



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:07 PM UTC

PDB ID : 8P3L / pdb_00008p3l
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.; Der-gousova, 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 ⓘ](#)) 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
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

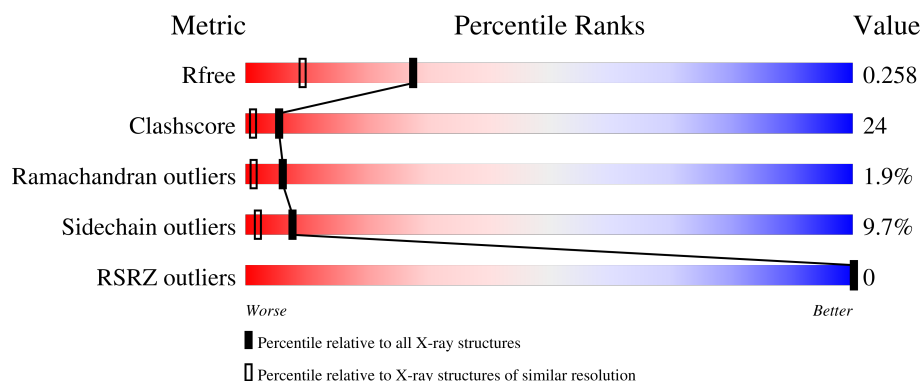
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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	 44% 36% 13% • 5%
1	D	494	 44% 35% 12% • 5%
1	G	494	 44% 35% 13% • 5%
1	J	494	 45% 35% 13% • 5%

2 Entry composition

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

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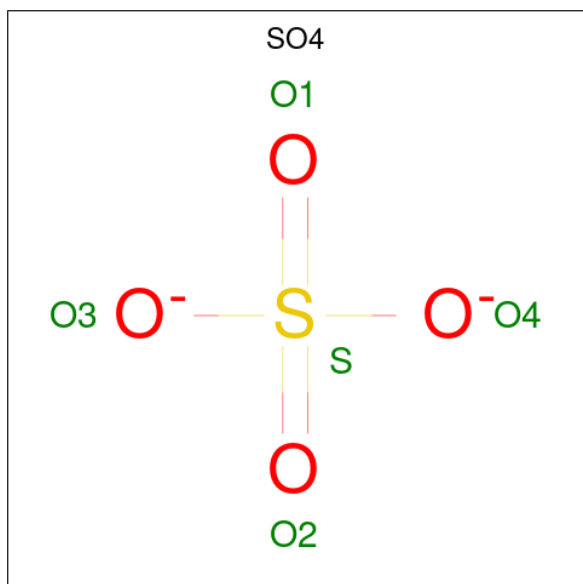
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Chain	Residue	Modelled	Actual	Comment	Reference
J	76	PHE	-	expression tag	UNP W0DP94
J	77	GLN	-	expression tag	UNP W0DP94
J	78	GLY	-	expression tag	UNP W0DP94
J	79	ALA	-	expression tag	UNP W0DP94
J	80	MET	-	expression tag	UNP W0DP94
J	81	GLY	-	expression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

- Molecule 2 is COPPER (II) ION (CCD ID: 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 (CCD ID: 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	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	1
			5	4	1		

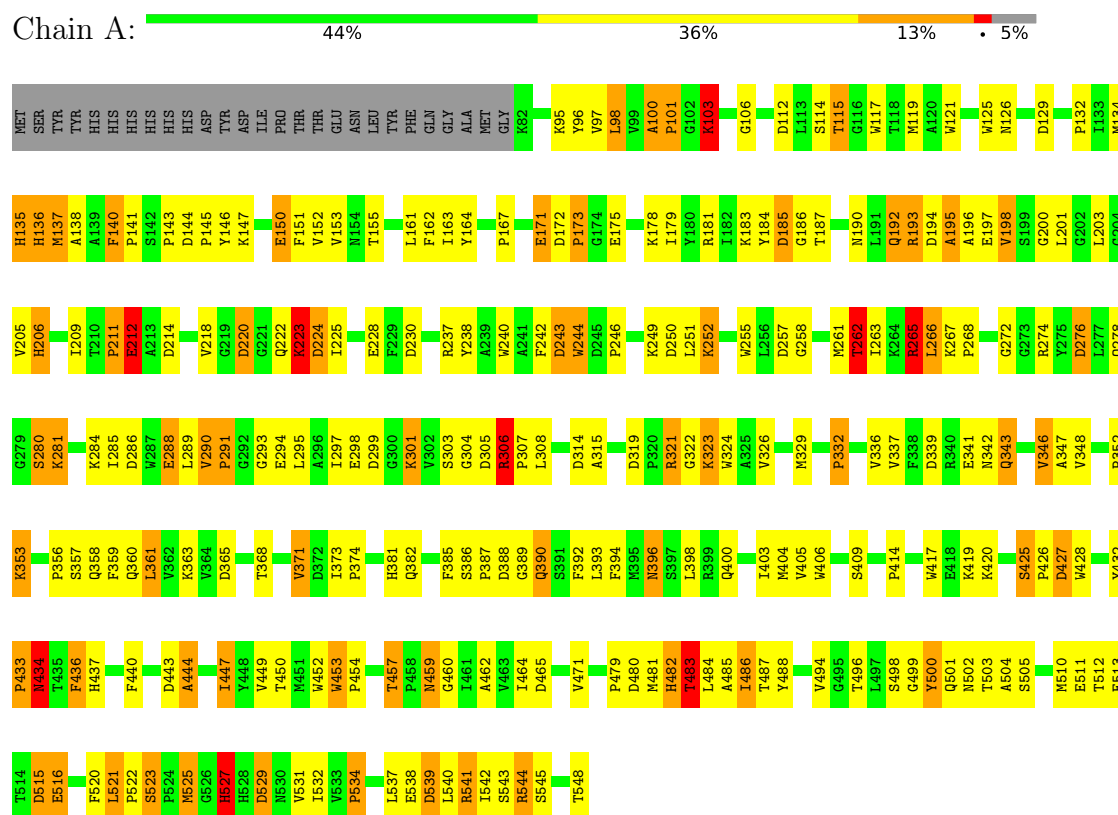
- Molecule 4 is water.

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

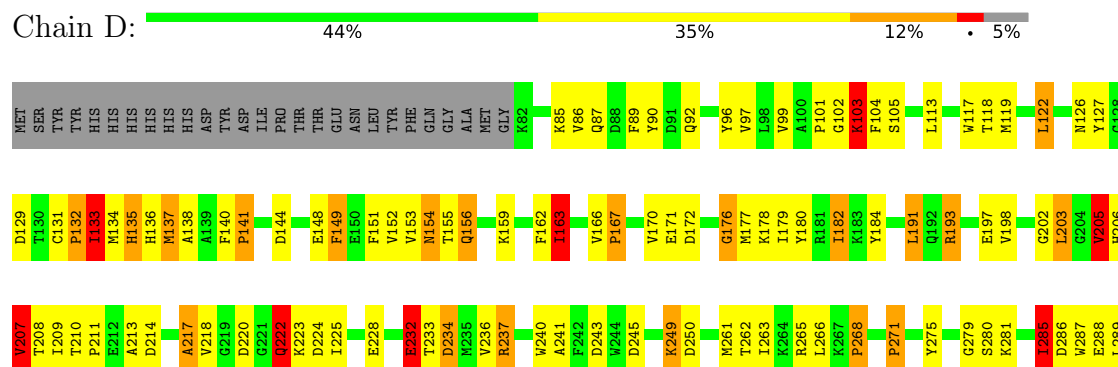
3 Residue-property plots

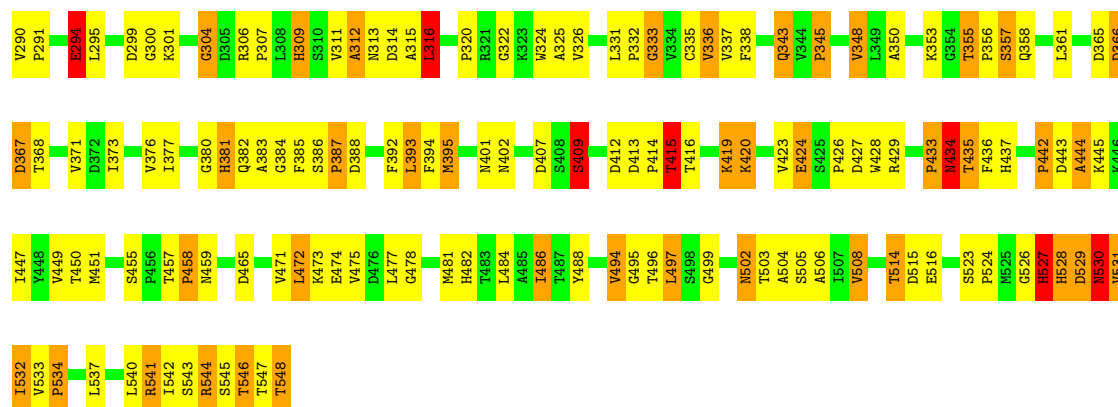
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



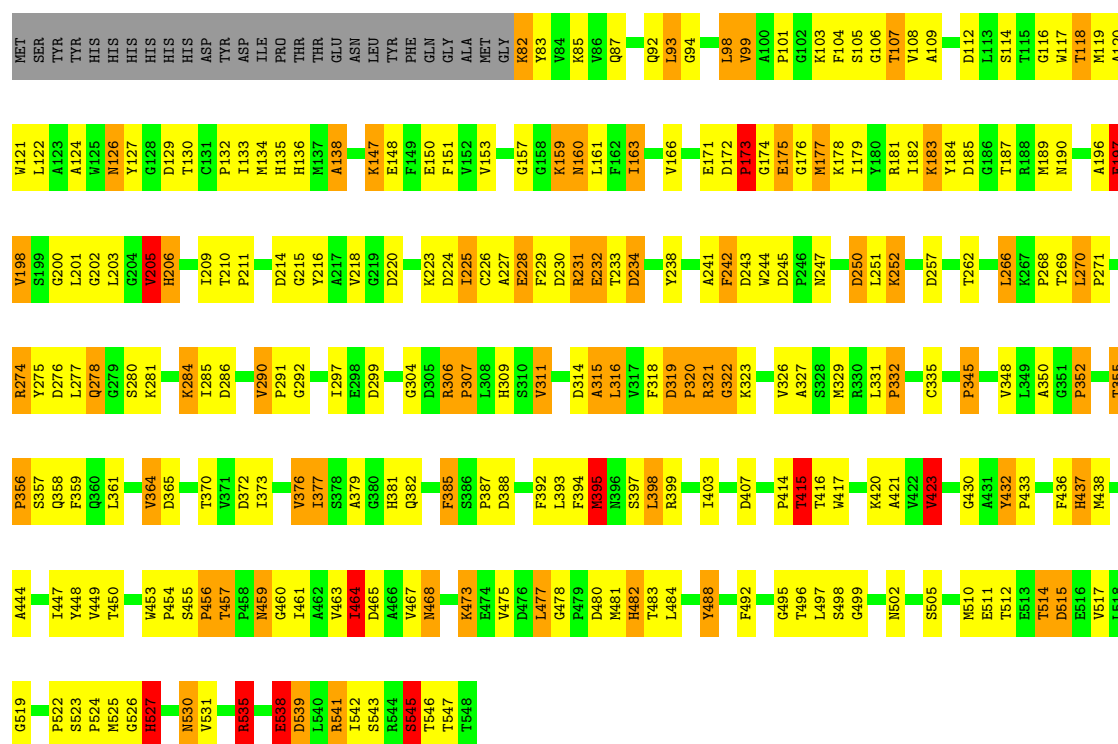
- Molecule 1: Twin-arginine translocation signal domain-containing protein





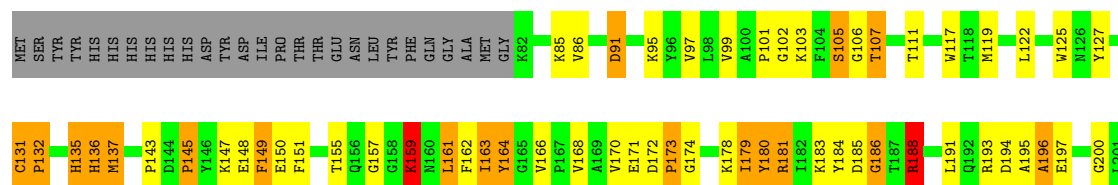
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain G: 44% 35% 13% 5%



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

Chain J: 45% 35% 13% 5%



G202	V290	L361	H437	E511
V206	P291	V362	M438	T512
H206	G292	K363	V439	E513
E212	G293	V364	D443	T514
V218	E294	D365	A444	D515
G219	E298	D366	K445	E516
D220	D299	D367	K446	
G221	D299	T368	I447	L521
G222	V302	W369	Y448	P522
K223	V371	V370	V449	
D224	D306	G375	T450	M525
I225	R306	V376	W453	G526
D230	P307	I377		H527
R231	L308	S378	P456	H528
E232	H309	A379	T457	D529
T233	S310	G380	P458	I532
D234	V311	H381	K459	V533
M235	A312	Q382	G460	P534
V236	N313	A383	I464	R535
R237	D314	G384	D465	T536
	A315	F385	A466	L540
	I316	S386	V467	
	V317	P387	M468	R544
V240	P320	Q390	W469	S545
A241	R321	L393	E470	T546
F242	G322	F394	E474	T548
D243	K323	M395		
P246	W324	K396	L477	
	A325	S397	G478	
K249	V326	L398	P479	
D250	M329	R399	D480	
L251	R330	Q400	M481	
K252	L331	N401	H482	
R253	P332	W404	T483	
A254	V337	V405	L484	
W255	F338	W406	A485	
L256	D339	D407	I486	
M261	R340	D407	T487	
	E341	H411	Y488	
K264	P345	P414	K491	
L266	V346		P492	
K267	A347	E418	V493	
P268	V348	K419	V494	
T269	I349	W422	T496	
	A350		L497	
G272	G351	P426	S498	
R273	P352	A431	Q501	
R274	T355	Y432	N502	
Q278	P356	P433	T503	
N283	S357	M434	A504	
K284	Q358	T435	S505	
I285	F359	F436	V508	
D286	Q360			

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 0.190 , 0.258	Depositor DCC
R_{free} test set	10643 reflections (5.06%)	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)	0.38 , 18.7	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	0.95	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	1.05	3/3752 (0.1%)	1.98	134/5119 (2.6%)
1	D	1.19	10/3755 (0.3%)	2.10	142/5124 (2.8%)
1	G	1.24	11/3740 (0.3%)	2.07	134/5104 (2.6%)
1	J	1.06	6/3743 (0.2%)	1.96	131/5110 (2.6%)
All	All	1.14	30/14990 (0.2%)	2.03	541/20457 (2.6%)

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 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	535	ARG	CD-NE	-13.20	1.27	1.46
1	D	528	HIS	CE1-NE2	10.96	1.43	1.32
1	G	206	HIS	CE1-NE2	10.82	1.43	1.32
1	J	135	HIS	CE1-NE2	9.69	1.42	1.32
1	G	136	HIS	CE1-NE2	9.27	1.41	1.32

The worst 5 of 541 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	311	VAL	N-CA-C	-12.59	101.75	113.71
1	D	141	PRO	CB-CA-C	-12.36	95.95	111.64
1	G	233	THR	CA-CB-OG1	-12.27	91.20	109.60
1	A	262	THR	CA-CB-OG1	-12.21	91.28	109.60
1	D	435	THR	CA-CB-OG1	-11.63	92.16	109.60

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	171	0
1	D	3644	0	3509	156	0
1	G	3628	0	3491	173	0
1	J	3631	0	3493	189	0
2	A	2	0	0	0	0
2	D	3	0	0	0	0
2	G	3	0	0	0	0
2	J	2	0	0	0	0
3	A	5	0	0	0	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	12	0
4	D	205	0	0	9	0
4	G	194	0	0	4	0
4	J	160	0	0	13	0
All	All	15340	0	14010	678	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 24.

The worst 5 of 678 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: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:443:ASP:CG	1:D:445:LYS:HE2	1.80	1.06
1:D:465:ASP:HB2	1:D:472:LEU:CD1	1.85	1.06
1:J:99:VAL:HG11	1:J:137:MET:HE1	1.38	1.05

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%)	6	1
1	D	467/494 (94%)	405 (87%)	51 (11%)	11 (2%)	4	1
1	G	467/494 (94%)	416 (89%)	40 (9%)	11 (2%)	4	1
1	J	467/494 (94%)	411 (88%)	52 (11%)	4 (1%)	14	5
All	All	1867/1976 (94%)	1652 (88%)	180 (10%)	35 (2%)	6	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%)	352 (90%)	40 (10%)	7	2
1	D	392/415 (94%)	353 (90%)	39 (10%)	7	2
1	G	388/415 (94%)	354 (91%)	34 (9%)	9	2
1	J	389/415 (94%)	349 (90%)	40 (10%)	7	2
All	All	1561/1660 (94%)	1408 (90%)	153 (10%)	8	2

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	111	THR
1	J	377	ILE
1	J	143	PRO
1	J	252	LYS
1	J	522	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	278	GLN
1	G	309	HIS
1	J	482	HIS
1	J	342	ASN
1	J	382	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 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	603	-	4,4,4	0.71	0	6,6,6	0.17	0
3	SO4	A	603[A]	-	4,4,4	0.46	0	6,6,6	1.16	0
3	SO4	G	606	-	4,4,4	0.33	0	6,6,6	0.69	0
3	SO4	D	604	-	4,4,4	0.44	0	6,6,6	0.68	0
3	SO4	J	603[A]	-	4,4,4	0.47	0	6,6,6	0.41	0
3	SO4	G	605	-	4,4,4	0.74	0	6,6,6	0.62	0
3	SO4	G	604	-	4,4,4	0.49	0	6,6,6	0.17	0
3	SO4	D	603	-	4,4,4	0.64	0	6,6,6	0.44	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	606	SO4	1	0
3	D	604	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%)	-1.15	0 100 100	9, 19, 28, 42	4 (0%)
1	D	467/494 (94%)	-1.19	0 100 100	8, 17, 26, 37	3 (0%)
1	G	467/494 (94%)	-1.19	0 100 100	8, 17, 25, 38	3 (0%)
1	J	467/494 (94%)	-1.15	0 100 100	10, 19, 30, 37	4 (0%)
All	All	1868/1976 (94%)	-1.17	0 100 100	8, 18, 27, 42	14 (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 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
3	SO4	D	603	5/5	0.99	0.04	19,20,24,26	5
3	SO4	D	604	5/5	0.99	0.03	9,12,13,14	5
3	SO4	G	603	5/5	0.99	0.04	15,19,22,23	0
3	SO4	G	604	5/5	0.99	0.04	17,17,20,25	5

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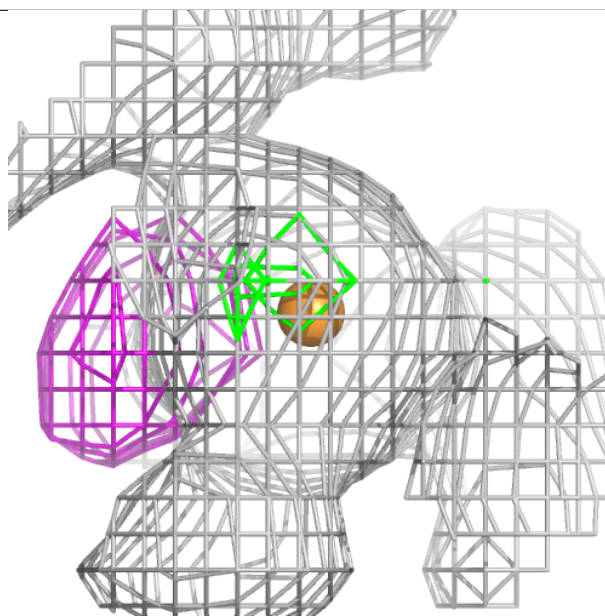
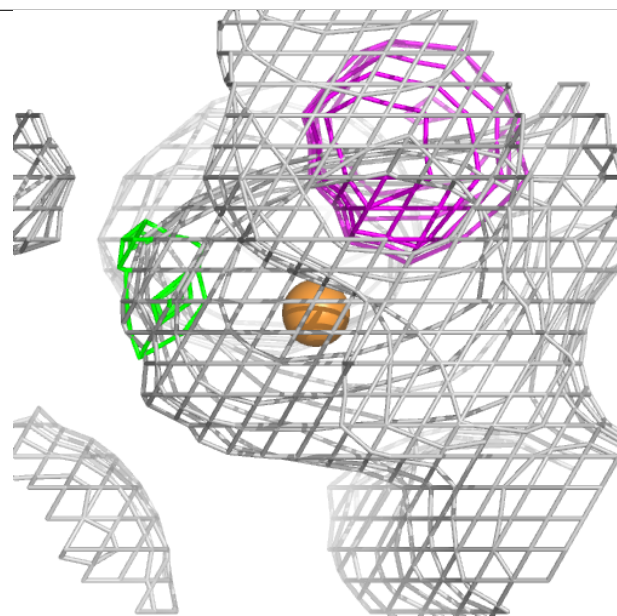
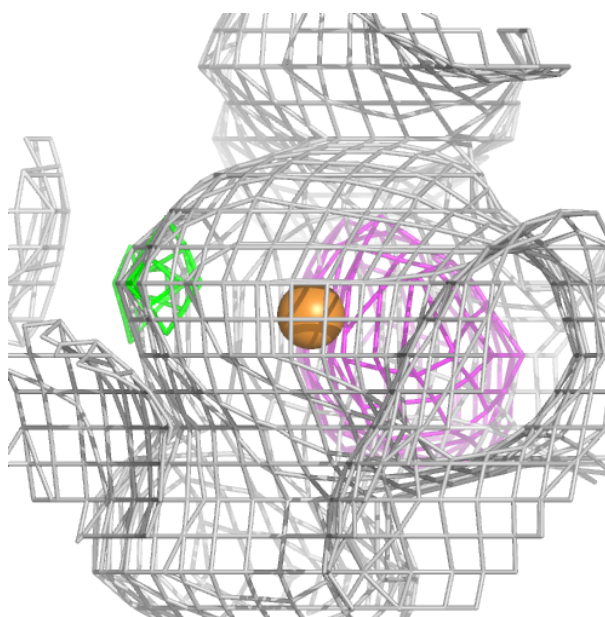
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	G	605	5/5	0.99	0.04	17,18,19,22	5
3	SO4	G	606	5/5	0.99	0.05	18,19,22,23	0
3	SO4	J	603[A]	5/5	0.99	0.04	18,18,19,23	0
2	CU	G	602[B]	1/1	1.00	0.02	15,15,15,15	1
2	CU	J	601	1/1	1.00	0.01	23,23,23,23	0
2	CU	J	602	1/1	1.00	0.02	19,19,19,19	0
3	SO4	A	603[A]	5/5	1.00	0.04	8,8,8,11	5
2	CU	A	601	1/1	1.00	0.03	15,15,15,15	0
2	CU	A	602	1/1	1.00	0.02	22,22,22,22	0
2	CU	D	601	1/1	1.00	0.02	18,18,18,18	0
2	CU	D	602[A]	1/1	1.00	0.02	14,14,14,14	1
2	CU	D	602[B]	1/1	1.00	0.02	6,6,6,6	1
2	CU	G	601	1/1	1.00	0.02	12,12,12,12	0
2	CU	G	602[A]	1/1	1.00	0.02	17,17,17,17	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.

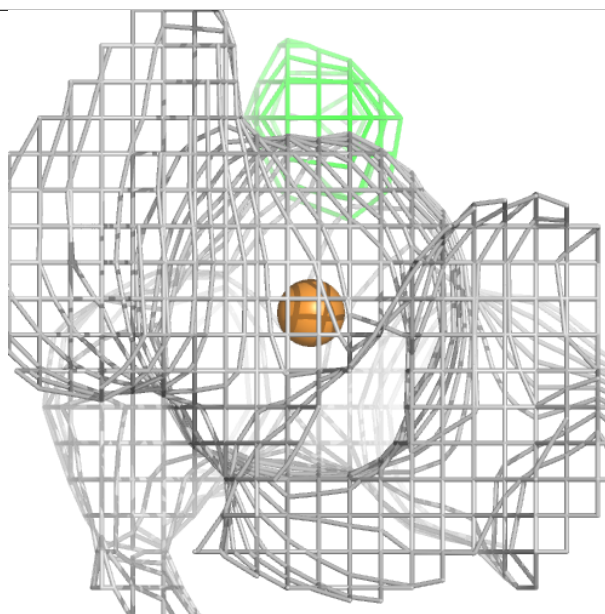
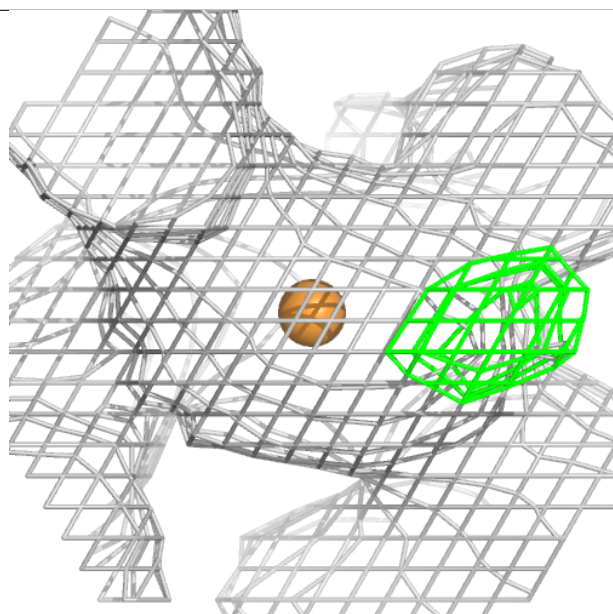
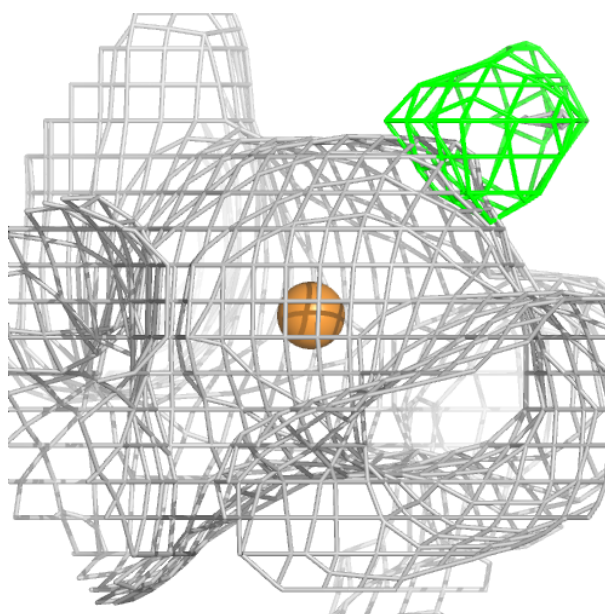
Electron density around CU G 602 (B):

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



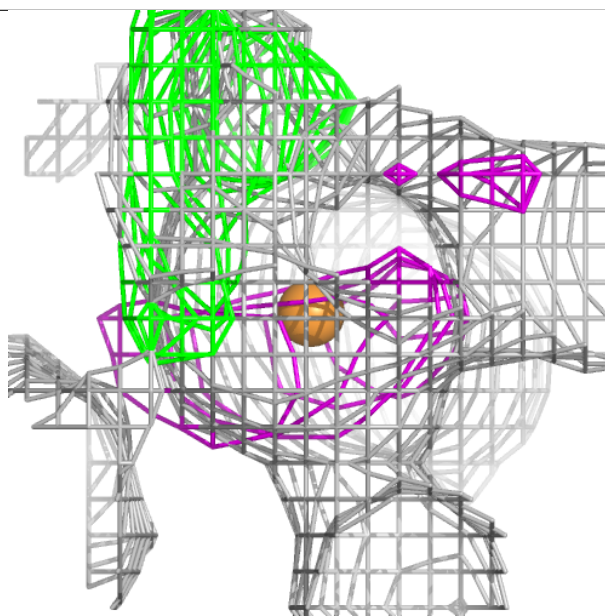
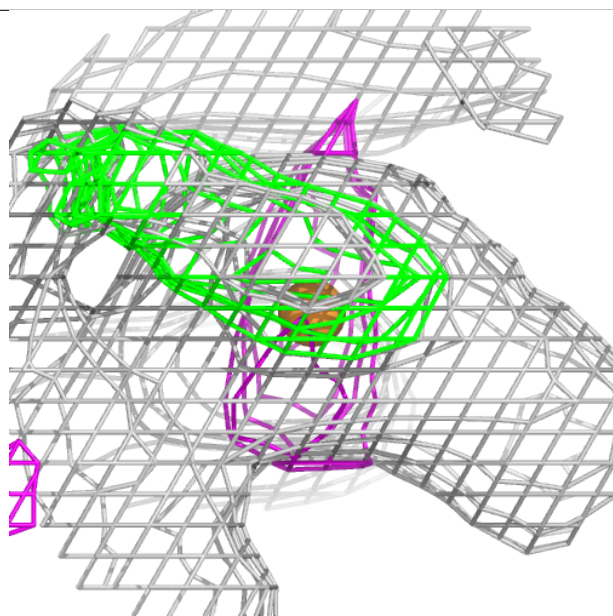
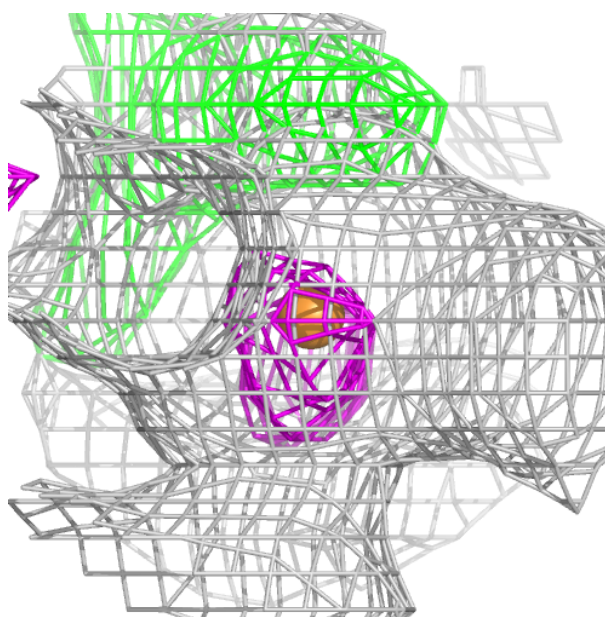
Electron density around CU J 601:

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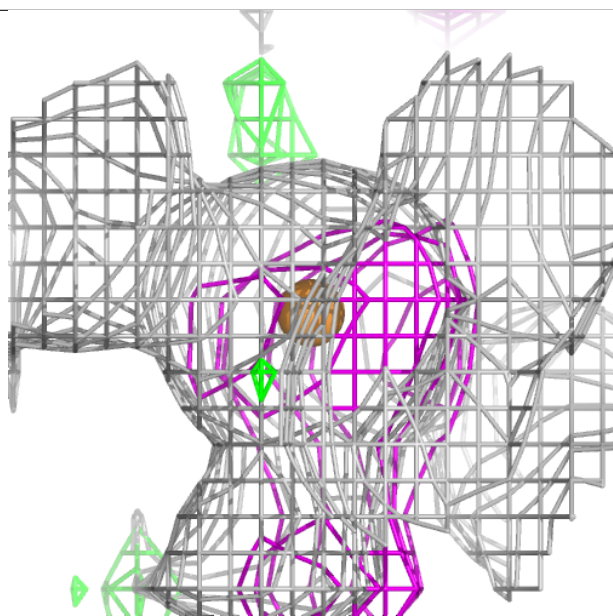
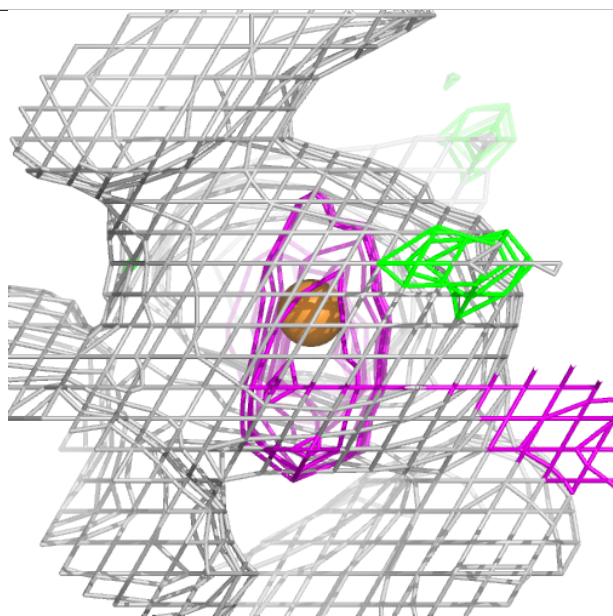
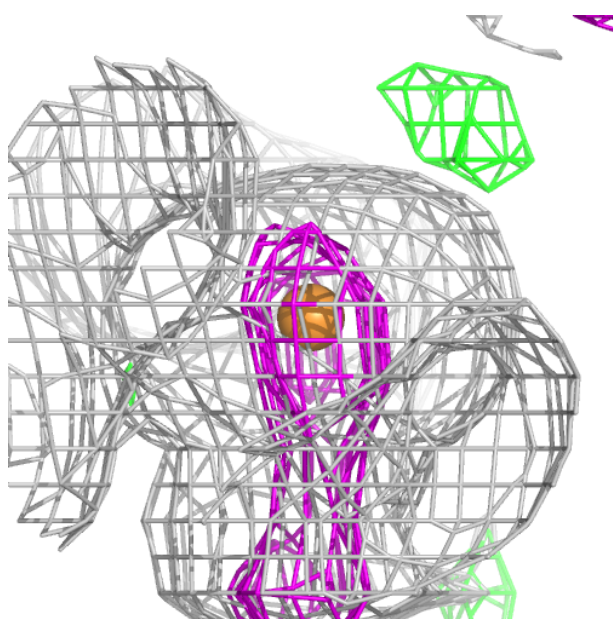
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and green (positive)



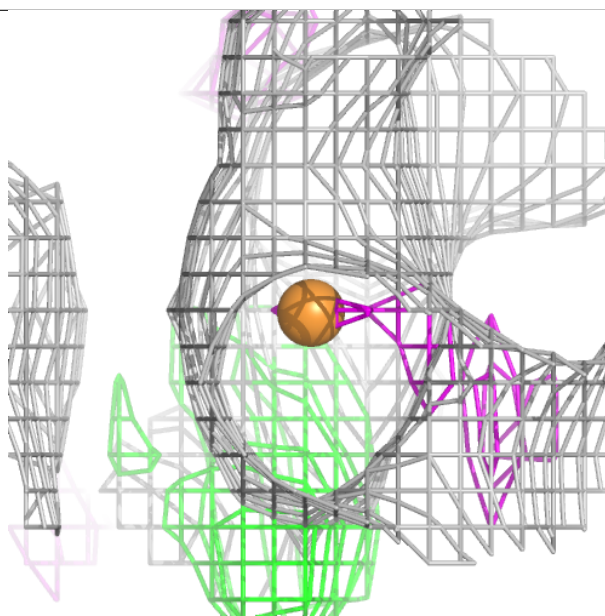
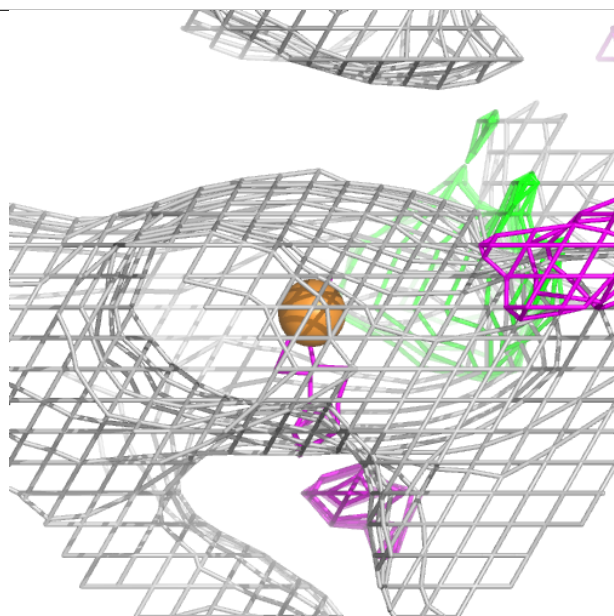
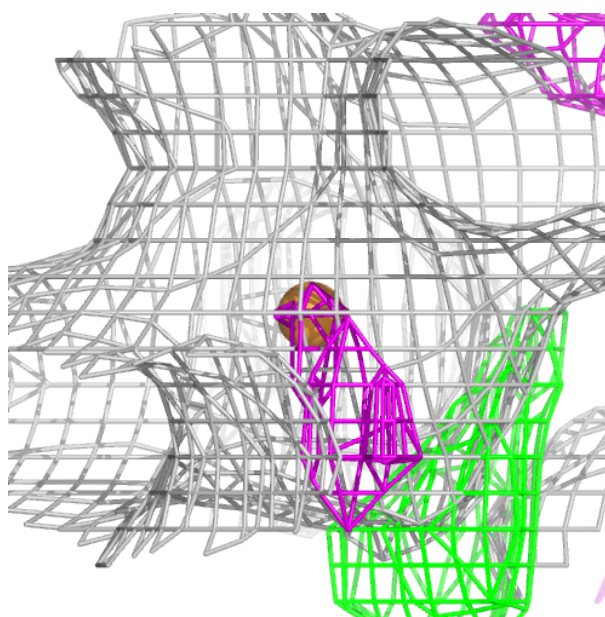
Electron density around CU A 601:

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and green (positive)



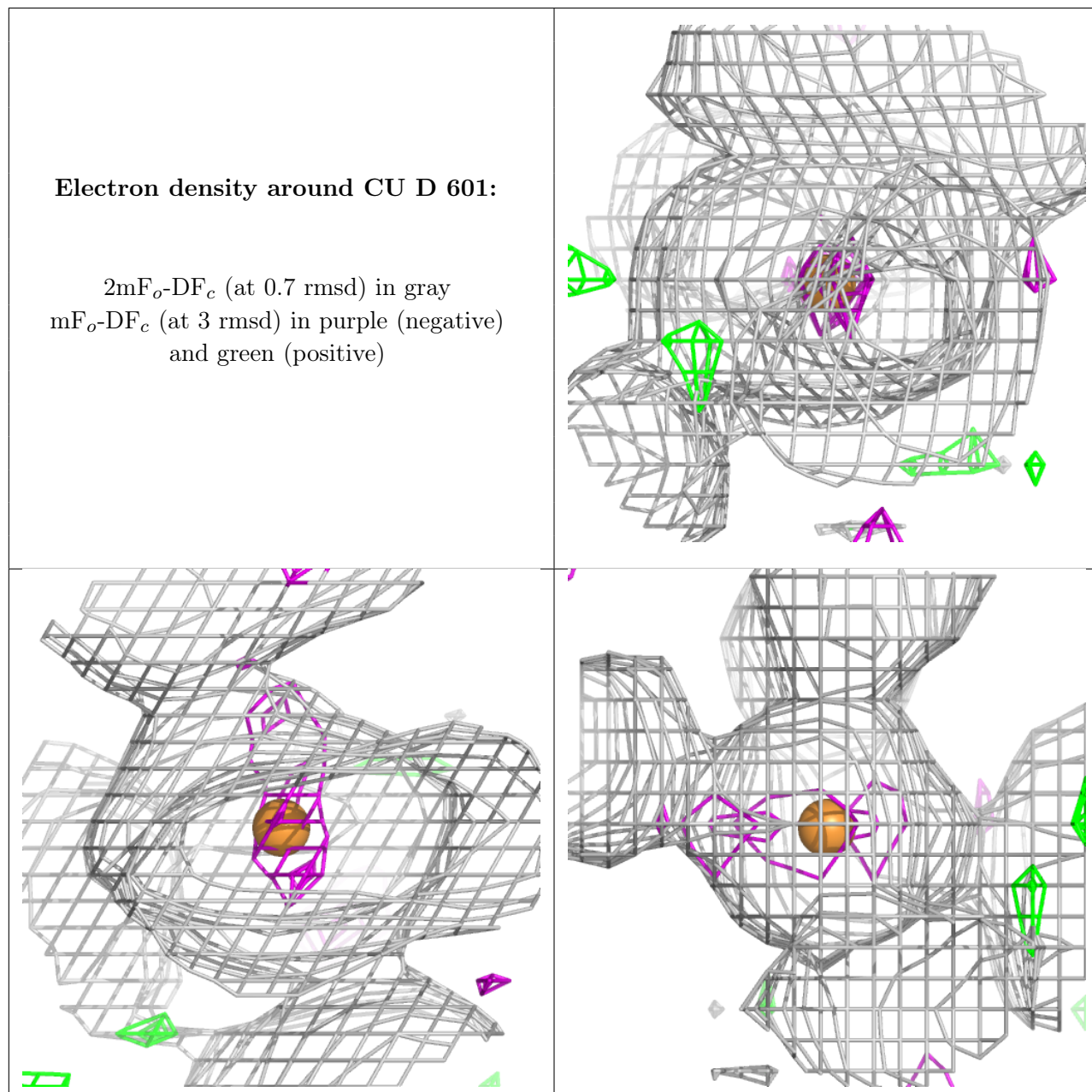
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and green (positive)



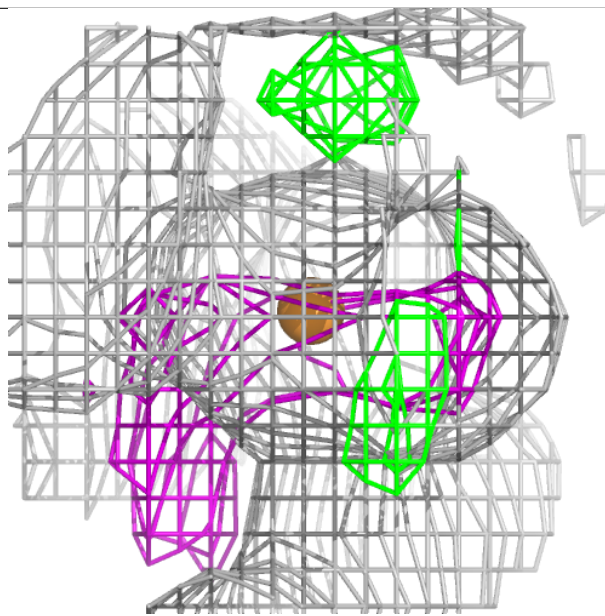
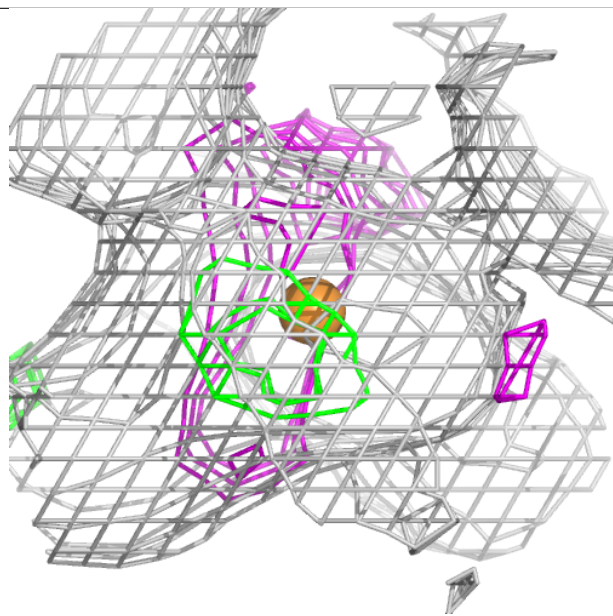
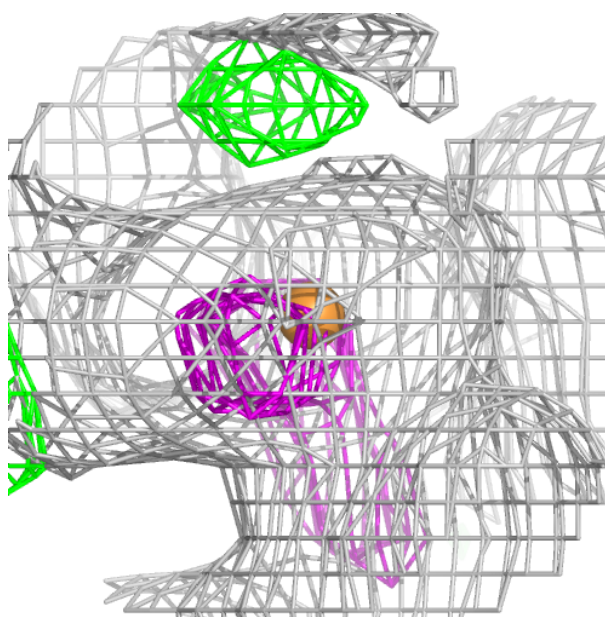
Electron density around CU D 601:

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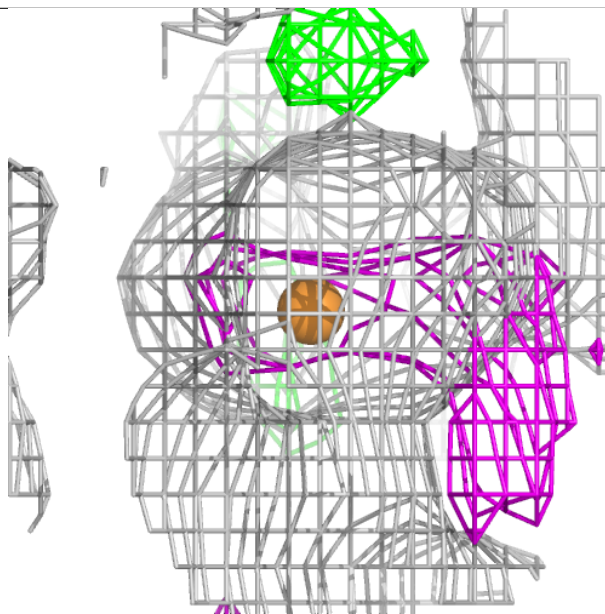
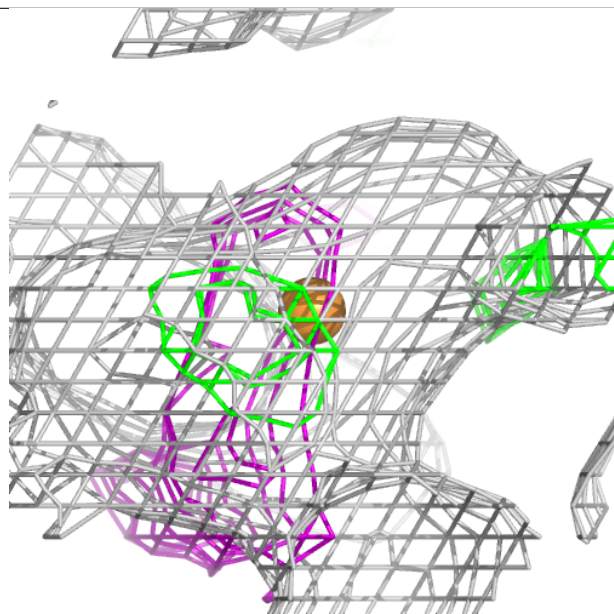
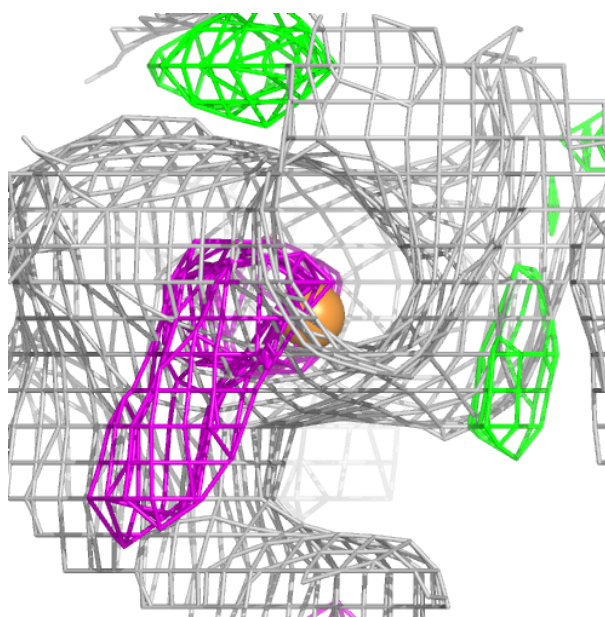
Electron density around CU D 602 (A):

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and green (positive)



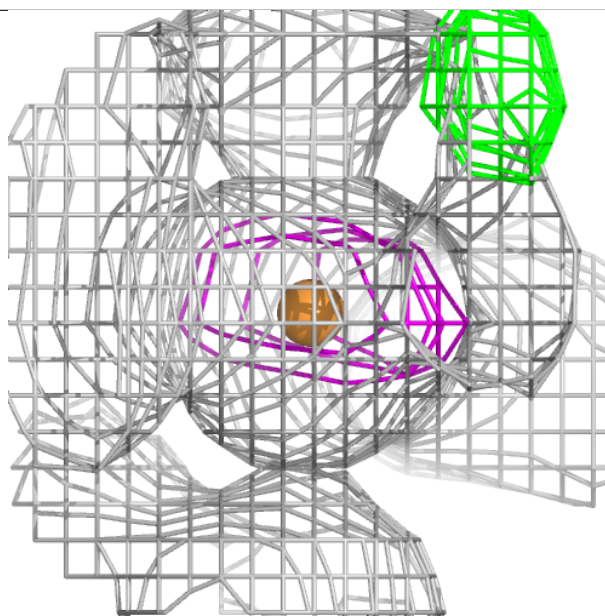
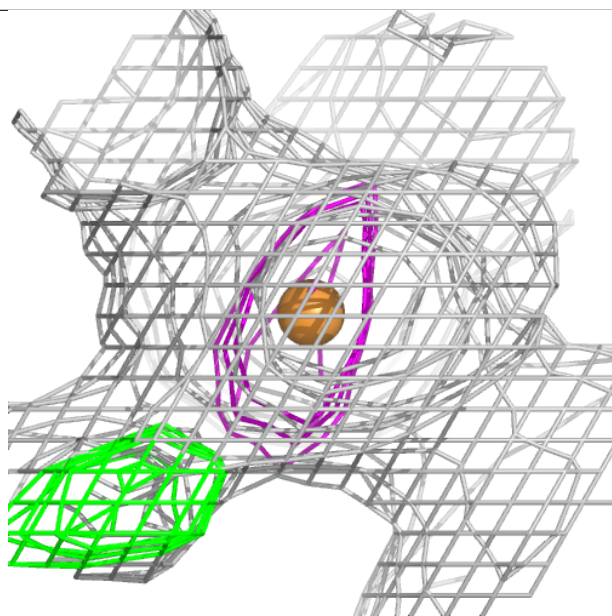
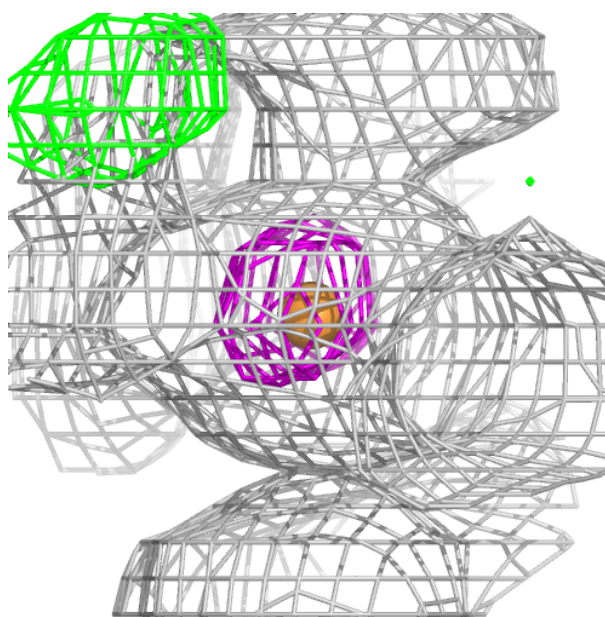
Electron density around CU D 602 (B):

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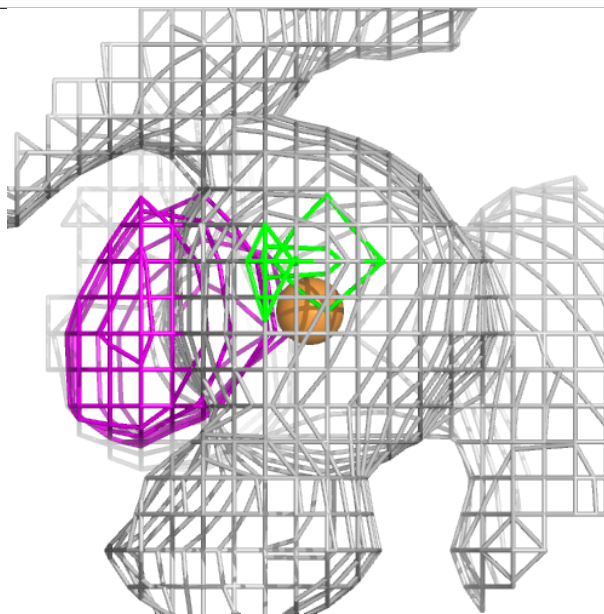
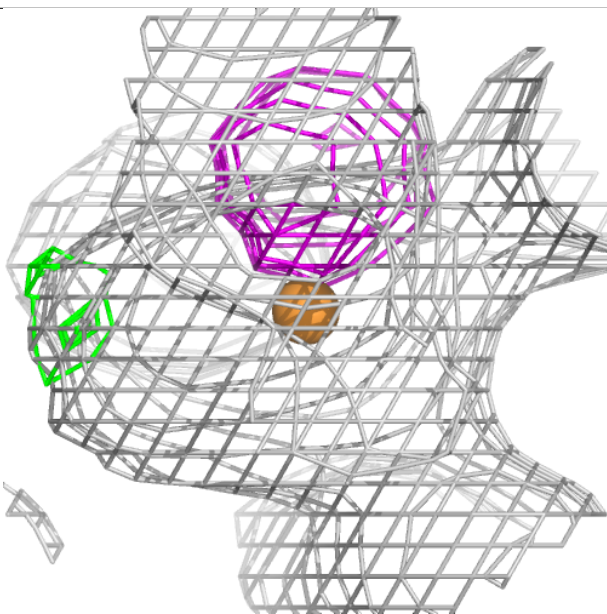
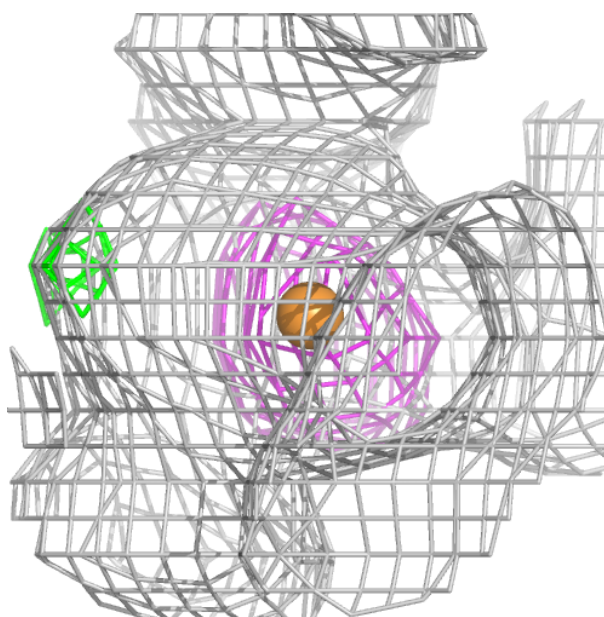
Electron density around CU G 601:

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and green (positive)



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.