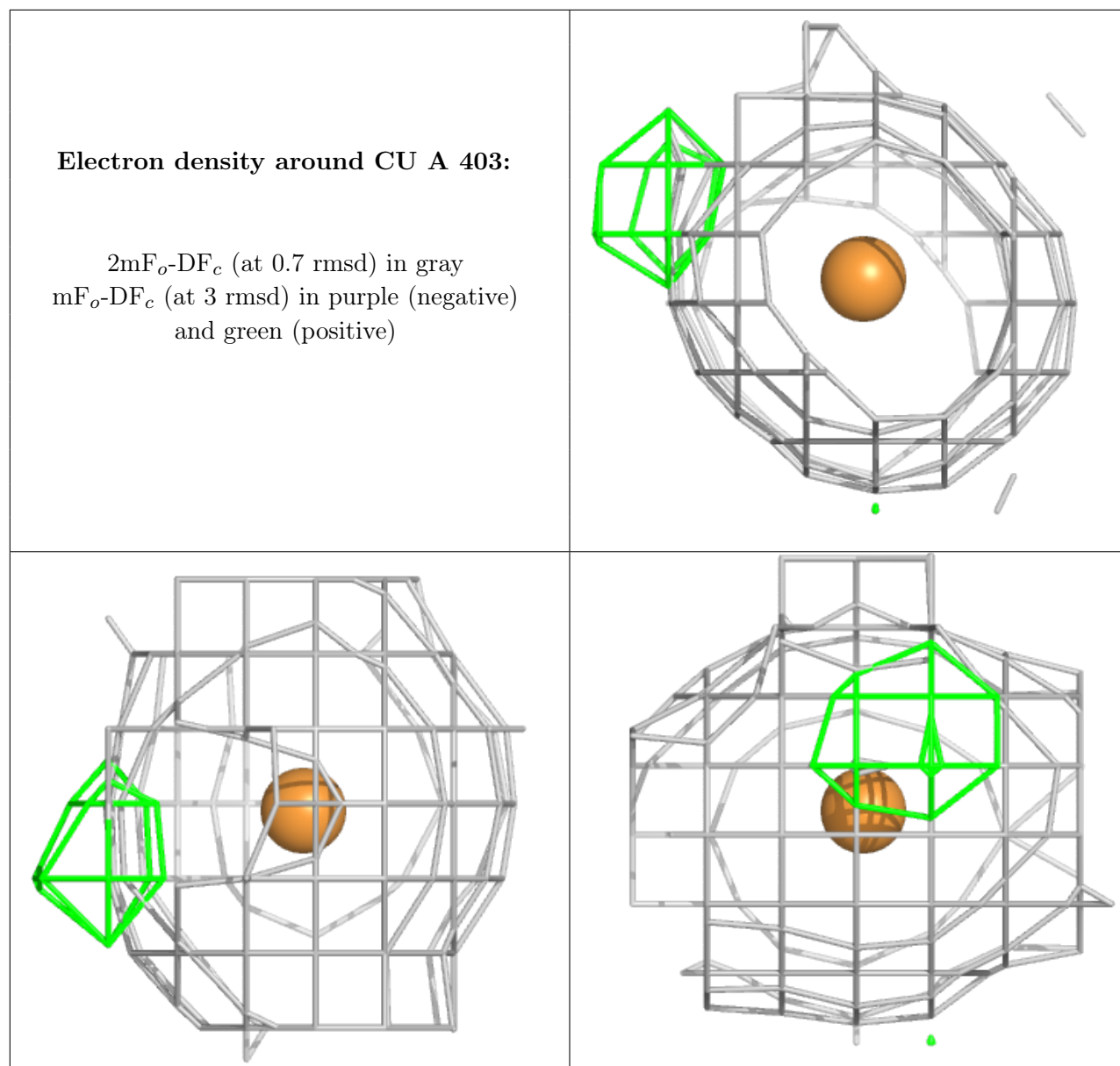
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	A	418	1/1	0.87	0.15	51,51,51,51	1
5	CL	A	422	1/1	0.88	0.26	70,70,70,70	0
5	CL	A	411	1/1	0.92	0.20	72,72,72,72	0
5	CL	A	417	1/1	0.93	0.03	67,67,67,67	0
3	SO4	A	402	5/5	0.95	0.11	29,31,34,38	5
5	CL	A	407	1/1	0.95	0.04	71,71,71,71	0
5	CL	A	408	1/1	0.96	0.24	75,75,75,75	0
5	CL	A	409	1/1	0.96	0.08	55,55,55,55	0
5	CL	A	405	1/1	0.97	0.11	44,44,44,44	0
5	CL	A	406	1/1	0.97	0.06	56,56,56,56	0
5	CL	A	415	1/1	0.97	0.05	29,29,29,29	1
5	CL	A	412	1/1	0.98	0.11	65,65,65,65	0
5	CL	A	413	1/1	0.98	0.09	35,35,35,35	1
5	CL	A	421	1/1	0.98	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	A	404	1/1	0.98	0.04	44,44,44,44	0
5	CL	A	414	1/1	0.99	0.09	36,36,36,36	1
5	CL	A	419	1/1	0.99	0.03	25,25,25,25	1
5	CL	A	420	1/1	0.99	0.09	35,35,35,35	1
5	CL	A	410	1/1	0.99	0.16	52,52,52,52	0
3	SO4	A	401	5/5	0.99	0.06	21,22,29,30	5
4	CU	A	403	1/1	1.00	0.05	18,18,18,18	0
5	CL	A	416	1/1	1.00	0.07	25,25,25,25	1

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.



5.5 Other polymers [i](#)

There are no such residues in this entry.