



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2023 – 04:20 pm BST

PDB ID : 8P3L
Title : The structure of thiocyanate dehydrogenase mutant form with Thr 169 replaced by Ala from Thioalkalivibrio paradoxus
Authors : Varfolomeeva, L.A.; Polyakov, K.M.; Komolov, A.S.; Rakitina, T.V.; Dergousova, N.I.; Dorovatovskii, P.V.; Boyko, K.M.; Tikhonova, T.V.; Popov, V.O.
Deposited on : 2023-05-18
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.33
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

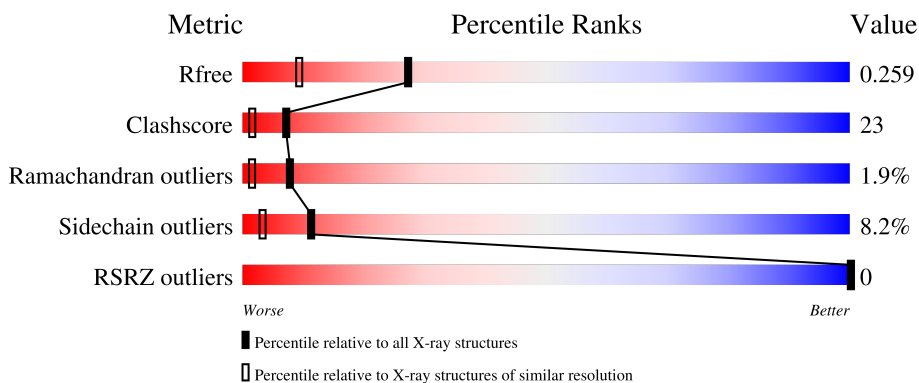
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	494	
1	D	494	
1	G	494	
1	J	494	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15340 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 Twin-arginine translocation signal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	3644	2325	608	693	18	6	1	0
1	D	467	3644	2325	607	694	18	4	2	0
1	G	467	3628	2320	599	691	18	4	2	0
1	J	467	3631	2321	601	691	18	3	2	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	initiating methionine	UNP W0DP94
A	56	SER	-	expression tag	UNP W0DP94
A	57	TYR	-	expression tag	UNP W0DP94
A	58	TYR	-	expression tag	UNP W0DP94
A	59	HIS	-	expression tag	UNP W0DP94
A	60	HIS	-	expression tag	UNP W0DP94
A	61	HIS	-	expression tag	UNP W0DP94
A	62	HIS	-	expression tag	UNP W0DP94
A	63	HIS	-	expression tag	UNP W0DP94
A	64	HIS	-	expression tag	UNP W0DP94
A	65	ASP	-	expression tag	UNP W0DP94
A	66	TYR	-	expression tag	UNP W0DP94
A	67	ASP	-	expression tag	UNP W0DP94
A	68	ILE	-	expression tag	UNP W0DP94
A	69	PRO	-	expression tag	UNP W0DP94
A	70	THR	-	expression tag	UNP W0DP94
A	71	THR	-	expression tag	UNP W0DP94
A	72	GLU	-	expression tag	UNP W0DP94
A	73	ASN	-	expression tag	UNP W0DP94
A	74	LEU	-	expression tag	UNP W0DP94
A	75	TYR	-	expression tag	UNP W0DP94

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Chain	Residue	Modelled	Actual	Comment	Reference
A	76	PHE	-	expression tag	UNP W0DP94
A	77	GLN	-	expression tag	UNP W0DP94
A	78	GLY	-	expression tag	UNP W0DP94
A	79	ALA	-	expression tag	UNP W0DP94
A	80	MET	-	expression tag	UNP W0DP94
A	81	GLY	-	expression tag	UNP W0DP94
A	169	ALA	THR	engineered mutation	UNP W0DP94
D	55	MET	-	initiating methionine	UNP W0DP94
D	56	SER	-	expression tag	UNP W0DP94
D	57	TYR	-	expression tag	UNP W0DP94
D	58	TYR	-	expression tag	UNP W0DP94
D	59	HIS	-	expression tag	UNP W0DP94
D	60	HIS	-	expression tag	UNP W0DP94
D	61	HIS	-	expression tag	UNP W0DP94
D	62	HIS	-	expression tag	UNP W0DP94
D	63	HIS	-	expression tag	UNP W0DP94
D	64	HIS	-	expression tag	UNP W0DP94
D	65	ASP	-	expression tag	UNP W0DP94
D	66	TYR	-	expression tag	UNP W0DP94
D	67	ASP	-	expression tag	UNP W0DP94
D	68	ILE	-	expression tag	UNP W0DP94
D	69	PRO	-	expression tag	UNP W0DP94
D	70	THR	-	expression tag	UNP W0DP94
D	71	THR	-	expression tag	UNP W0DP94
D	72	GLU	-	expression tag	UNP W0DP94
D	73	ASN	-	expression tag	UNP W0DP94
D	74	LEU	-	expression tag	UNP W0DP94
D	75	TYR	-	expression tag	UNP W0DP94
D	76	PHE	-	expression tag	UNP W0DP94
D	77	GLN	-	expression tag	UNP W0DP94
D	78	GLY	-	expression tag	UNP W0DP94
D	79	ALA	-	expression tag	UNP W0DP94
D	80	MET	-	expression tag	UNP W0DP94
D	81	GLY	-	expression tag	UNP W0DP94
D	169	ALA	THR	engineered mutation	UNP W0DP94
G	55	MET	-	initiating methionine	UNP W0DP94
G	56	SER	-	expression tag	UNP W0DP94
G	57	TYR	-	expression tag	UNP W0DP94
G	58	TYR	-	expression tag	UNP W0DP94
G	59	HIS	-	expression tag	UNP W0DP94
G	60	HIS	-	expression tag	UNP W0DP94
G	61	HIS	-	expression tag	UNP W0DP94

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Chain	Residue	Modelled	Actual	Comment	Reference
G	62	HIS	-	expression tag	UNP W0DP94
G	63	HIS	-	expression tag	UNP W0DP94
G	64	HIS	-	expression tag	UNP W0DP94
G	65	ASP	-	expression tag	UNP W0DP94
G	66	TYR	-	expression tag	UNP W0DP94
G	67	ASP	-	expression tag	UNP W0DP94
G	68	ILE	-	expression tag	UNP W0DP94
G	69	PRO	-	expression tag	UNP W0DP94
G	70	THR	-	expression tag	UNP W0DP94
G	71	THR	-	expression tag	UNP W0DP94
G	72	GLU	-	expression tag	UNP W0DP94
G	73	ASN	-	expression tag	UNP W0DP94
G	74	LEU	-	expression tag	UNP W0DP94
G	75	TYR	-	expression tag	UNP W0DP94
G	76	PHE	-	expression tag	UNP W0DP94
G	77	GLN	-	expression tag	UNP W0DP94
G	78	GLY	-	expression tag	UNP W0DP94
G	79	ALA	-	expression tag	UNP W0DP94
G	80	MET	-	expression tag	UNP W0DP94
G	81	GLY	-	expression tag	UNP W0DP94
G	169	ALA	THR	engineered mutation	UNP W0DP94
J	55	MET	-	initiating methionine	UNP W0DP94
J	56	SER	-	expression tag	UNP W0DP94
J	57	TYR	-	expression tag	UNP W0DP94
J	58	TYR	-	expression tag	UNP W0DP94
J	59	HIS	-	expression tag	UNP W0DP94
J	60	HIS	-	expression tag	UNP W0DP94
J	61	HIS	-	expression tag	UNP W0DP94
J	62	HIS	-	expression tag	UNP W0DP94
J	63	HIS	-	expression tag	UNP W0DP94
J	64	HIS	-	expression tag	UNP W0DP94
J	65	ASP	-	expression tag	UNP W0DP94
J	66	TYR	-	expression tag	UNP W0DP94
J	67	ASP	-	expression tag	UNP W0DP94
J	68	ILE	-	expression tag	UNP W0DP94
J	69	PRO	-	expression tag	UNP W0DP94
J	70	THR	-	expression tag	UNP W0DP94
J	71	THR	-	expression tag	UNP W0DP94
J	72	GLU	-	expression tag	UNP W0DP94
J	73	ASN	-	expression tag	UNP W0DP94
J	74	LEU	-	expression tag	UNP W0DP94
J	75	TYR	-	expression tag	UNP W0DP94

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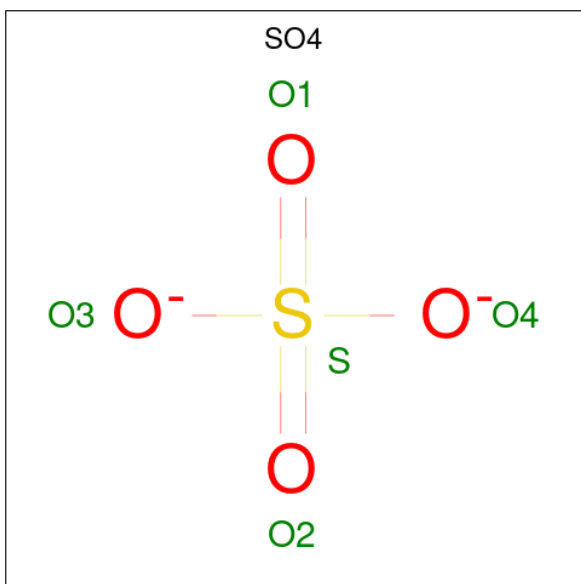
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Chain	Residue	Modelled	Actual	Comment	Reference
J	76	PHE	-	expression tag	UNP W0DP94
J	77	GLN	-	expression tag	UNP W0DP94
J	78	GLY	-	expression tag	UNP W0DP94
J	79	ALA	-	expression tag	UNP W0DP94
J	80	MET	-	expression tag	UNP W0DP94
J	81	GLY	-	expression tag	UNP W0DP94
J	169	ALA	THR	engineered mutation	UNP W0DP94

- 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	2	Total Cu 2 2	0	0
2	D	2	Total Cu 3 3	0	1
2	G	2	Total Cu 3 3	0	1
2	J	2	Total Cu 2 2	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	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	1

- Molecule 4 is water.

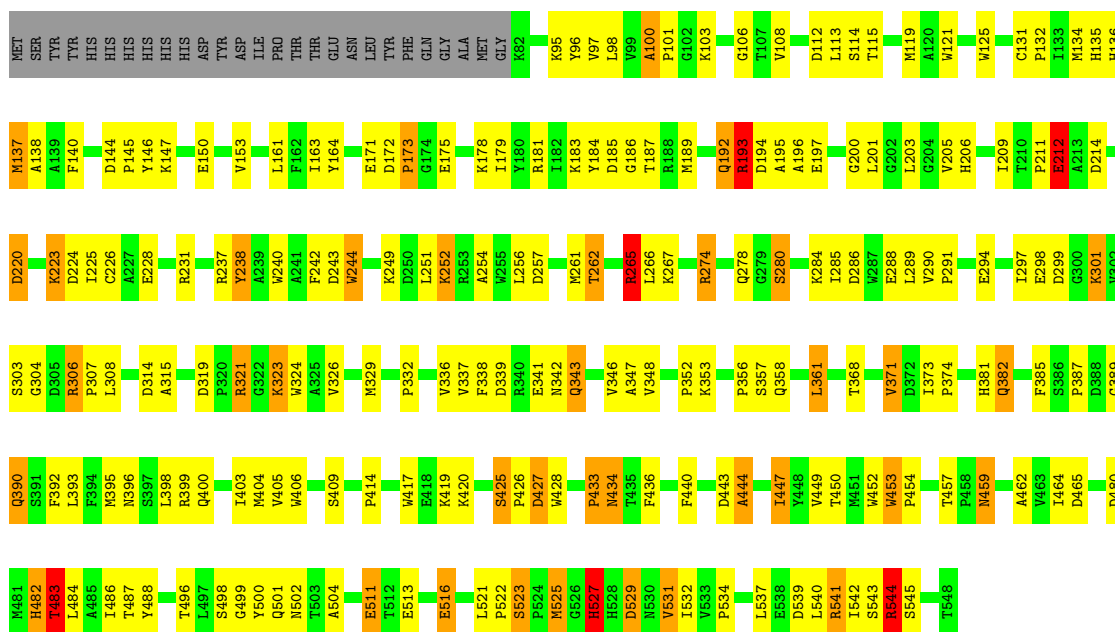
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	184	Total O 184 184	0	0
4	D	205	Total O 205 205	0	0
4	G	194	Total O 194 194	0	0
4	J	160	Total O 160 160	0	0

3 Residue-property plots

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.

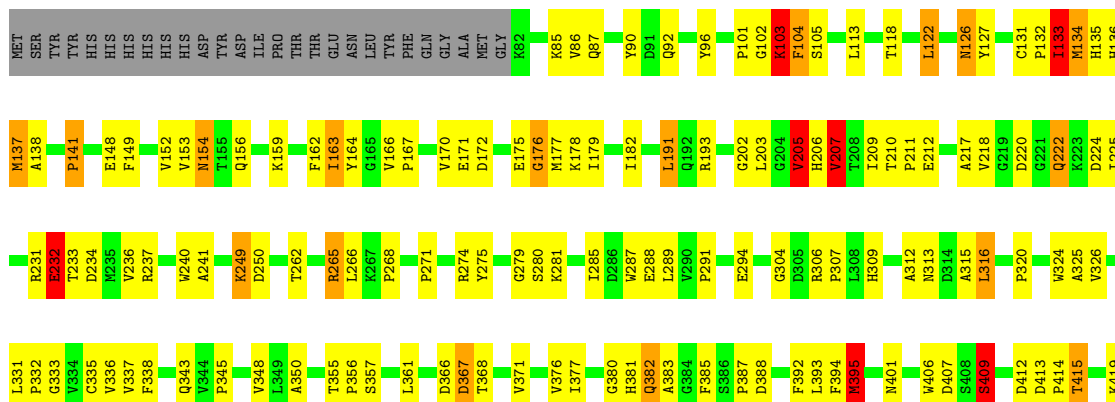
- Molecule 1: Twin-arginine translocation signal domain-containing protein

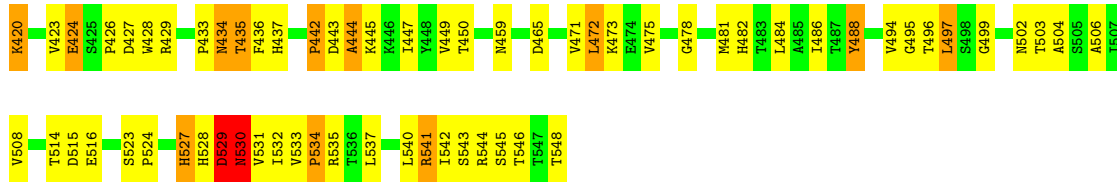
Chain A: 



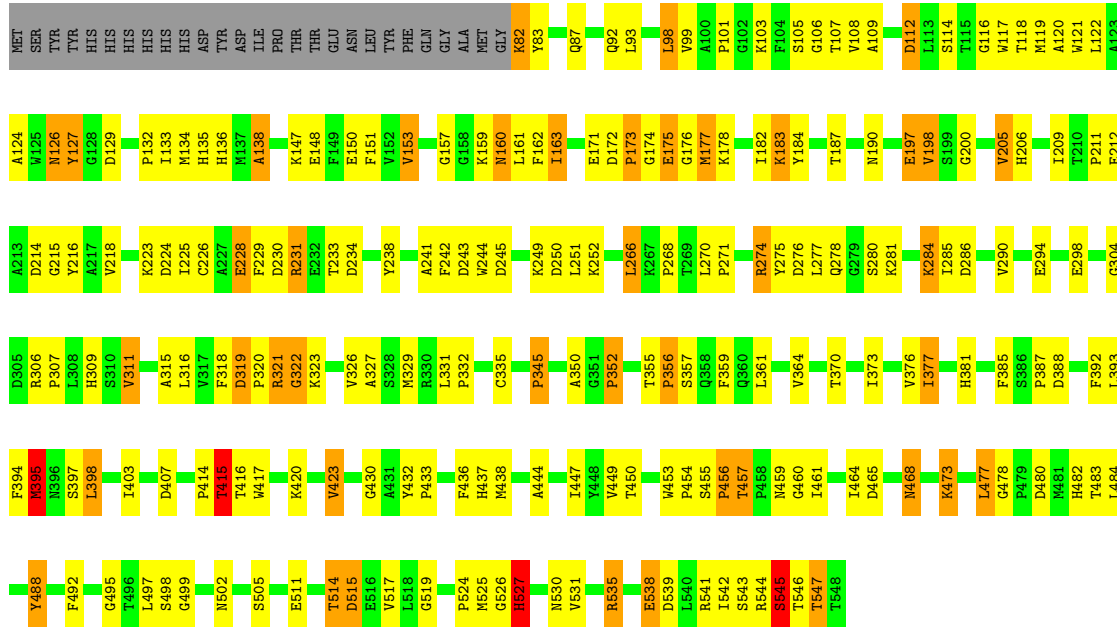
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain D: 

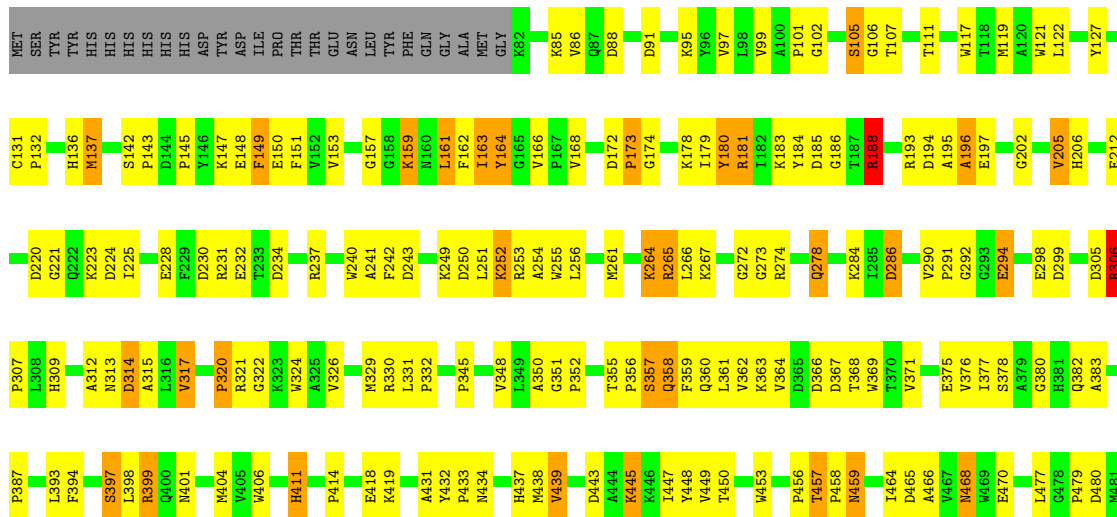




• Molecule 1: Twin-arginine translocation signal domain-containing protein



• Molecule 1: Twin-arginine translocation signal domain-containing protein



H482	T483	L484	A485	I486	T487	Y488	K491	F492	V493	V494	L497	S498	Q501	N502	S505	V508	V509	M510	E511	T512	E513	T514	D515	E516	L521	P522	M525	G526	H527	H528	D529	I532	V533	P534	R536	T536	R544	S545	T546	T547	T548
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.81Å 162.24Å 90.76Å 90.00° 119.74° 90.00°	Depositor
Resolution (Å)	81.12 – 1.80 81.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (81.12-1.80) 98.9 (81.12-1.80)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.254 0.191 , 0.259	Depositor DCC
R_{free} test set	10643 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	1.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.046 for l,k,-h-l 0.046 for -h-l,k,h 0.048 for -h-l,-k,l 0.045 for h,-k,-h-l 0.447 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15340	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.81	2/3752 (0.1%)	1.48	37/5119 (0.7%)
1	D	0.93	6/3755 (0.2%)	1.59	43/5124 (0.8%)
1	G	0.94	8/3740 (0.2%)	1.54	39/5104 (0.8%)
1	J	0.80	2/3743 (0.1%)	1.47	33/5110 (0.6%)
All	All	0.87	18/14990 (0.1%)	1.52	152/20457 (0.7%)

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	5
1	D	0	7
1	G	0	9
1	J	0	5
All	All	0	26

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	288	GLU	CD-OE1	11.34	1.38	1.25
1	G	535	ARG	CD-NE	-10.99	1.27	1.46
1	G	228	GLU	CD-OE1	-10.06	1.14	1.25
1	A	498	SER	CA-CB	-8.71	1.39	1.52
1	D	175	GLU	CD-OE2	-8.57	1.16	1.25

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	249	LYS	CB-CA-C	-10.58	89.25	110.40
1	J	188	ARG	CG-CD-NE	-9.62	91.60	111.80
1	D	535	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	G	456	PRO	N-CA-CB	-9.47	91.94	103.30
1	D	426	PRO	N-CD-CG	-9.36	89.17	103.20

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ALA	Mainchain
1	A	266	LEU	Mainchain
1	A	343	GLN	Peptide
1	A	385	PHE	Peptide
1	A	453	TRP	Peptide

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	A	3644	0	3517	160	0
1	D	3644	0	3509	149	0
1	G	3628	0	3491	169	0
1	J	3631	0	3493	178	0
2	A	2	0	0	0	0
2	D	3	0	0	1	0
2	G	3	0	0	0	0
2	J	2	0	0	0	0
3	A	5	0	0	1	0
3	D	10	0	0	1	0
3	G	20	0	0	1	0
3	J	5	0	0	0	0
4	A	184	0	0	13	0
4	D	205	0	0	10	0
4	G	194	0	0	4	0
4	J	160	0	0	14	0
All	All	15340	0	14010	647	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 23.

The worst 5 of 647 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)
2:D:602[B]:CU:CU	4:D:747:HOH:O	0.94	1.12
1:A:265:ARG:HG3	1:A:265:ARG:HH11	1.14	1.09
1:D:236:VAL:HG11	1:D:275:TYR:CE1	1.86	1.08
1:D:465:ASP:HB2	1:D:472:LEU:CD1	1.85	1.06
1:D:103:LYS:HE2	1:D:528:HIS:CE1	1.91	1.04

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	466/494 (94%)	420 (90%)	37 (8%)	9 (2%)	8	1
1	D	467/494 (94%)	405 (87%)	51 (11%)	11 (2%)	6	1
1	G	467/494 (94%)	416 (89%)	40 (9%)	11 (2%)	6	1
1	J	467/494 (94%)	411 (88%)	52 (11%)	4 (1%)	17	6
All	All	1867/1976 (94%)	1652 (88%)	180 (10%)	35 (2%)	8	1

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	280	SER
1	D	444	ALA
1	G	398	LEU
1	A	323	LYS
1	A	389	GLY

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	392/415 (94%)	359 (92%)	33 (8%)	11	3
1	D	392/415 (94%)	358 (91%)	34 (9%)	10	3
1	G	388/415 (94%)	361 (93%)	27 (7%)	15	5
1	J	389/415 (94%)	354 (91%)	35 (9%)	9	2
All	All	1561/1660 (94%)	1432 (92%)	129 (8%)	11	3

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	317	VAL
1	J	366[B]	ASP
1	D	336	VAL
1	D	294	GLU
1	J	377	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	342	ASN
1	J	360	GLN
1	J	482	HIS
1	D	382	GLN
1	D	401	ASN

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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	G	606	-	4,4,4	0.28	0	6,6,6	0.69	0
3	SO4	G	604	-	4,4,4	0.62	0	6,6,6	0.24	0
3	SO4	G	605	-	4,4,4	0.86	0	6,6,6	0.62	0
3	SO4	D	604	-	4,4,4	0.55	0	6,6,6	0.66	0
3	SO4	J	603[A]	-	4,4,4	0.44	0	6,6,6	0.44	0
3	SO4	G	603	-	4,4,4	0.68	0	6,6,6	0.21	0
3	SO4	A	603[A]	-	4,4,4	0.47	0	6,6,6	1.14	0
3	SO4	D	603	-	4,4,4	0.72	0	6,6,6	0.43	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	606	SO4	1	0
3	D	604	SO4	1	0
3	A	603[A]	SO4	1	0

5.7 Other polymers [i](#)

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 [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, 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	467/494 (94%)	-0.62	0 100 100	9, 19, 28, 42	3 (0%)
1	D	467/494 (94%)	-0.65	0 100 100	8, 17, 26, 37	1 (0%)
1	G	467/494 (94%)	-0.69	0 100 100	9, 17, 25, 38	1 (0%)
1	J	467/494 (94%)	-0.62	0 100 100	10, 19, 30, 37	2 (0%)
All	All	1868/1976 (94%)	-0.65	0 100 100	8, 18, 27, 42	7 (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, 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
3	SO4	G	603	5/5	0.97	0.08	15,19,22,23	0
3	SO4	D	604	5/5	0.98	0.07	9,12,13,14	5
3	SO4	D	603	5/5	0.98	0.09	19,20,24,26	5
3	SO4	G	604	5/5	0.98	0.07	17,17,20,25	5

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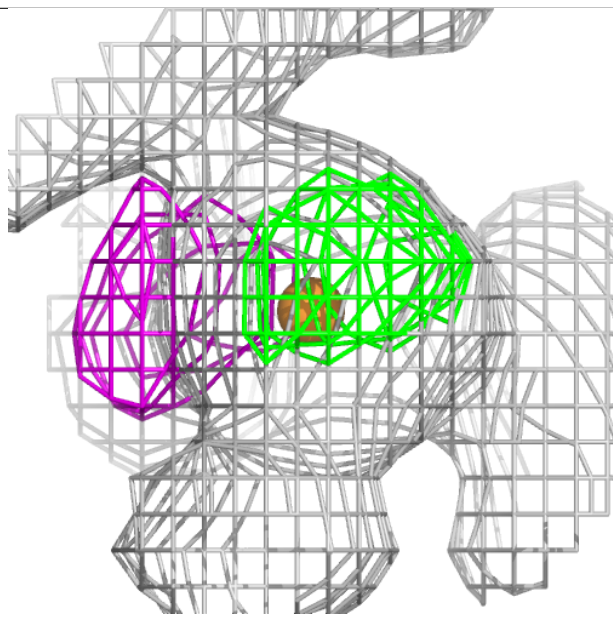
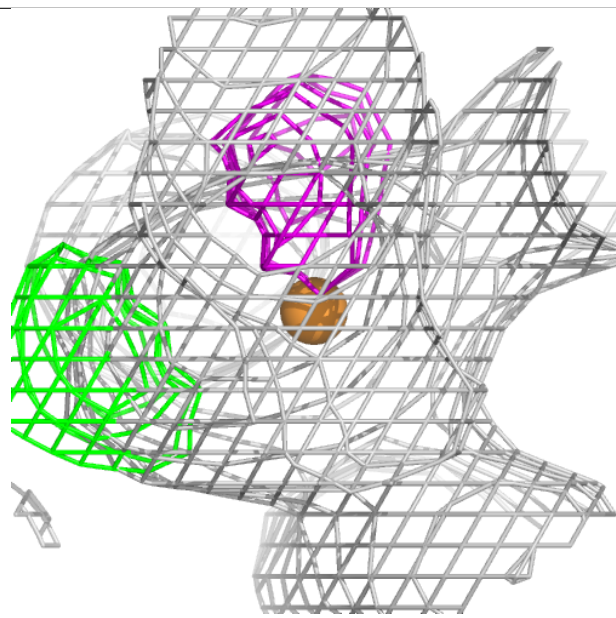
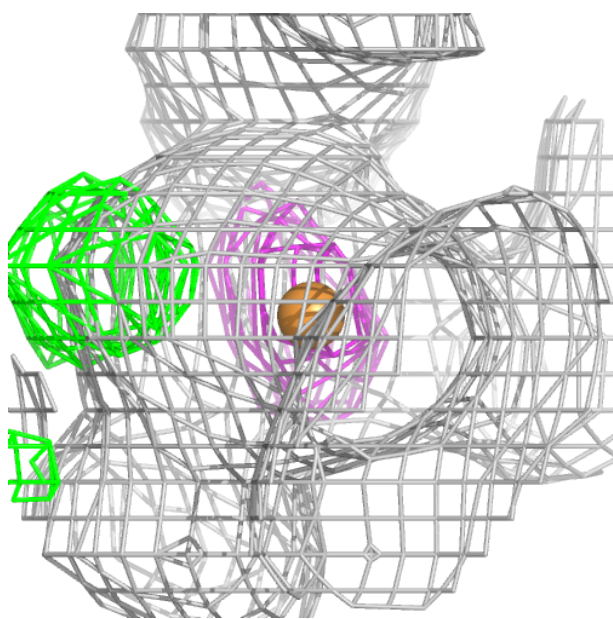
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	G	605	5/5	0.98	0.10	17,18,19,22	5
3	SO4	A	603[A]	5/5	0.99	0.09	8,8,8,11	5
2	CU	G	602[A]	1/1	0.99	0.06	17,17,17,17	1
2	CU	G	602[B]	1/1	0.99	0.06	15,15,15,15	1
3	SO4	G	606	5/5	0.99	0.05	18,19,22,23	0
3	SO4	J	603[A]	5/5	0.99	0.05	18,18,19,23	0
2	CU	D	601	1/1	1.00	0.05	18,18,18,18	0
2	CU	D	602[A]	1/1	1.00	0.05	14,14,14,14	1
2	CU	D	602[B]	1/1	1.00	0.05	6,6,6,6	1
2	CU	G	601	1/1	1.00	0.05	12,12,12,12	0
2	CU	A	601	1/1	1.00	0.05	15,15,15,15	0
2	CU	A	602	1/1	1.00	0.06	22,22,22,22	0
2	CU	J	601	1/1	1.00	0.07	23,23,23,23	0
2	CU	J	602	1/1	1.00	0.04	19,19,19,19	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.

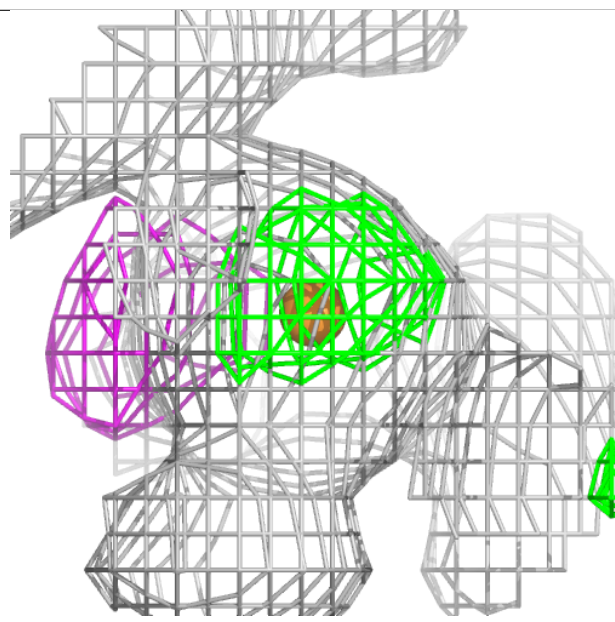
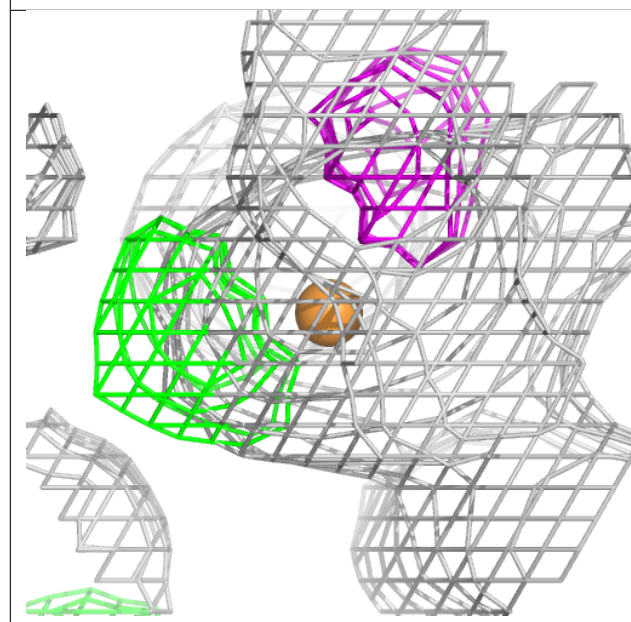
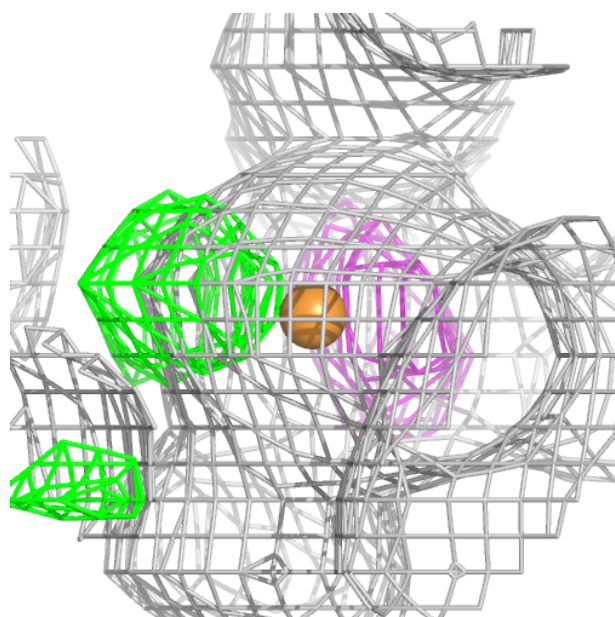
Electron density around CU G 602 (A):

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



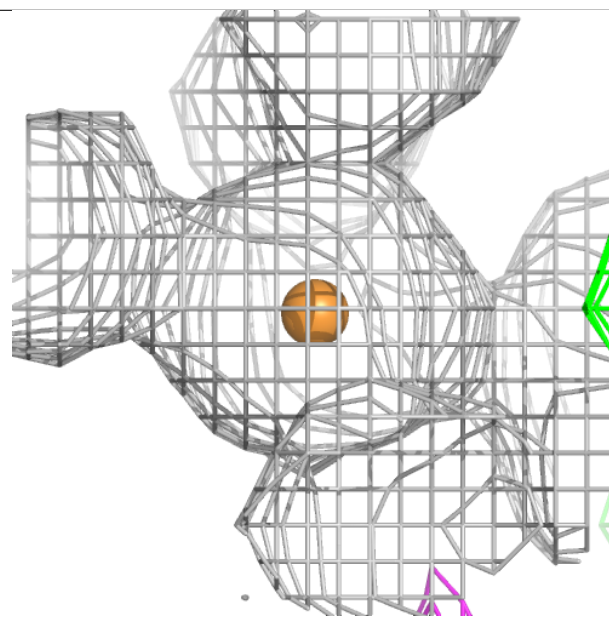
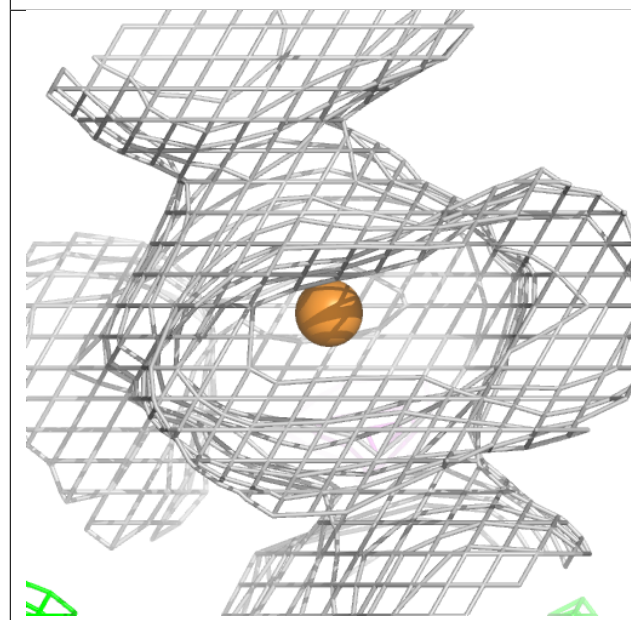
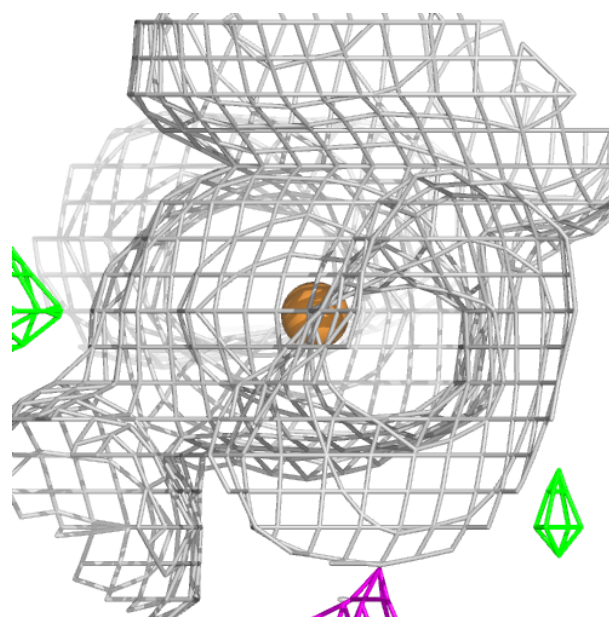
Electron density around CU G 602 (B):

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and green (positive)



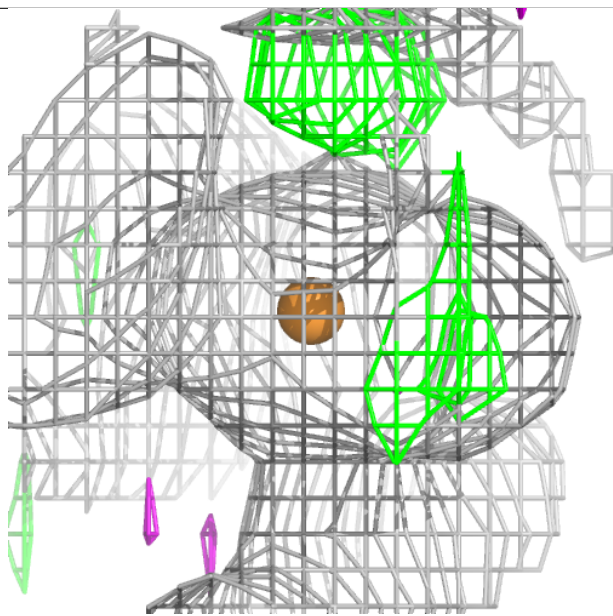
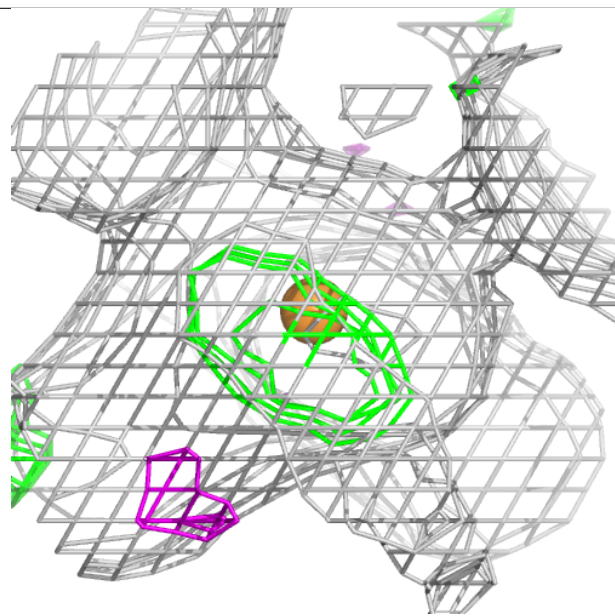
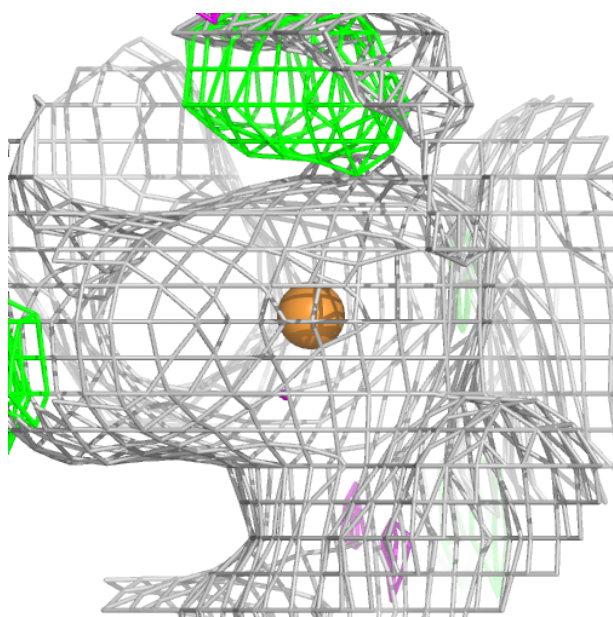
Electron density around CU D 601:

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



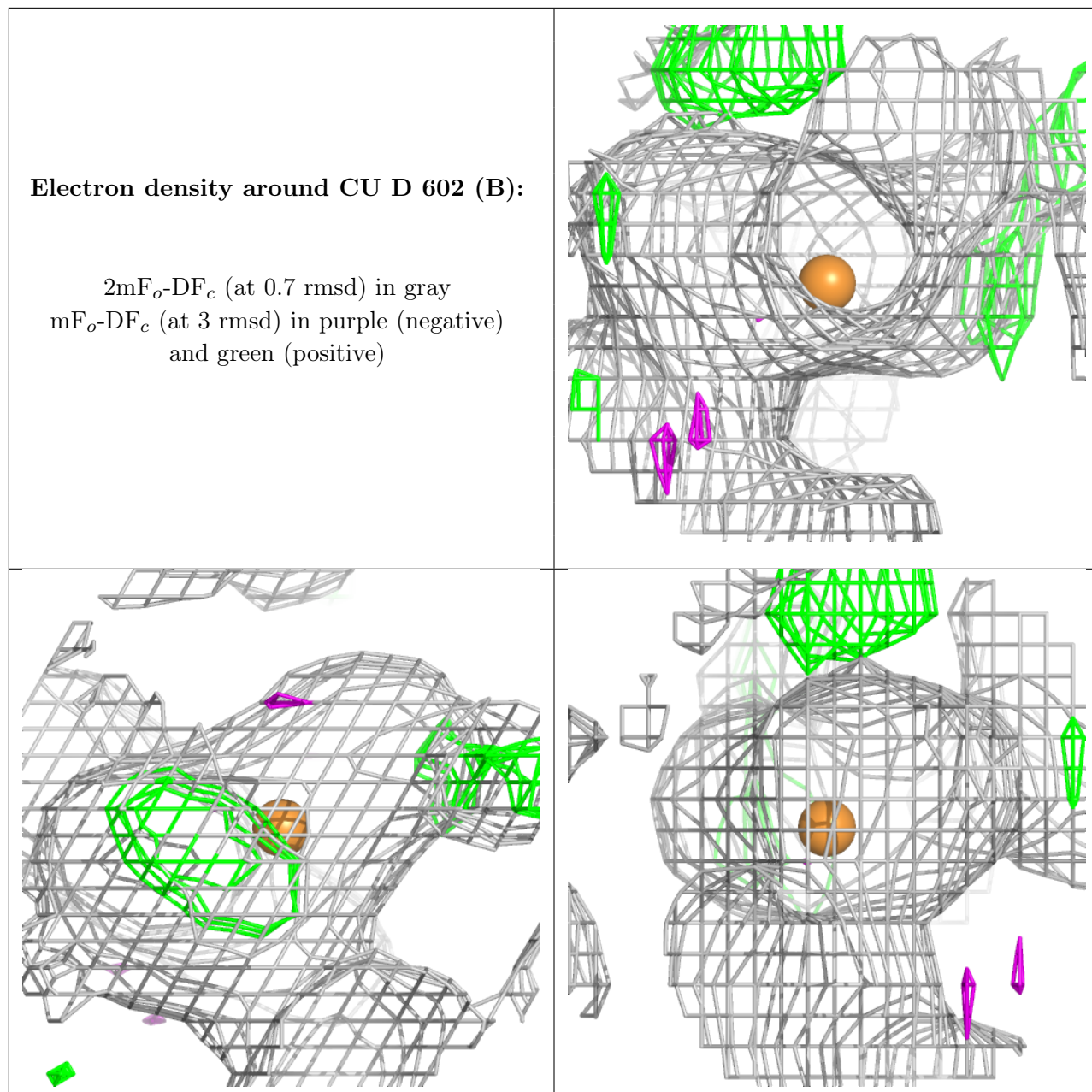
Electron density around CU D 602 (A):

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and green (positive)



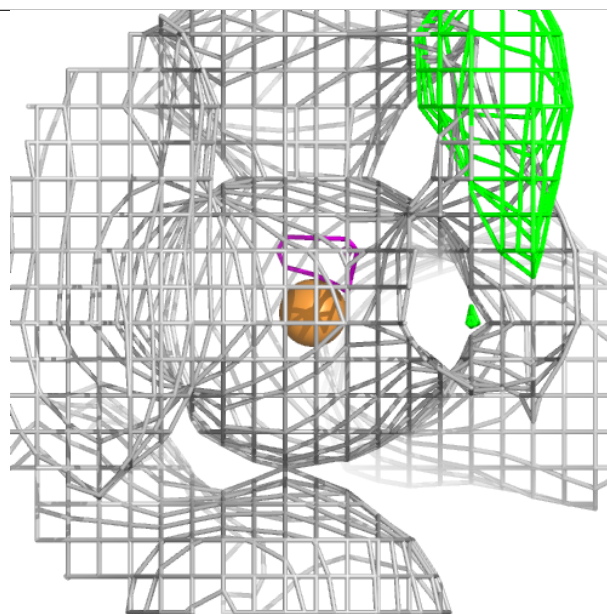
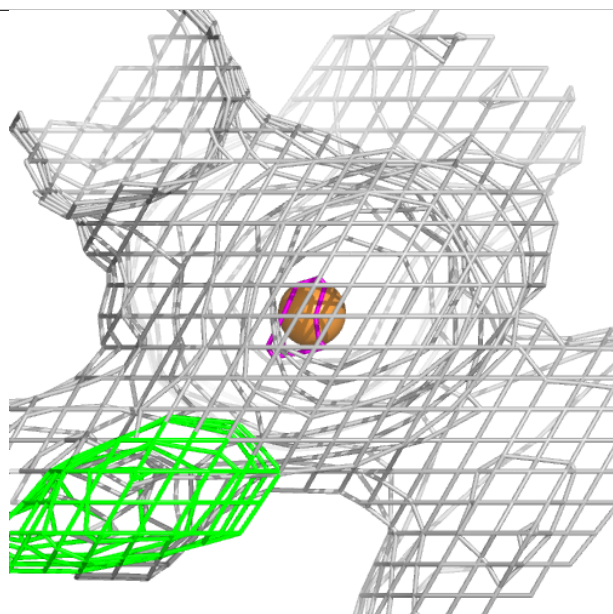
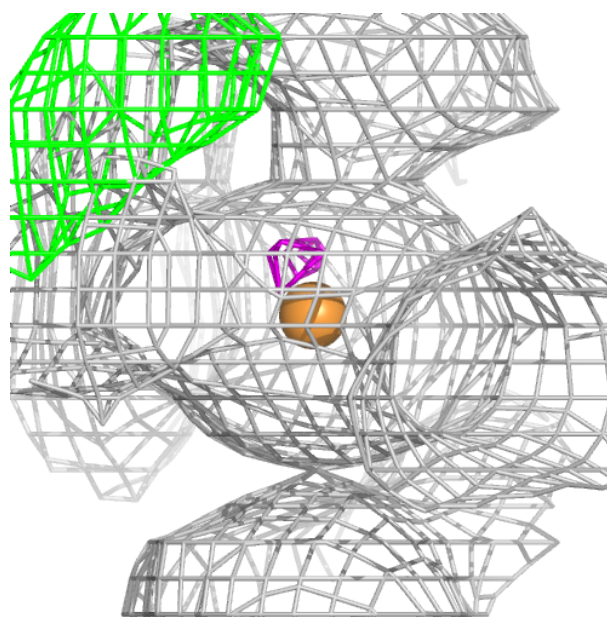
Electron density around CU D 602 (B):

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and green (positive)



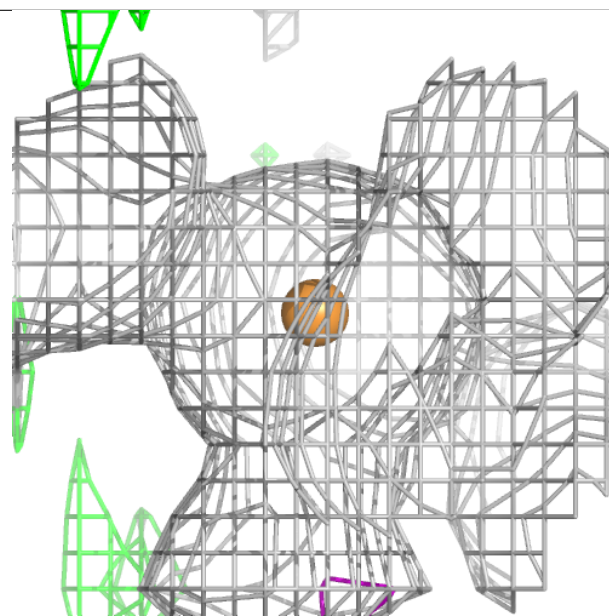
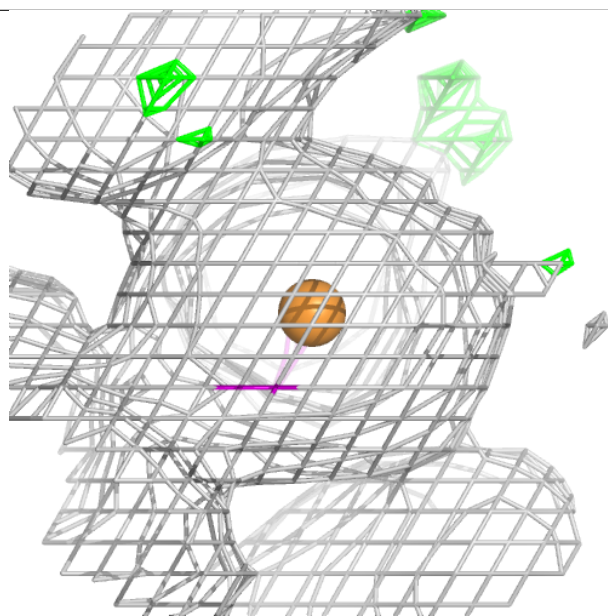
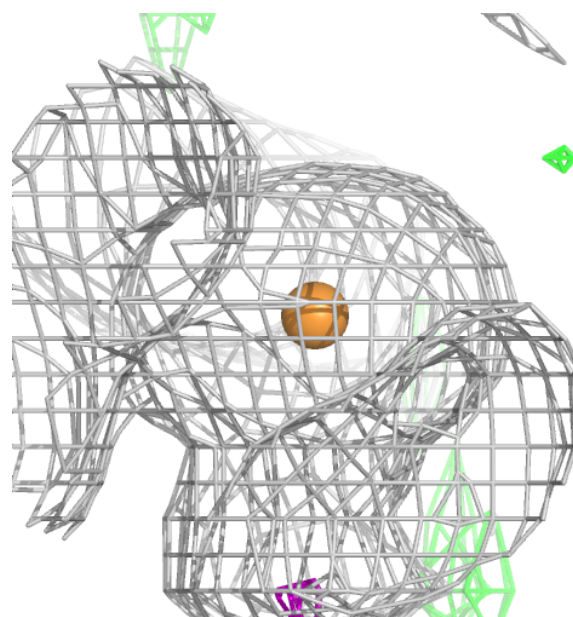
Electron density around CU G 601:

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and green (positive)



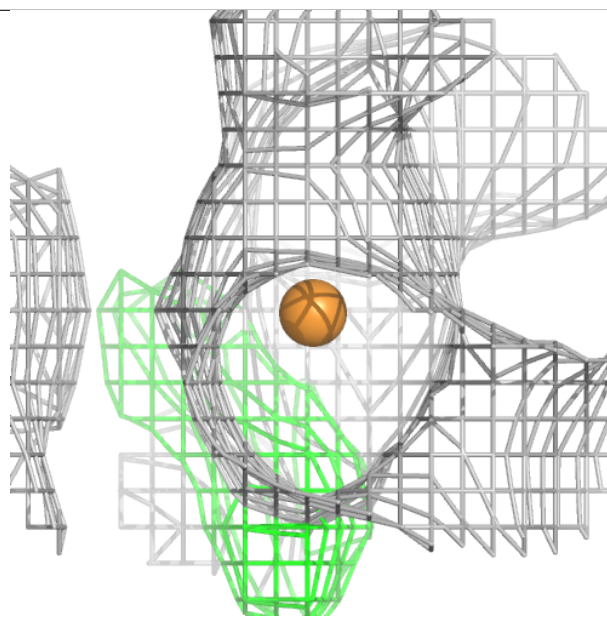
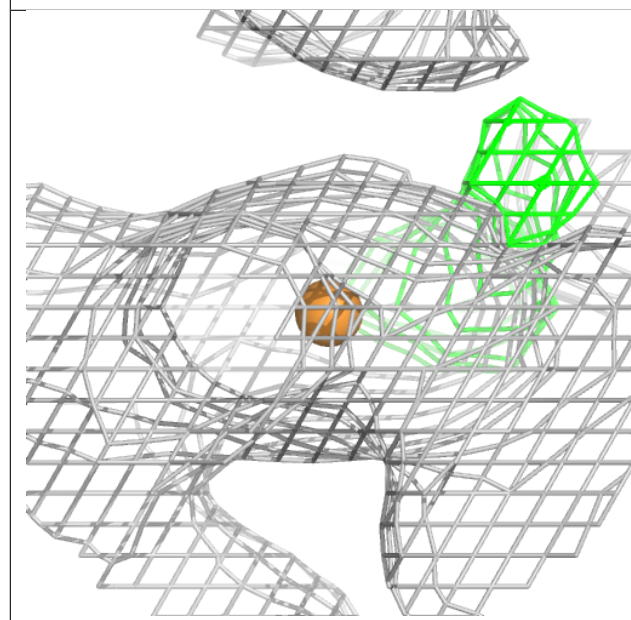
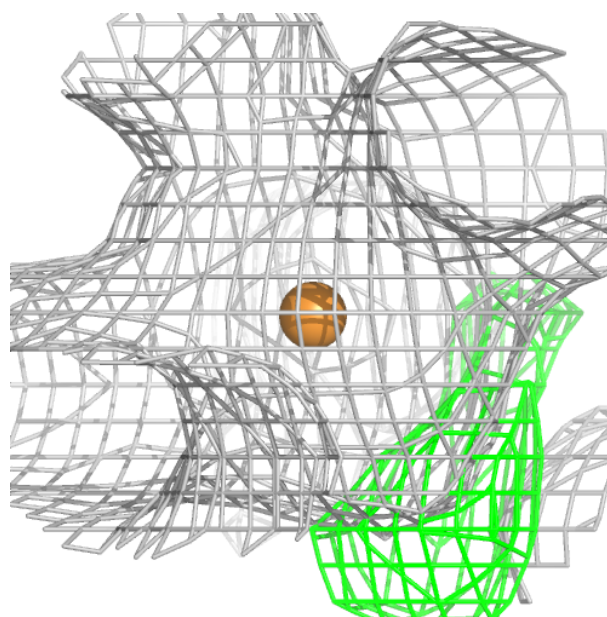
Electron density around CU A 601:

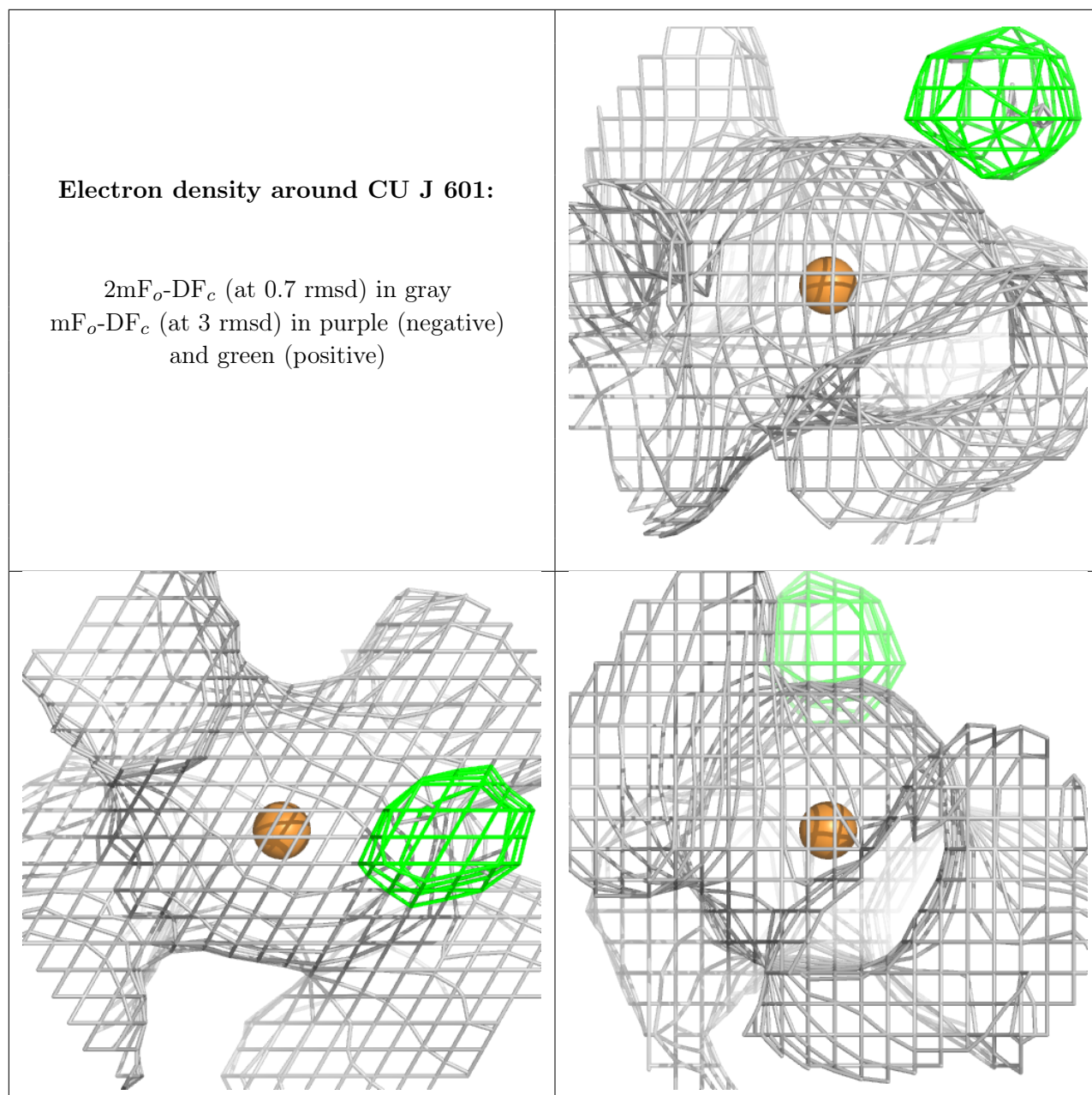
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

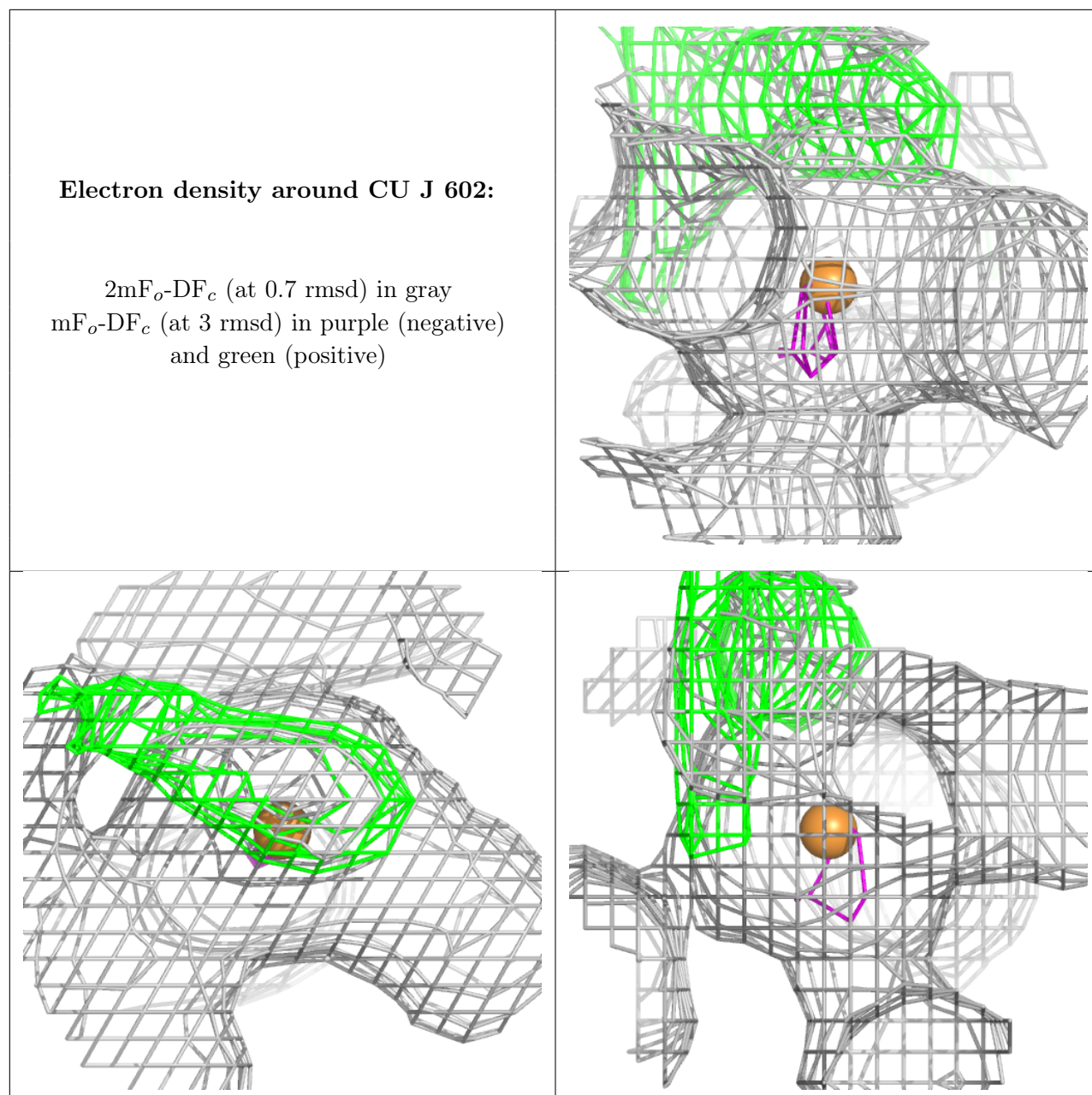


Electron density around CU A 602:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.