



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 AM UTC

PDB ID : 9RCN / pdb_00009rcn
Title : Laccase (multicopper oxidase) from *Pediococcus pentosaceus* 4618 mutant
E451L co-crystallized with Silver Nitrate (2 molecules in assymetric unit)
Authors : Paredes, F.; Casino, P.
Deposited on : 2025-05-29
Resolution : 2.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

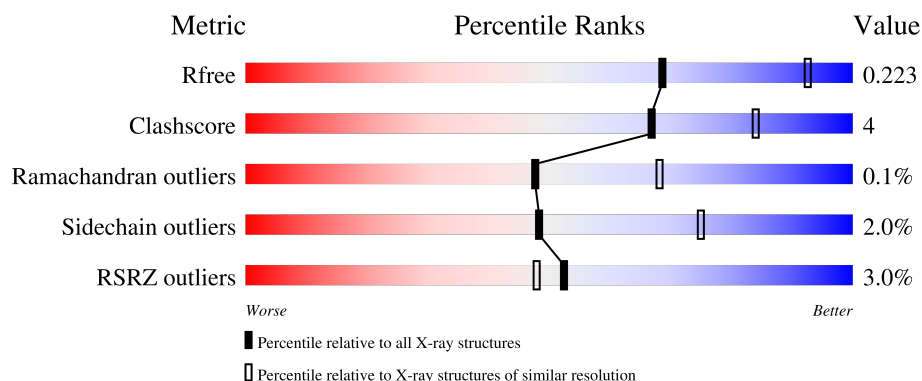
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

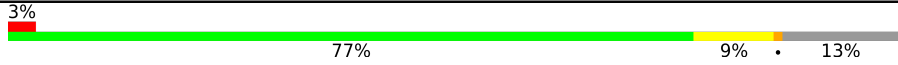
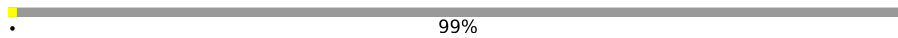
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	532	 3% 77% 9% • 13%
1	C	532	 2% 79% 7% • 13%
1	G	532	 • 99%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7457 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 Multicopper oxidase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3676	2349	627	686	14			
1	C	462	Total	C	N	O	S	0	0	0
			3661	2340	624	683	14			
1	G	5	Total	C	N	O		0	0	0
			45	27	13	5				

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0AB73HHR8
A	-21	GLY	-	expression tag	UNP A0AB73HHR8
A	-20	SER	-	expression tag	UNP A0AB73HHR8
A	-19	SER	-	expression tag	UNP A0AB73HHR8
A	-18	HIS	-	expression tag	UNP A0AB73HHR8
A	-17	HIS	-	expression tag	UNP A0AB73HHR8
A	-16	HIS	-	expression tag	UNP A0AB73HHR8
A	-15	HIS	-	expression tag	UNP A0AB73HHR8
A	-14	HIS	-	expression tag	UNP A0AB73HHR8
A	-13	HIS	-	expression tag	UNP A0AB73HHR8
A	-12	SER	-	expression tag	UNP A0AB73HHR8
A	-11	SER	-	expression tag	UNP A0AB73HHR8
A	-10	GLY	-	expression tag	UNP A0AB73HHR8
A	-9	LEU	-	expression tag	UNP A0AB73HHR8
A	-8	VAL	-	expression tag	UNP A0AB73HHR8
A	-7	PRO	-	expression tag	UNP A0AB73HHR8
A	-6	ARG	-	expression tag	UNP A0AB73HHR8
A	-5	GLY	-	expression tag	UNP A0AB73HHR8
A	-4	SER	-	expression tag	UNP A0AB73HHR8
A	-3	HIS	-	expression tag	UNP A0AB73HHR8
A	-2	MET	-	expression tag	UNP A0AB73HHR8
A	-1	ALA	-	expression tag	UNP A0AB73HHR8
A	0	SER	-	expression tag	UNP A0AB73HHR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	PRO	GLN	variant	UNP A0AB73HHR8
A	241	ASN	ASP	variant	UNP A0AB73HHR8
A	253	ALA	SER	variant	UNP A0AB73HHR8
A	451	LEU	GLU	engineered mutation	UNP A0AB73HHR8
C	-22	MET	-	initiating methionine	UNP A0AB73HHR8
C	-21	GLY	-	expression tag	UNP A0AB73HHR8
C	-20	SER	-	expression tag	UNP A0AB73HHR8
C	-19	SER	-	expression tag	UNP A0AB73HHR8
C	-18	HIS	-	expression tag	UNP A0AB73HHR8
C	-17	HIS	-	expression tag	UNP A0AB73HHR8
C	-16	HIS	-	expression tag	UNP A0AB73HHR8
C	-15	HIS	-	expression tag	UNP A0AB73HHR8
C	-14	HIS	-	expression tag	UNP A0AB73HHR8
C	-13	HIS	-	expression tag	UNP A0AB73HHR8
C	-12	SER	-	expression tag	UNP A0AB73HHR8
C	-11	SER	-	expression tag	UNP A0AB73HHR8
C	-10	GLY	-	expression tag	UNP A0AB73HHR8
C	-9	LEU	-	expression tag	UNP A0AB73HHR8
C	-8	VAL	-	expression tag	UNP A0AB73HHR8
C	-7	PRO	-	expression tag	UNP A0AB73HHR8
C	-6	ARG	-	expression tag	UNP A0AB73HHR8
C	-5	GLY	-	expression tag	UNP A0AB73HHR8
C	-4	SER	-	expression tag	UNP A0AB73HHR8
C	-3	HIS	-	expression tag	UNP A0AB73HHR8
C	-2	MET	-	expression tag	UNP A0AB73HHR8
C	-1	ALA	-	expression tag	UNP A0AB73HHR8
C	0	SER	-	expression tag	UNP A0AB73HHR8
C	12	PRO	GLN	variant	UNP A0AB73HHR8
C	241	ASN	ASP	variant	UNP A0AB73HHR8
C	253	ALA	SER	variant	UNP A0AB73HHR8
C	451	LEU	GLU	engineered mutation	UNP A0AB73HHR8
G	-1	MET	-	initiating methionine	UNP A0AB73HHR8
G	0	GLY	-	expression tag	UNP A0AB73HHR8
G	1	SER	-	expression tag	UNP A0AB73HHR8
G	2	SER	-	expression tag	UNP A0AB73HHR8
G	3	HIS	-	expression tag	UNP A0AB73HHR8
G	4	HIS	-	expression tag	UNP A0AB73HHR8
G	5	HIS	-	expression tag	UNP A0AB73HHR8
G	6	HIS	-	expression tag	UNP A0AB73HHR8
G	7	HIS	-	expression tag	UNP A0AB73HHR8
G	8	HIS	-	expression tag	UNP A0AB73HHR8
G	9	SER	-	expression tag	UNP A0AB73HHR8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	10	SER	-	expression tag	UNP A0AB73HHR8
G	11	GLY	-	expression tag	UNP A0AB73HHR8
G	12	LEU	-	expression tag	UNP A0AB73HHR8
G	13	VAL	-	expression tag	UNP A0AB73HHR8
G	14	PRO	-	expression tag	UNP A0AB73HHR8
G	15	ARG	-	expression tag	UNP A0AB73HHR8
G	16	GLY	-	expression tag	UNP A0AB73HHR8
G	17	SER	-	expression tag	UNP A0AB73HHR8
G	18	HIS	-	expression tag	UNP A0AB73HHR8
G	19	MET	-	expression tag	UNP A0AB73HHR8
G	20	ALA	-	expression tag	UNP A0AB73HHR8
G	21	SER	-	expression tag	UNP A0AB73HHR8
G	33	PRO	GLN	variant	UNP A0AB73HHR8
G	262	ASN	ASP	variant	UNP A0AB73HHR8
G	274	ALA	SER	variant	UNP A0AB73HHR8
G	472	LEU	GLU	engineered mutation	UNP A0AB73HHR8

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cu 4 4	0	0
2	C	4	Total Cu 4 4	0	0

- Molecule 3 is SILVER ION (CCD ID: AG) (formula: Ag) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ag 2 2	0	0
3	C	1	Total Ag 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	C	26	Total	O	0	0
			26	26		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.81Å 119.81Å 174.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	103.76 – 2.50 103.76 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (103.76-2.50) 98.9 (103.76-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.179 , 0.218 0.191 , 0.223	Depositor DCC
R_{free} test set	2536 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: AG, SO4, 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	1/3792 (0.0%)	0.98	9/5187 (0.2%)
1	C	0.52	0/3777	0.94	6/5166 (0.1%)
1	G	0.83	0/48	1.89	1/64 (1.6%)
All	All	0.53	1/7617 (0.0%)	0.97	16/10417 (0.2%)

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
1	C	0	5
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	ALA	CA-C	-5.36	1.46	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ILE	N-CA-C	-9.23	94.87	108.54
1	G	5	HIS	CA-CB-CG	-7.86	105.94	113.80
1	A	160	HIS	CB-CA-C	-7.34	96.78	110.36
1	A	139	GLN	CB-CA-C	-6.89	98.72	109.55
1	A	386	ALA	CA-C-N	-6.49	111.73	119.84
1	A	386	ALA	C-N-CA	-6.49	111.73	119.84
1	A	154	THR	CA-CB-OG1	-6.25	100.23	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASN	N-CA-C	-5.74	104.94	111.14
1	C	209	ASP	CA-CB-CG	5.61	118.20	112.60
1	A	298	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	15	ASP	CA-CB-CG	5.50	118.10	112.60
1	C	254	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	305	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	160	HIS	N-CA-C	-5.19	106.97	113.15
1	C	290	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	298	ASP	CA-CB-CG	5.07	117.67	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	ARG	Sidechain
1	C	180	ARG	Sidechain
1	C	205	ARG	Sidechain
1	C	245	ARG	Sidechain
1	C	249	ARG	Sidechain
1	C	434	ARG	Sidechain

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	3676	0	3503	30	1
1	C	3661	0	3491	22	1
1	G	45	0	29	3	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
4	C	10	0	0	0	0
4	G	5	0	0	0	0
5	A	23	0	0	1	0
5	C	26	0	0	1	0
All	All	7457	0	7023	53	1

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 (53) 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:347:MET:SD	5:A:709:HOH:O	2.39	0.80
1:C:260:GLN:HE22	1:C:413:ASN:HD22	1.31	0.79
1:A:384:ASN:O	1:A:385:ASP:OD1	2.03	0.77
1:A:260:GLN:HE22	1:A:413:ASN:HD22	1.37	0.72
1:A:386:ALA:HB1	1:A:387:PRO:HD2	1.73	0.71
1:C:104:THR:HG23	1:C:119:GLY:O	1.94	0.68
1:A:384:ASN:C	1:A:385:ASP:OD1	2.36	0.67
1:A:336:VAL:HG21	1:A:377:TYR:CZ	2.34	0.62
1:A:253:ALA:O	1:G:3:HIS:HE1	1.83	0.62
1:A:202:TRP:HZ2	1:A:219:MET:HE1	1.65	0.62
1:C:104:THR:CG2	1:C:119:GLY:O	2.48	0.61
1:C:104:THR:HG21	1:C:149:HIS:HB3	1.85	0.59
1:C:251:HIS:HE1	1:C:305:ASP:O	1.88	0.56
1:C:120:GLY:HA3	1:C:442:MET:HE3	1.90	0.54
1:C:264:ASP:HB2	1:C:418:LYS:HA	1.90	0.54
1:A:386:ALA:HB1	1:A:387:PRO:CD	2.40	0.51
1:A:386:ALA:CB	1:A:387:PRO:HD2	2.41	0.50
1:A:334:PRO:HB3	1:A:434:ARG:NH2	2.26	0.50
1:A:15:ASP:HB3	1:A:245:ARG:NH1	2.27	0.50
1:A:282:ALA:HB2	1:A:446:HIS:CD2	2.48	0.49
1:C:276:HIS:NE2	5:C:701:HOH:O	2.13	0.49
1:C:451:LEU:HD23	1:C:451:LEU:C	2.38	0.48
1:A:253:ALA:O	1:G:3:HIS:CE1	2.64	0.48
1:C:152:PRO:HB2	1:C:153:SER:HA	1.96	0.48
1:A:386:ALA:CB	1:A:387:PRO:CD	2.92	0.47
1:A:451:LEU:C	1:A:451:LEU:HD23	2.39	0.47
1:A:234:LYS:HE2	1:A:290:ASP:OD2	2.14	0.47
1:C:370:GLN:HE22	1:C:378:TRP:HE1	1.62	0.47
1:C:149:HIS:N	1:C:150:PRO:CD	2.78	0.46
1:A:336:VAL:HG21	1:A:377:TYR:CE1	2.51	0.45
1:A:386:ALA:O	1:A:387:PRO:C	2.54	0.45
1:C:211:ASP:O	1:C:389:MET:HE1	2.17	0.45
1:A:320:ASP:OD1	1:A:322:THR:HG22	2.17	0.44
1:A:382:ASN:ND2	1:A:391:HIS:HD2	2.16	0.44
1:A:212:GLY:HA2	1:A:449:GLU:OE1	2.16	0.44
1:A:264:ASP:HB2	1:A:418:LYS:HA	1.98	0.44
1:A:1:MET:HA	1:A:4:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:HIS:CE1	1:C:305:ASP:O	2.70	0.44
1:A:347:MET:HB3	1:A:455:MET:HE2	2.01	0.43
1:A:11:GLU:N	1:A:12:PRO:CD	2.82	0.43
1:C:7:TYR:CE1	1:C:276:HIS:HB3	2.54	0.42
1:C:109:GLY:HA3	1:C:144:LEU:HD22	2.01	0.42
1:A:370:GLN:HE22	1:A:378:TRP:HE1	1.68	0.42
1:C:152:PRO:CB	1:C:153:SER:HA	2.50	0.41
1:C:347:MET:HB3	1:C:455:MET:HE2	2.02	0.41
1:A:149:HIS:CD2	1:A:149:HIS:O	2.73	0.41
1:C:170:ASP:OD1	1:C:170:ASP:C	2.64	0.41
1:A:245:ARG:HA	1:A:281:CYS:SG	2.61	0.41
1:C:337:ASP:OD2	1:C:374:LYS:HD3	2.20	0.41
1:C:369:THR:HA	1:C:460:GLU:O	2.20	0.41
1:A:152:PRO:HB2	1:A:153:SER:HA	2.04	0.40
1:C:451:LEU:HG	1:C:456:MET:HE3	2.02	0.40
1:G:5:HIS:O	1:G:6:HIS:CB	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:OE2	1:C:313:ARG:NH2[6_664]	2.07	0.13

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	463/532 (87%)	446 (96%)	16 (4%)	1 (0%)	43	63
1	C	460/532 (86%)	444 (96%)	16 (4%)	0	100	100
1	G	3/532 (1%)	3 (100%)	0	0	100	100
All	All	926/1596 (58%)	893 (96%)	32 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	ALA

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	394/454 (87%)	386 (98%)	8 (2%)	48	75
1	C	394/454 (87%)	387 (98%)	7 (2%)	51	77
1	G	4/454 (1%)	3 (75%)	1 (25%)	0	1
All	All	792/1362 (58%)	776 (98%)	16 (2%)	48	75

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	THR
1	A	205	ARG
1	A	245	ARG
1	A	385	ASP
1	A	387	PRO
1	A	389	MET
1	A	442	MET
1	A	458	GLN
1	C	104	THR
1	C	205	ARG
1	C	211	ASP
1	C	245	ARG
1	C	323	THR
1	C	389	MET
1	C	442	MET
1	G	4	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	149	HIS
1	A	260	GLN
1	A	364	GLN
1	A	370	GLN
1	A	391	HIS
1	A	396	HIS
1	A	446	HIS
1	C	89	GLN
1	C	90	HIS
1	C	92	HIS
1	C	244	ASN
1	C	251	HIS
1	C	260	GLN
1	C	315	HIS
1	C	344	HIS
1	C	370	GLN
1	C	396	HIS
1	C	458	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 14 ligands modelled in this entry, 11 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	SO4	C	606	-	4,4,4	0.32	0	6,6,6	0.10	0
4	SO4	C	607	-	4,4,4	0.40	0	6,6,6	0.08	0
4	SO4	G	601	-	4,4,4	0.29	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

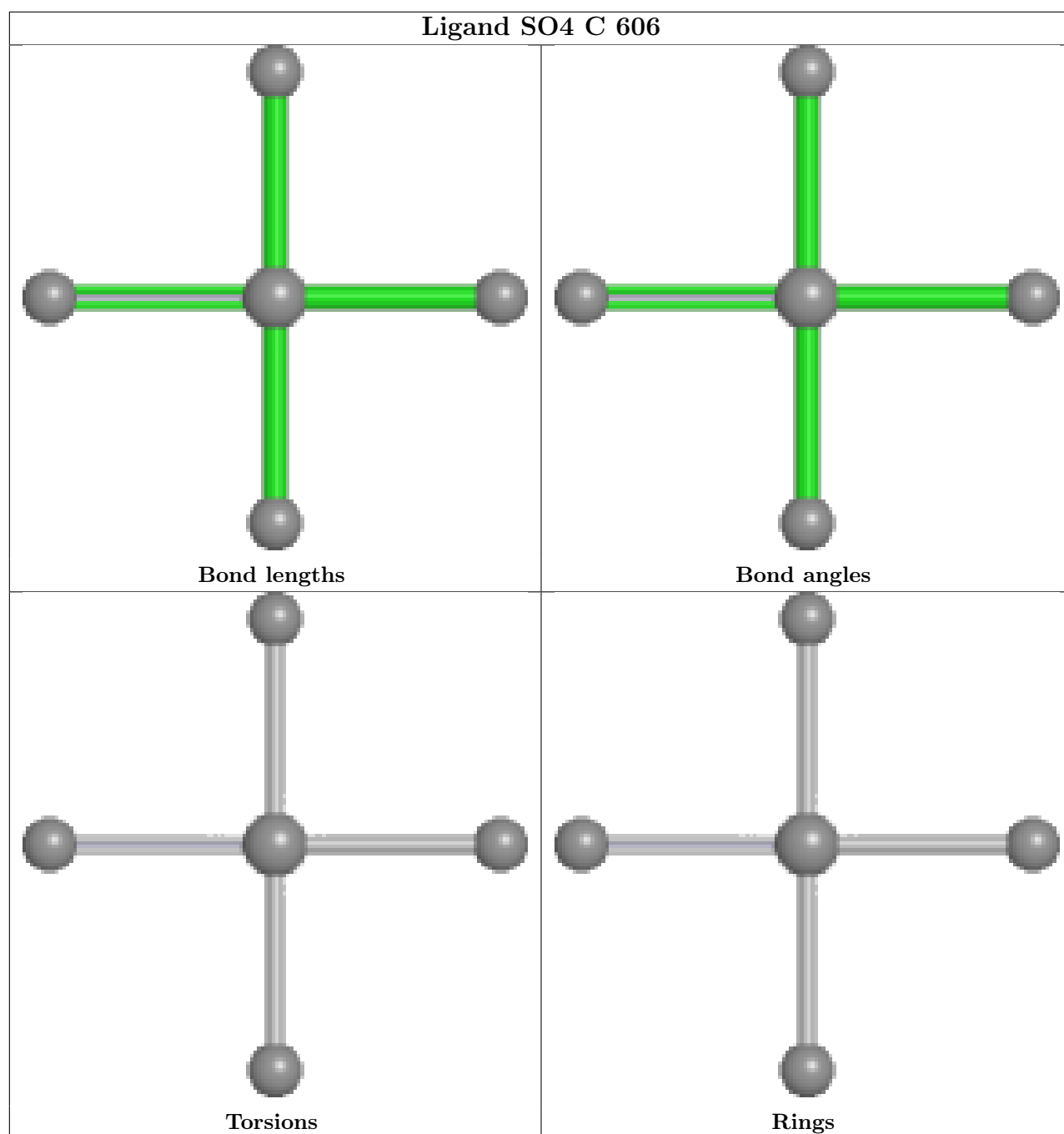
There are no chirality outliers.

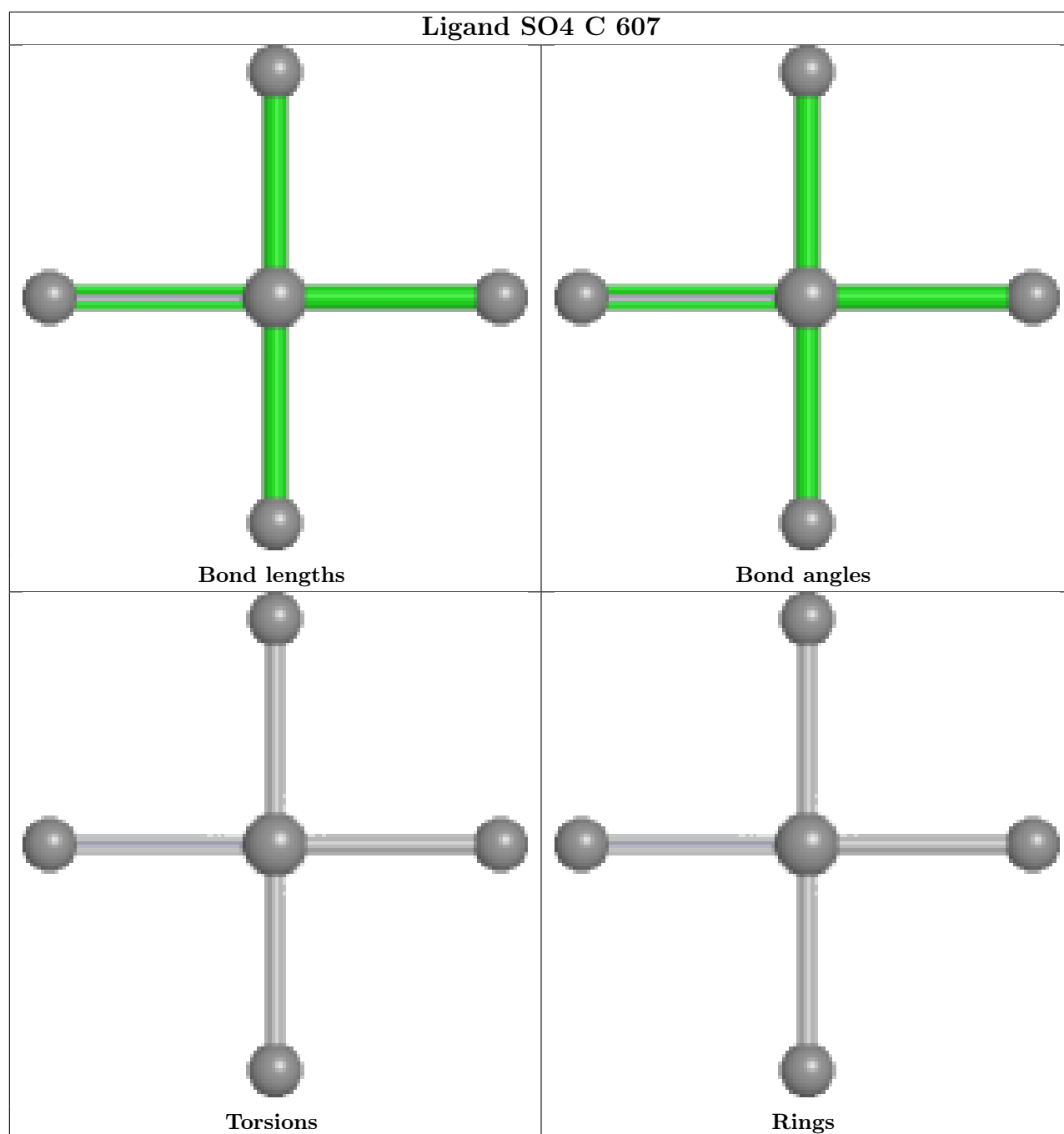
There are no torsion outliers.

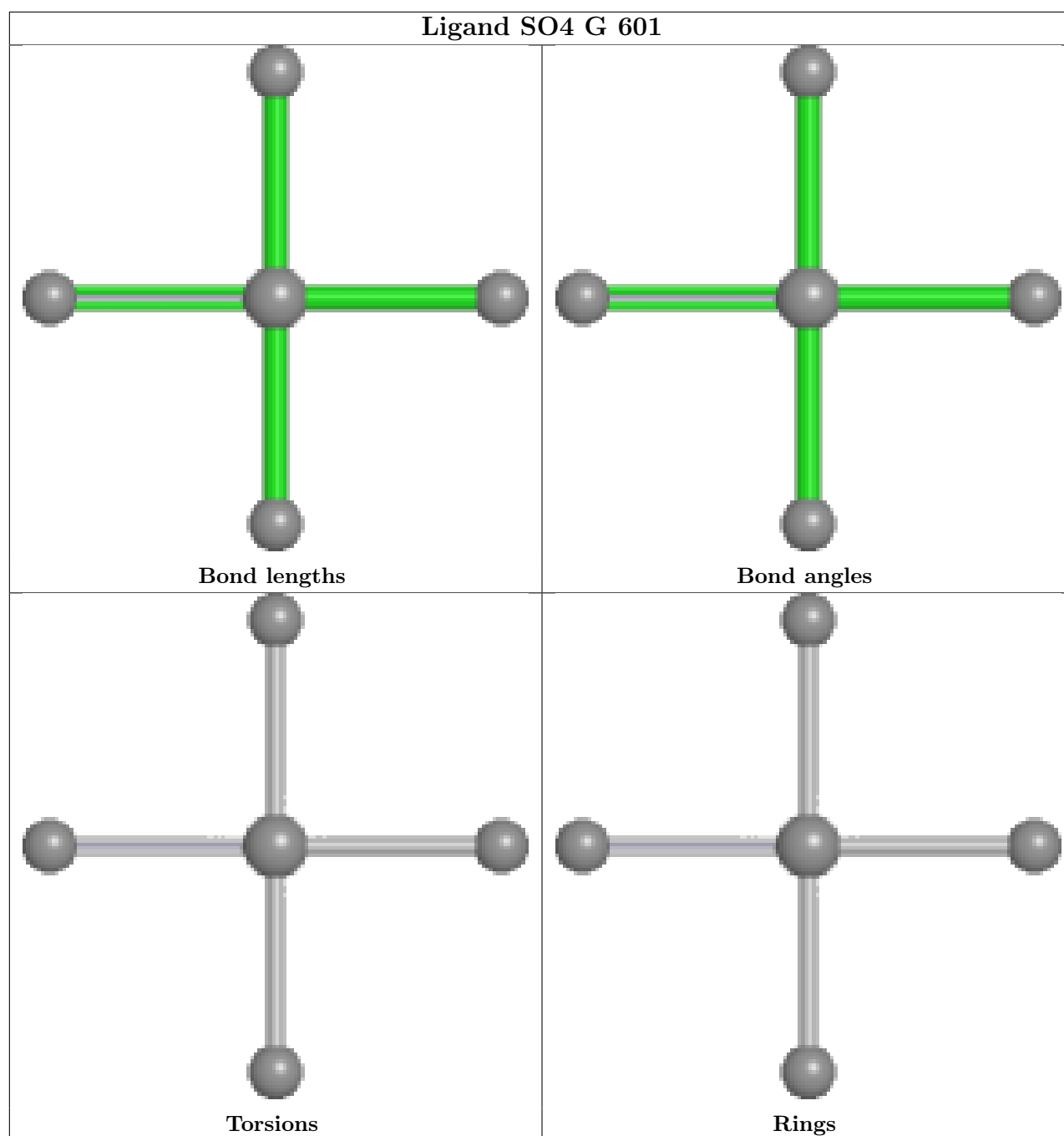
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	465/532 (87%)	0.05	18 (3%) 43 38	30, 54, 80, 123	0
1	C	462/532 (86%)	-0.09	8 (1%) 69 65	38, 52, 76, 107	0
1	G	5/532 (0%)	1.74	2 (40%) 1 0	64, 69, 80, 83	0
All	All	932/1596 (58%)	-0.01	28 (3%) 52 48	30, 53, 80, 123	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	ASN	5.9
1	A	385	ASP	4.9
1	A	465	ALA	4.5
1	A	387	PRO	4.3
1	A	1	MET	4.2
1	G	2	SER	3.4
1	A	3	ASN	3.1
1	A	384	ASN	3.0
1	A	386	ALA	2.9
1	A	350	MET	2.8
1	C	384	ASN	2.8
1	A	2	LYS	2.7
1	C	387	PRO	2.4
1	C	464	PRO	2.4
1	A	364	GLN	2.4
1	A	389	MET	2.3
1	C	350	MET	2.3
1	A	336	VAL	2.2
1	A	44	LYS	2.2
1	C	351	ASP	2.2
1	A	321	GLN	2.1
1	A	383	SER	2.1
1	A	31	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	385	ASP	2.1
1	A	116	TYR	2.1
1	C	386	ALA	2.0
1	A	344	HIS	2.0
1	G	4	HIS	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](#)

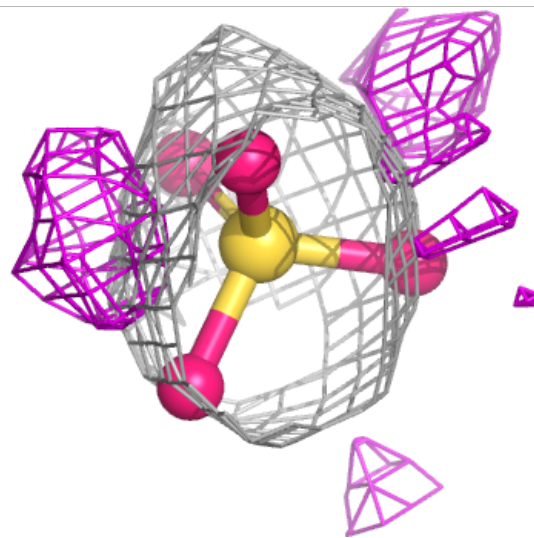
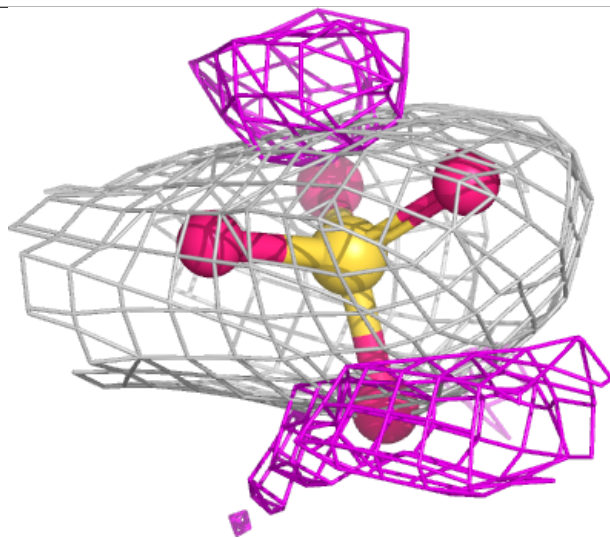
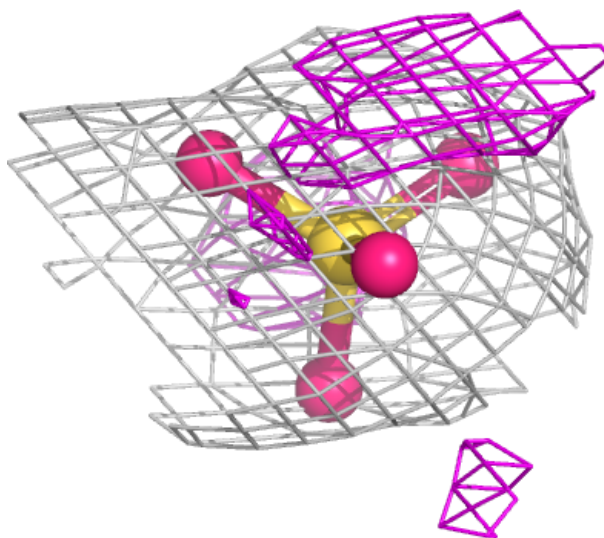
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	606	5/5	0.69	0.11	104,115,116,117	0
3	AG	A	605	1/1	0.79	0.29	154,154,154,154	1
4	SO4	C	607	5/5	0.84	0.12	84,88,90,100	0
3	AG	C	605	1/1	0.85	0.29	159,159,159,159	1
4	SO4	G	601	5/5	0.98	0.08	58,59,65,67	0
3	AG	A	606	1/1	0.99	0.08	75,75,75,75	1
2	CU	A	602	1/1	0.99	0.04	53,53,53,53	0
2	CU	A	604	1/1	0.99	0.02	43,43,43,43	0
2	CU	C	602	1/1	0.99	0.04	49,49,49,49	0
2	CU	A	601	1/1	0.99	0.03	48,48,48,48	0
2	CU	C	603	1/1	1.00	0.05	41,41,41,41	0
2	CU	C	604	1/1	1.00	0.03	40,40,40,40	0
2	CU	C	601	1/1	1.00	0.02	43,43,43,43	0
2	CU	A	603	1/1	1.00	0.06	41,41,41,41	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.

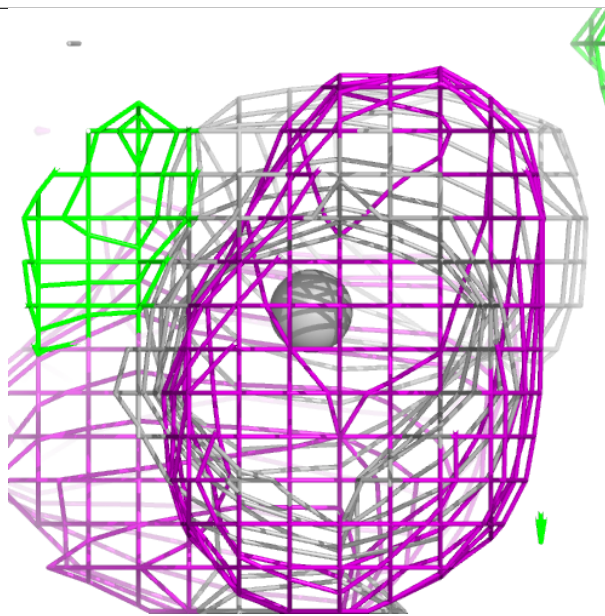
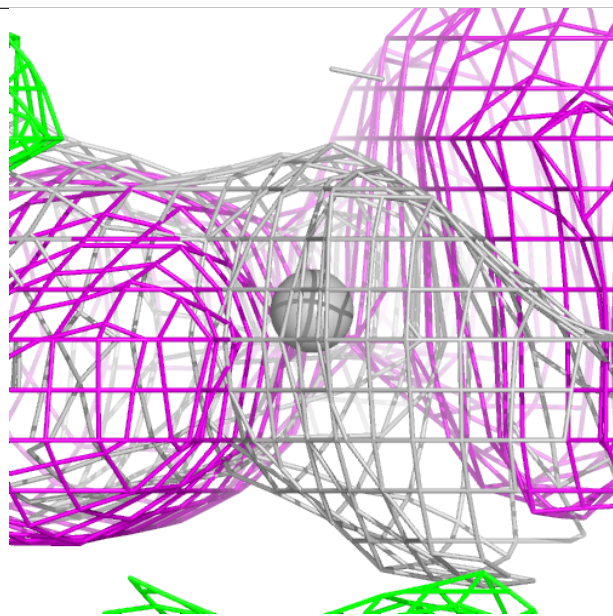
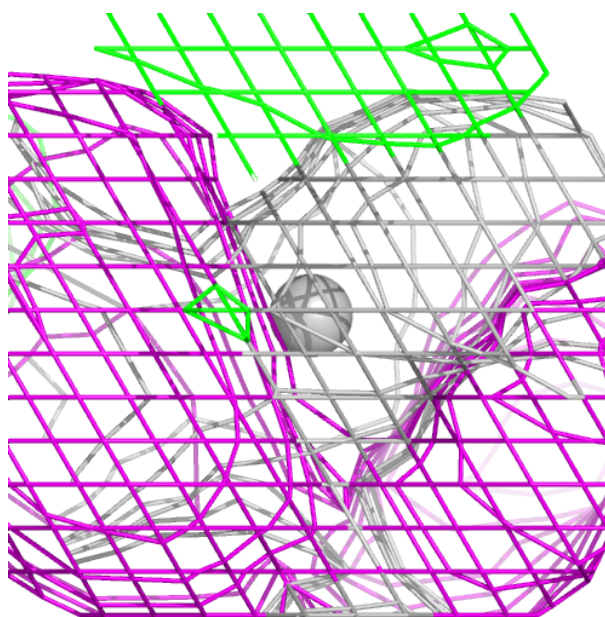
Electron density around SO4 C 606:

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



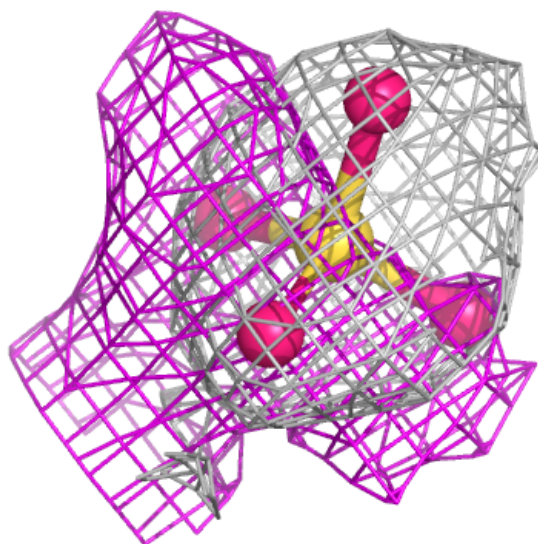
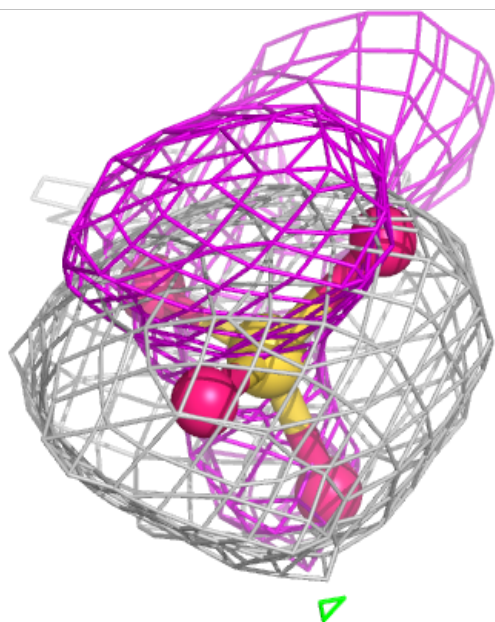
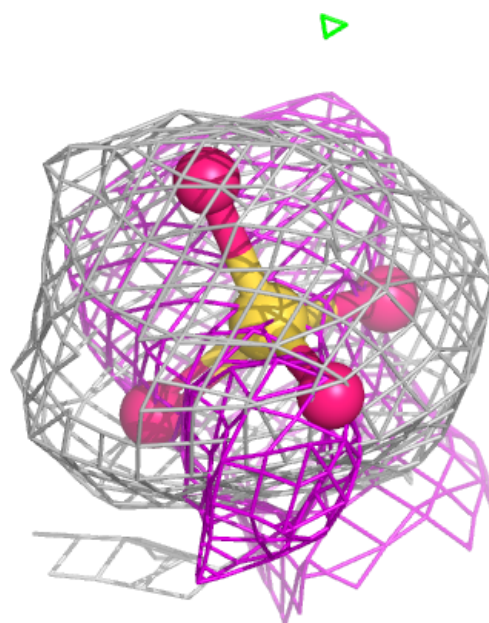
Electron density around AG A 605:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



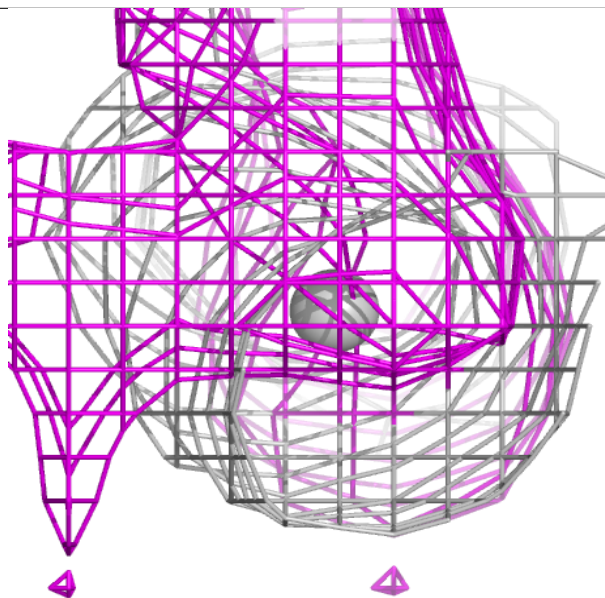
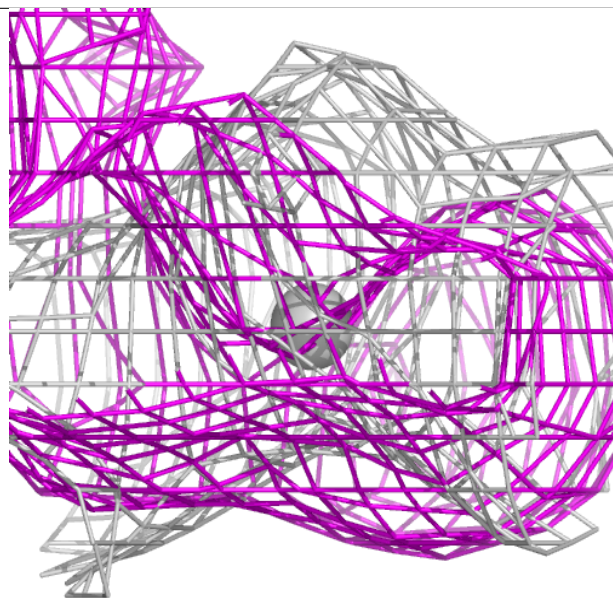
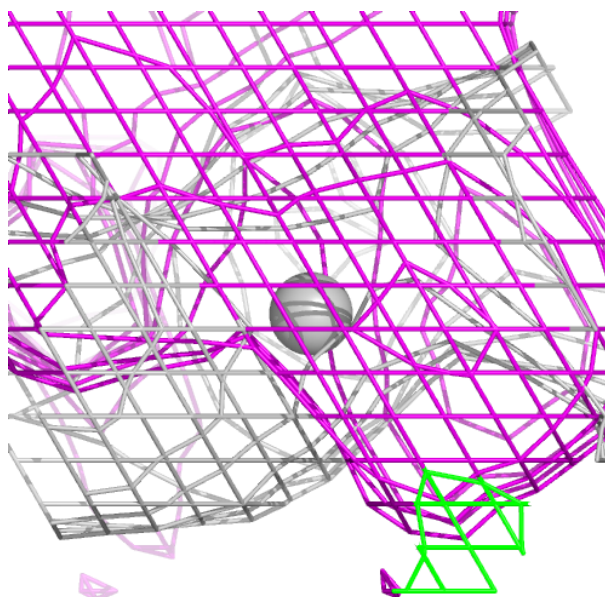
Electron density around SO4 C 607:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



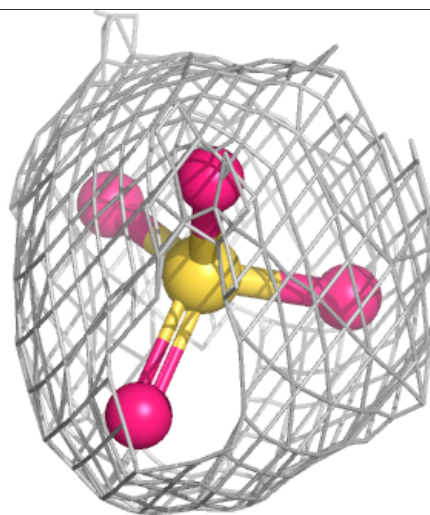
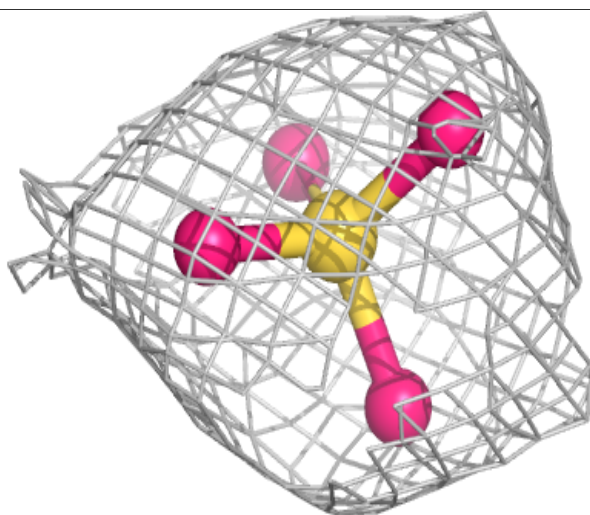
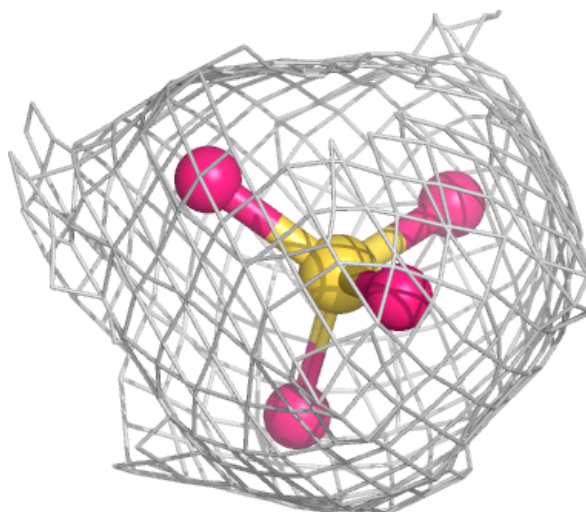
Electron density around AG C 605:

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and green (positive)



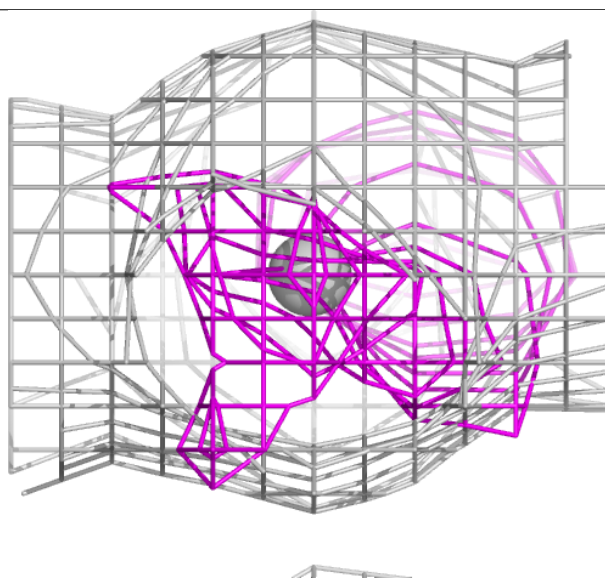
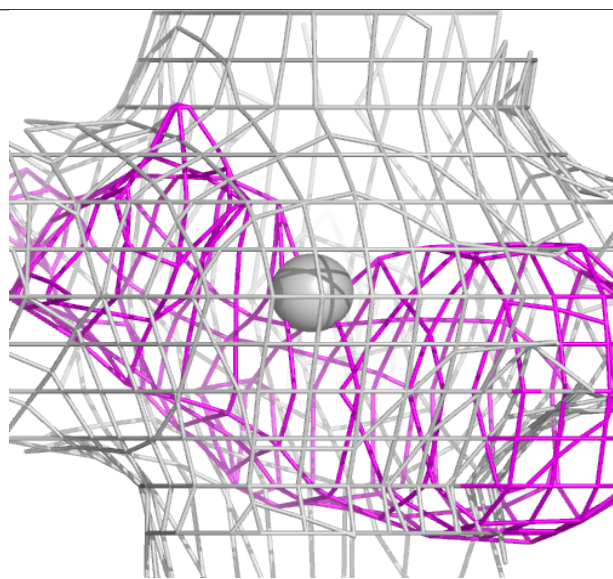
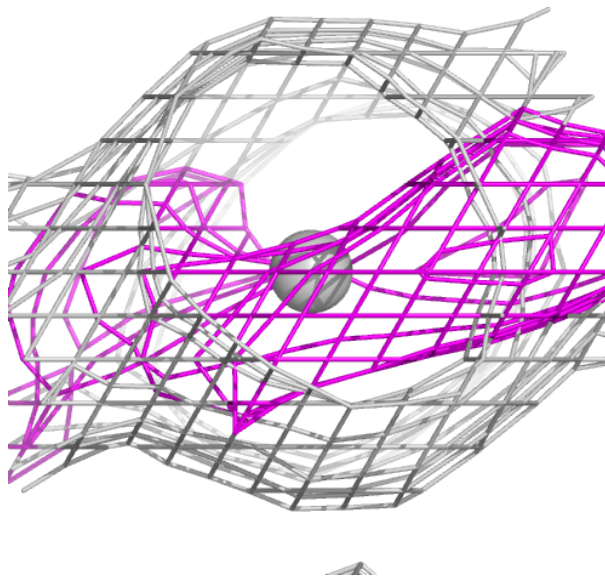
Electron density around SO4 G 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



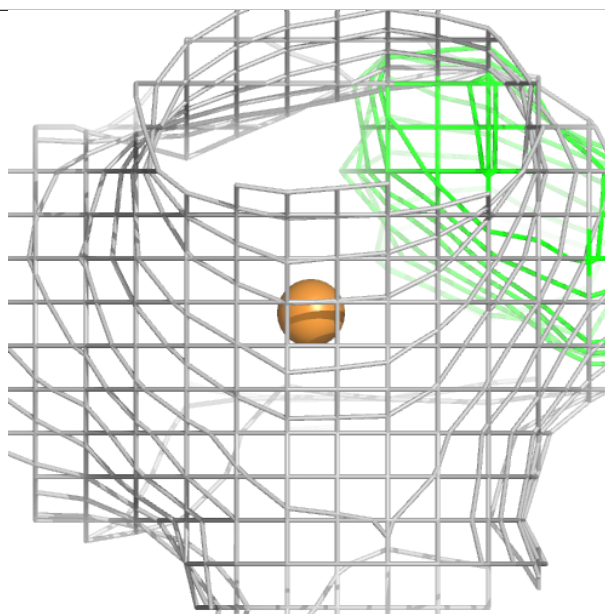
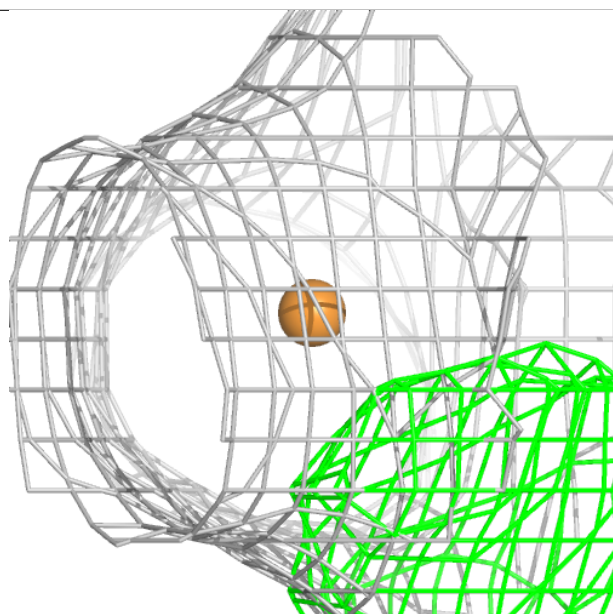
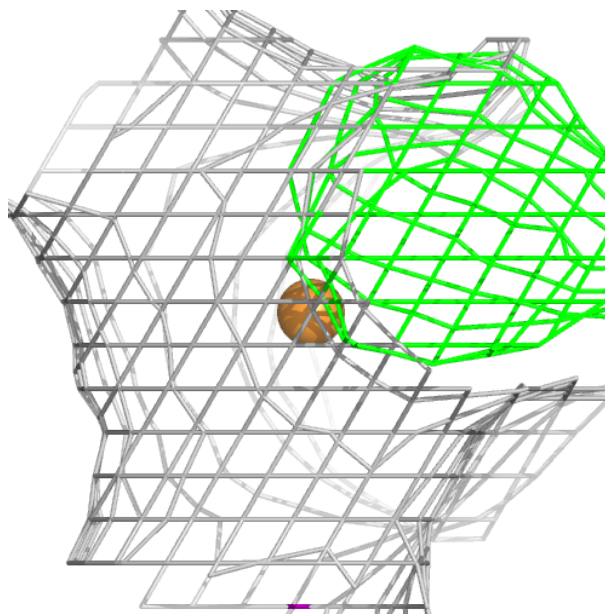
Electron density around AG A 606:

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and green (positive)



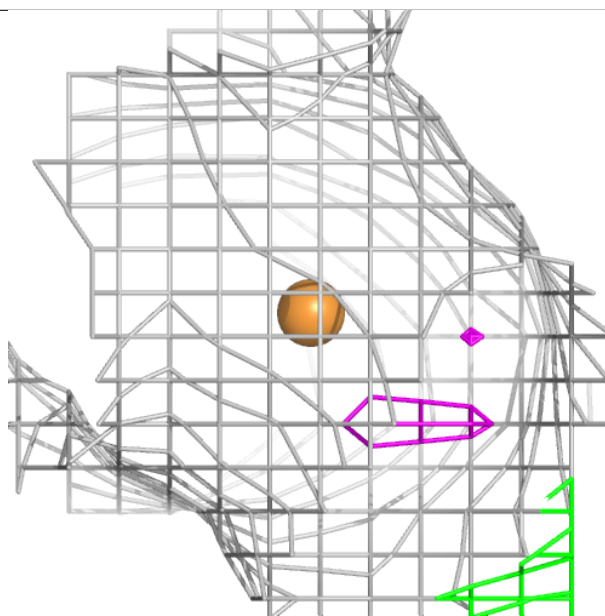
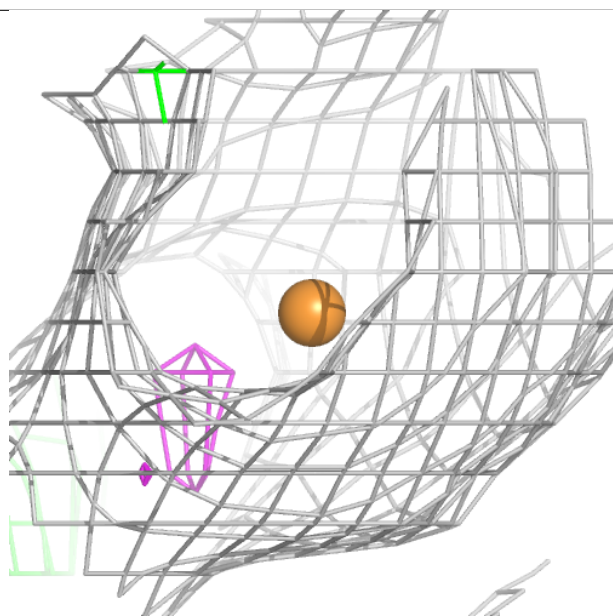
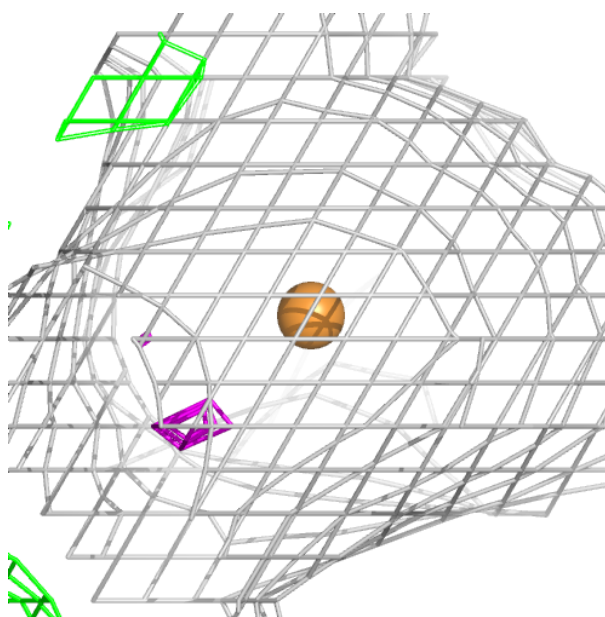
Electron density around CU A 602:

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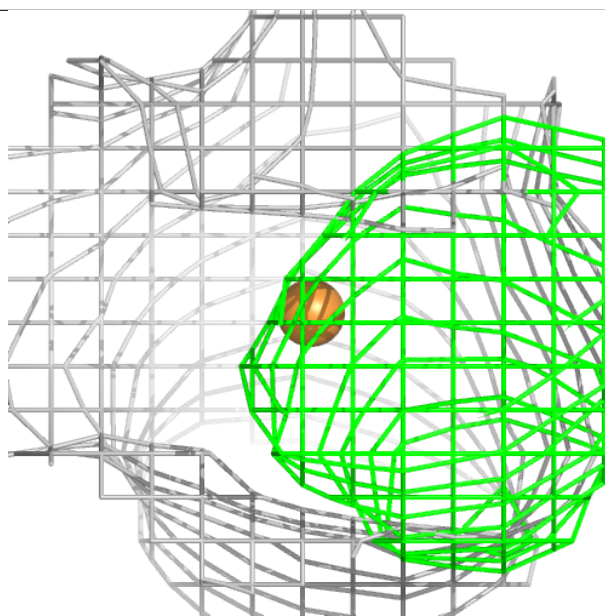
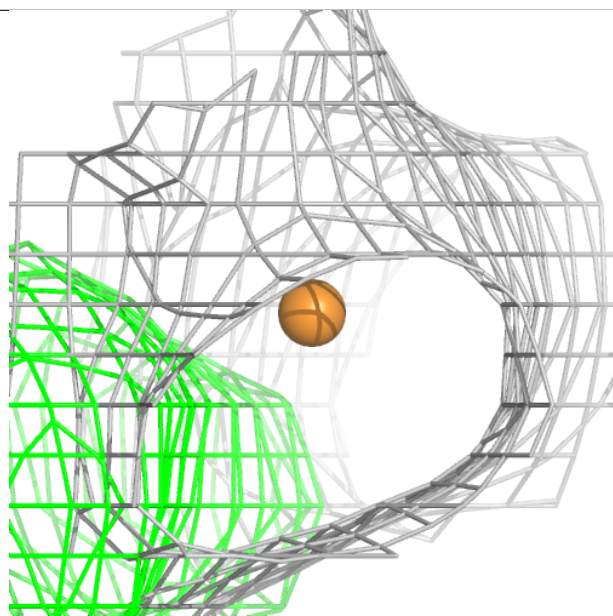
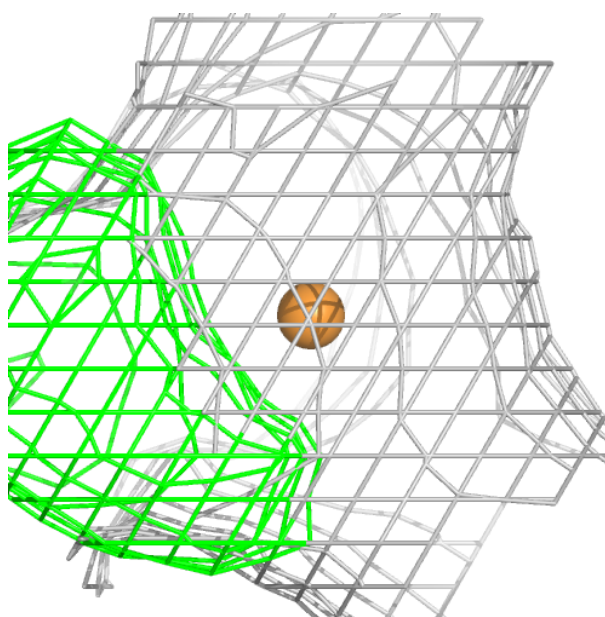
Electron density around CU A 604:

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and green (positive)



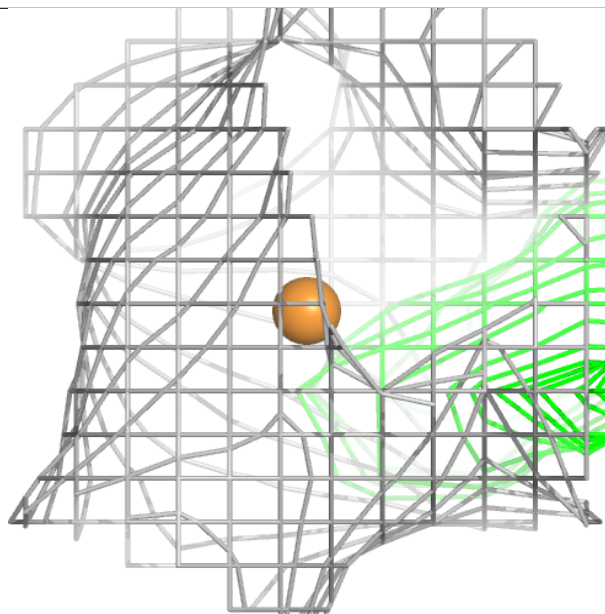
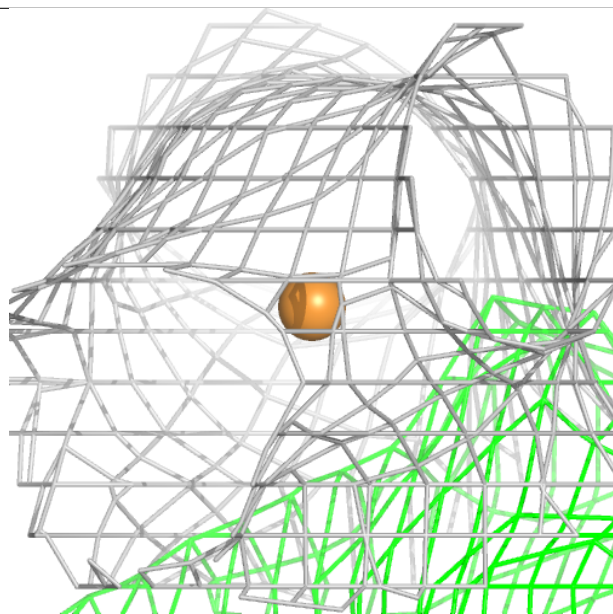
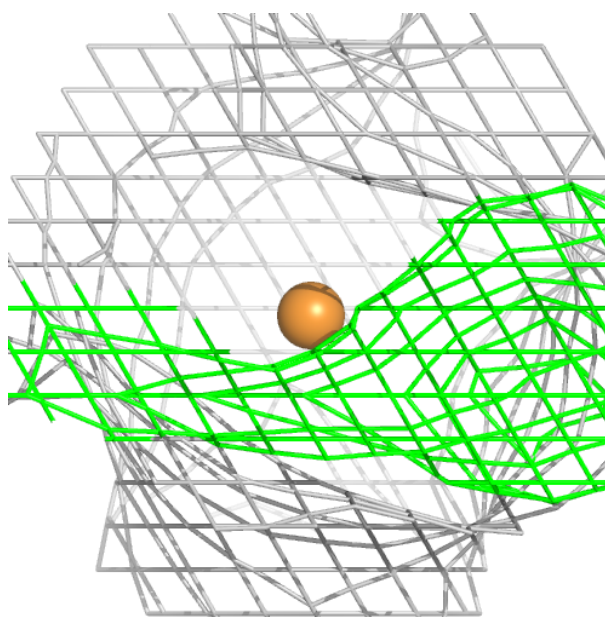
Electron density around CU C 602:

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and green (positive)



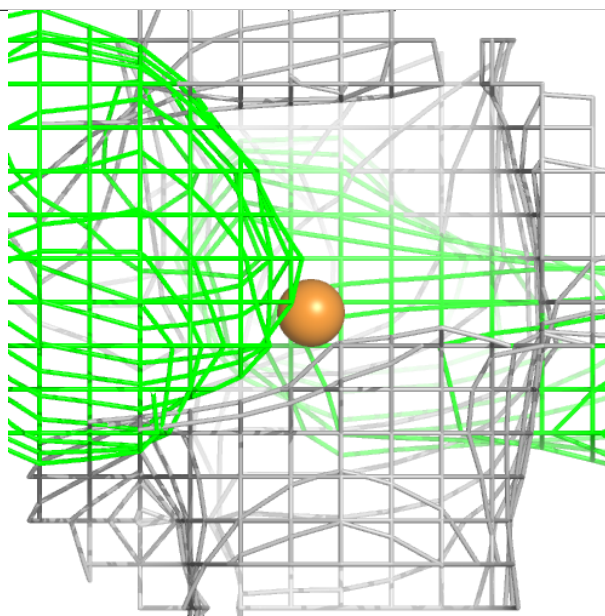
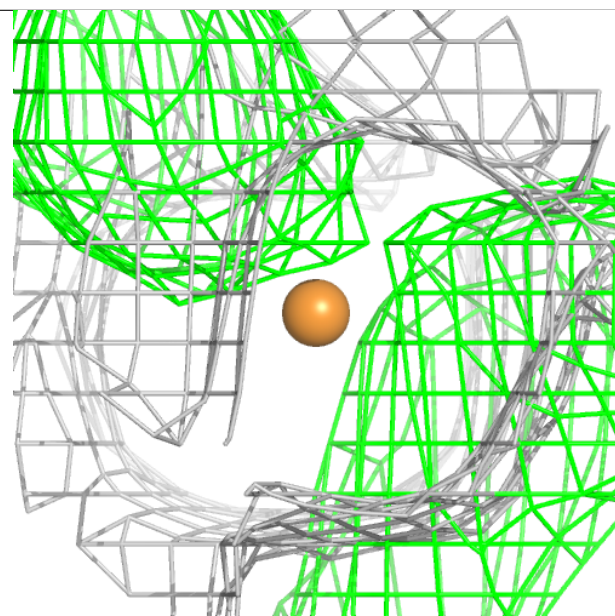
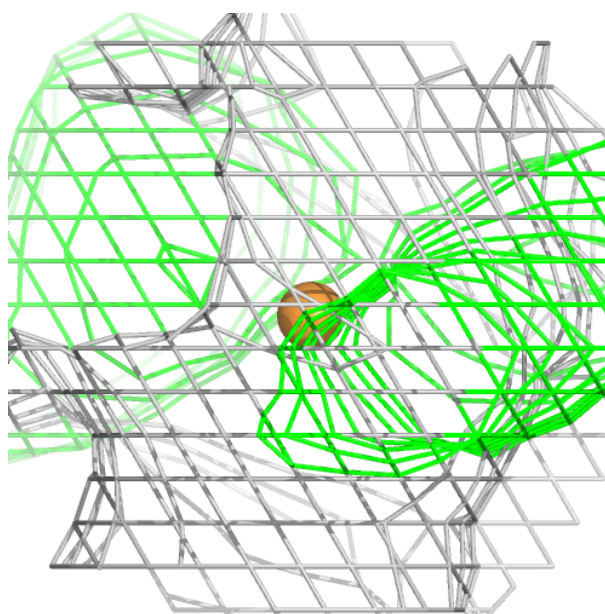
Electron density around CU A 601:

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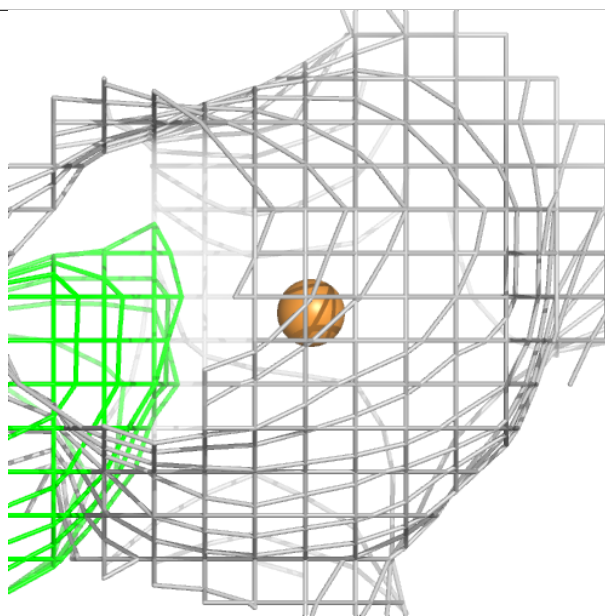
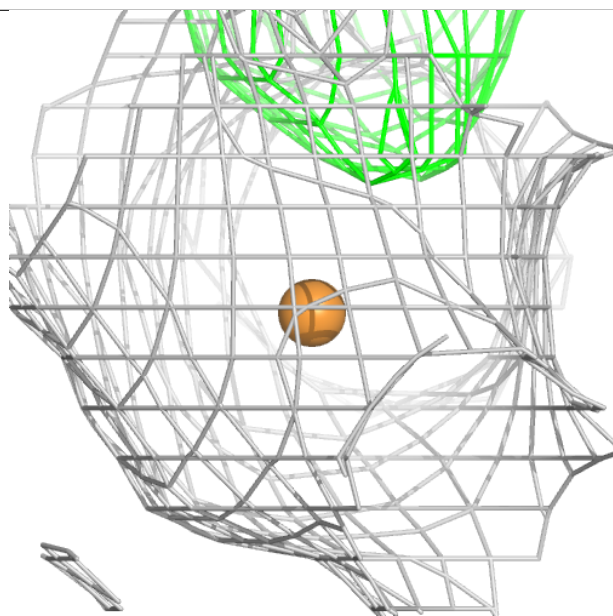
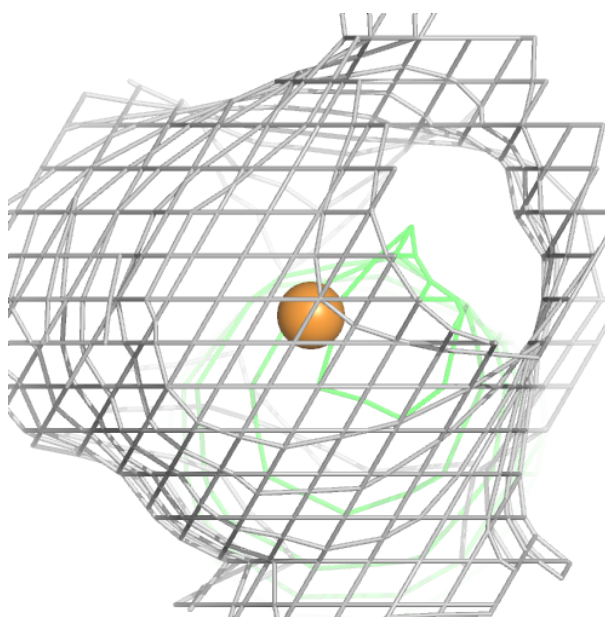
Electron density around CU C 603:

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and green (positive)



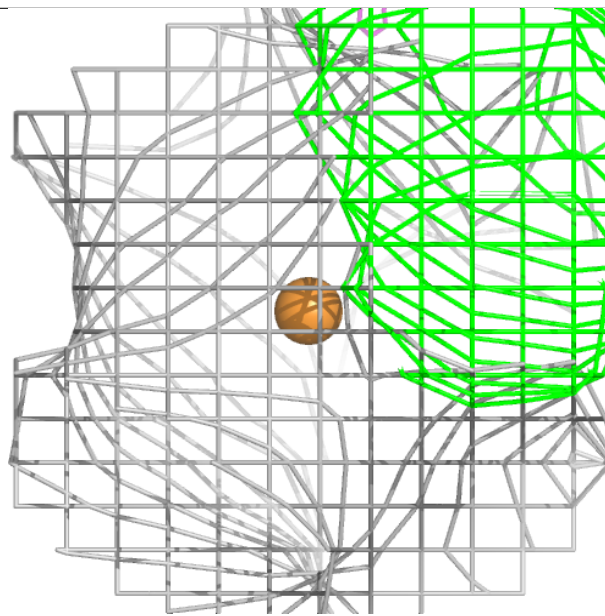
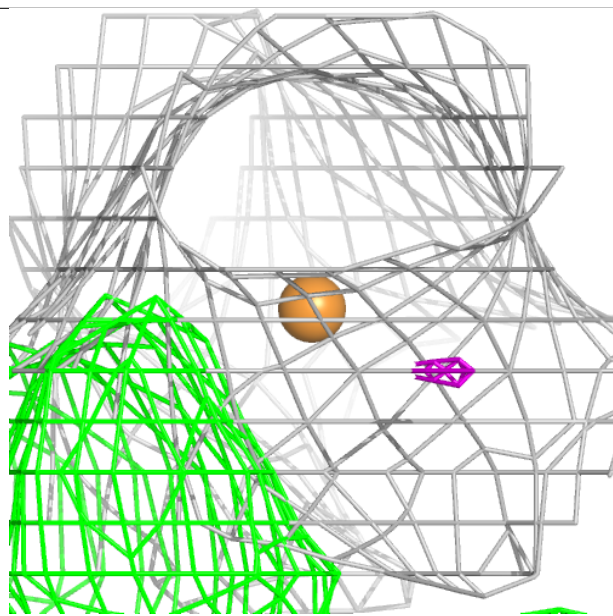
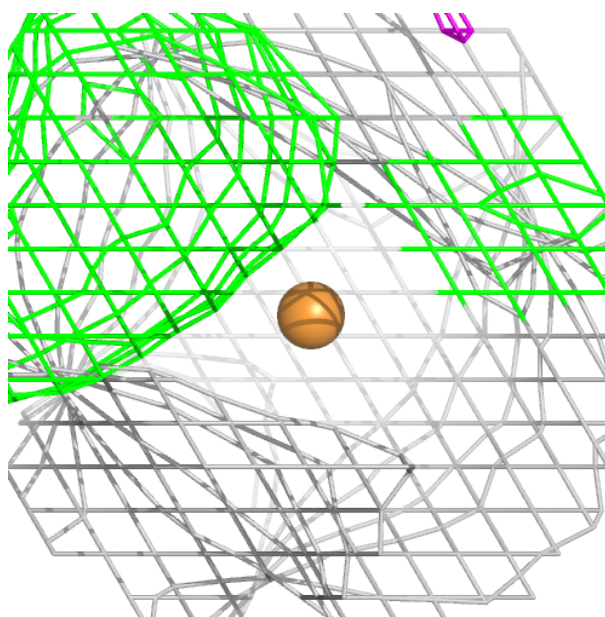
Electron density around CU C 604:

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and green (positive)



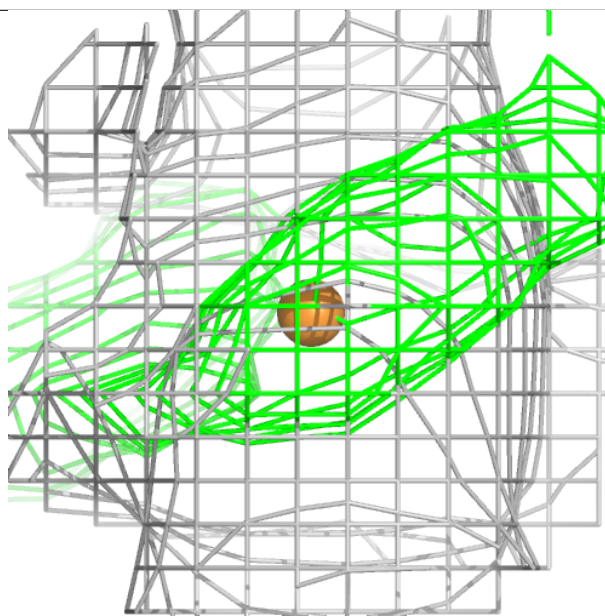
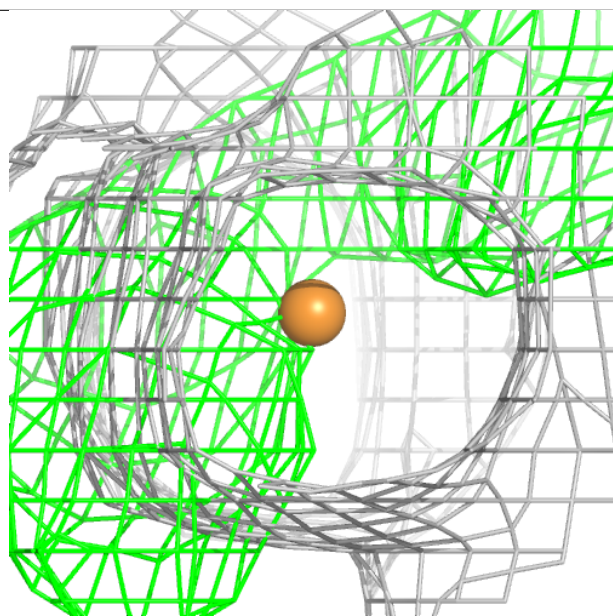
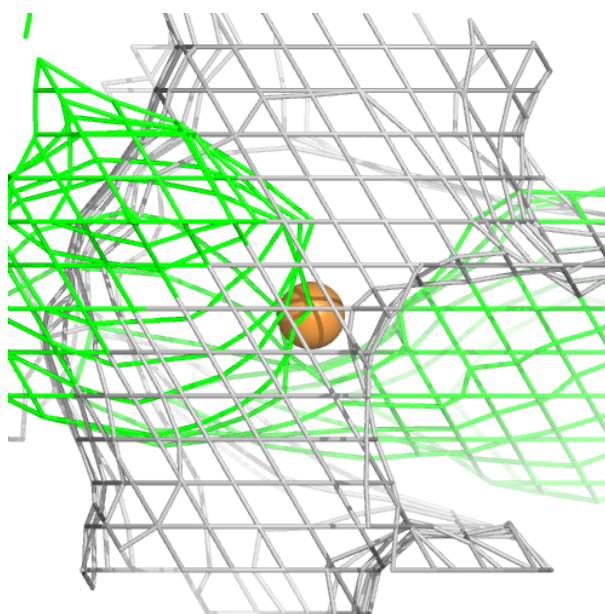
Electron density around CU C 601:

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



Electron density around CU A 603:

$2mF_o-DF_c$ (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.