



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 05:16 PM UTC

PDB ID : 9GKU / pdb_00009gku
Title : Crystal Structure of Propanil hydrolase (PrpH) from Sphingomonas sp. Y57
Authors : Graf, L.G.; Lammers, L.; Palm, G.J.; Schulze, S.
Deposited on : 2024-08-26
Resolution : 1.48 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

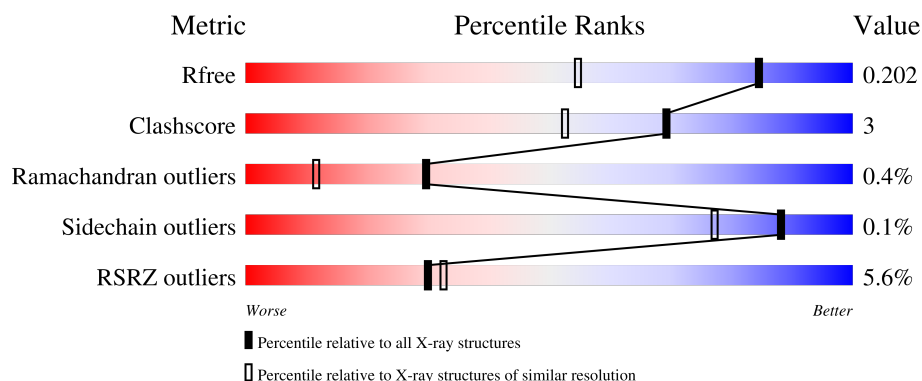
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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.



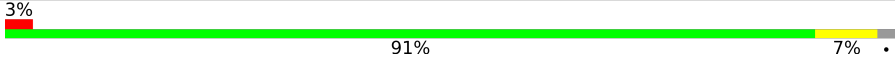
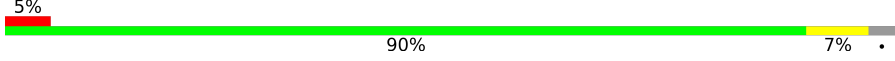
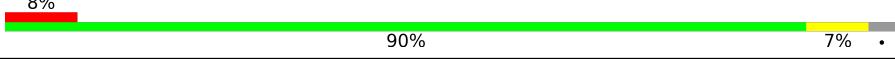
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	380	6% 91% 7%
1	B	380	10% 91% 6%
1	C	380	4% 92% 6%
1	D	380	5% 89% 8%
1	E	380	4% 91% 6%

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Mol	Chain	Length	Quality of chain
1	F	380	 3% 91% 7% •
1	G	380	 5% 90% 7% •
1	H	380	 8% 90% 7% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25009 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 Propanil hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	6	0
			2861	1806	501	533	21			
1	B	371	Total	C	N	O	S	0	3	0
			2856	1801	506	529	20			
1	C	371	Total	C	N	O	S	0	0	0
			2829	1785	499	526	19			
1	D	371	Total	C	N	O	S	0	2	0
			2842	1794	499	528	21			
1	E	369	Total	C	N	O	S	0	3	0
			2839	1792	500	527	20			
1	F	371	Total	C	N	O	S	0	2	0
			2845	1795	502	528	20			
1	G	369	Total	C	N	O	S	0	4	0
			2850	1800	503	526	21			
1	H	368	Total	C	N	O	S	0	0	0
			2817	1778	496	524	19			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP G3JWV8
A	1	ALA	-	expression tag	UNP G3JWV8
A	2	HIS	-	expression tag	UNP G3JWV8
A	3	HIS	-	expression tag	UNP G3JWV8
A	4	HIS	-	expression tag	UNP G3JWV8
A	5	HIS	-	expression tag	UNP G3JWV8
A	6	HIS	-	expression tag	UNP G3JWV8
A	7	HIS	-	expression tag	UNP G3JWV8
A	8	VAL	-	expression tag	UNP G3JWV8
A	9	GLY	-	expression tag	UNP G3JWV8
A	10	THR	-	expression tag	UNP G3JWV8
B	0	MET	-	initiating methionine	UNP G3JWV8
B	1	ALA	-	expression tag	UNP G3JWV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	HIS	-	expression tag	UNP G3JWV8
B	3	HIS	-	expression tag	UNP G3JWV8
B	4	HIS	-	expression tag	UNP G3JWV8
B	5	HIS	-	expression tag	UNP G3JWV8
B	6	HIS	-	expression tag	UNP G3JWV8
B	7	HIS	-	expression tag	UNP G3JWV8
B	8	VAL	-	expression tag	UNP G3JWV8
B	9	GLY	-	expression tag	UNP G3JWV8
B	10	THR	-	expression tag	UNP G3JWV8
C	0	MET	-	initiating methionine	UNP G3JWV8
C	1	ALA	-	expression tag	UNP G3JWV8
C	2	HIS	-	expression tag	UNP G3JWV8
C	3	HIS	-	expression tag	UNP G3JWV8
C	4	HIS	-	expression tag	UNP G3JWV8
C	5	HIS	-	expression tag	UNP G3JWV8
C	6	HIS	-	expression tag	UNP G3JWV8
C	7	HIS	-	expression tag	UNP G3JWV8
C	8	VAL	-	expression tag	UNP G3JWV8
C	9	GLY	-	expression tag	UNP G3JWV8
C	10	THR	-	expression tag	UNP G3JWV8
D	0	MET	-	initiating methionine	UNP G3JWV8
D	1	ALA	-	expression tag	UNP G3JWV8
D	2	HIS	-	expression tag	UNP G3JWV8
D	3	HIS	-	expression tag	UNP G3JWV8
D	4	HIS	-	expression tag	UNP G3JWV8
D	5	HIS	-	expression tag	UNP G3JWV8
D	6	HIS	-	expression tag	UNP G3JWV8
D	7	HIS	-	expression tag	UNP G3JWV8
D	8	VAL	-	expression tag	UNP G3JWV8
D	9	GLY	-	expression tag	UNP G3JWV8
D	10	THR	-	expression tag	UNP G3JWV8
E	0	MET	-	initiating methionine	UNP G3JWV8
E	1	ALA	-	expression tag	UNP G3JWV8
E	2	HIS	-	expression tag	UNP G3JWV8
E	3	HIS	-	expression tag	UNP G3JWV8
E	4	HIS	-	expression tag	UNP G3JWV8
E	5	HIS	-	expression tag	UNP G3JWV8
E	6	HIS	-	expression tag	UNP G3JWV8
E	7	HIS	-	expression tag	UNP G3JWV8
E	8	VAL	-	expression tag	UNP G3JWV8
E	9	GLY	-	expression tag	UNP G3JWV8
E	10	THR	-	expression tag	UNP G3JWV8

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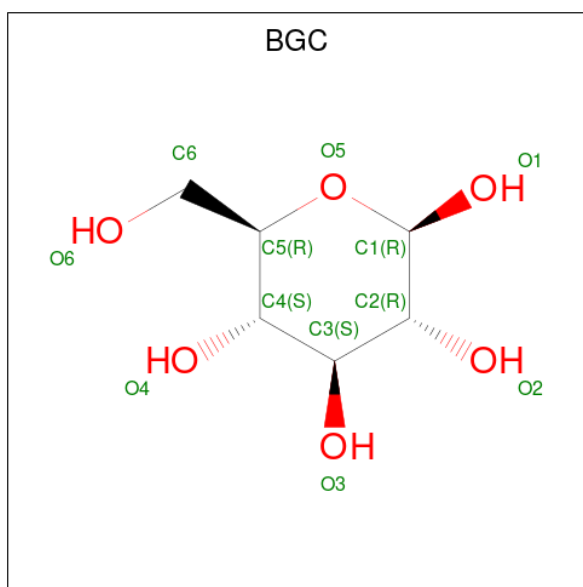
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	initiating methionine	UNP G3JWV8
F	1	ALA	-	expression tag	UNP G3JWV8
F	2	HIS	-	expression tag	UNP G3JWV8
F	3	HIS	-	expression tag	UNP G3JWV8
F	4	HIS	-	expression tag	UNP G3JWV8
F	5	HIS	-	expression tag	UNP G3JWV8
F	6	HIS	-	expression tag	UNP G3JWV8
F	7	HIS	-	expression tag	UNP G3JWV8
F	8	VAL	-	expression tag	UNP G3JWV8
F	9	GLY	-	expression tag	UNP G3JWV8
F	10	THR	-	expression tag	UNP G3JWV8
G	0	MET	-	initiating methionine	UNP G3JWV8
G	1	ALA	-	expression tag	UNP G3JWV8
G	2	HIS	-	expression tag	UNP G3JWV8
G	3	HIS	-	expression tag	UNP G3JWV8
G	4	HIS	-	expression tag	UNP G3JWV8
G	5	HIS	-	expression tag	UNP G3JWV8
G	6	HIS	-	expression tag	UNP G3JWV8
G	7	HIS	-	expression tag	UNP G3JWV8
G	8	VAL	-	expression tag	UNP G3JWV8
G	9	GLY	-	expression tag	UNP G3JWV8
G	10	THR	-	expression tag	UNP G3JWV8
H	0	MET	-	initiating methionine	UNP G3JWV8
H	1	ALA	-	expression tag	UNP G3JWV8
H	2	HIS	-	expression tag	UNP G3JWV8
H	3	HIS	-	expression tag	UNP G3JWV8
H	4	HIS	-	expression tag	UNP G3JWV8
H	5	HIS	-	expression tag	UNP G3JWV8
H	6	HIS	-	expression tag	UNP G3JWV8
H	7	HIS	-	expression tag	UNP G3JWV8
H	8	VAL	-	expression tag	UNP G3JWV8
H	9	GLY	-	expression tag	UNP G3JWV8
H	10	THR	-	expression tag	UNP G3JWV8

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		
3	G	1	Total	C	O	0	0
			12	6	6		
3	H	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0
4	E	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0
4	G	1	Total 1	Zn 1	0	0
4	H	1	Total 1	Zn 1	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	K 1	0	0
5	B	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0
5	E	1	Total 1	K 1	0	0
5	F	1	Total 1	K 1	0	0
5	G	1	Total 1	K 1	0	0
5	H	1	Total 1	K 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	267	Total 267	O 267	0	0
6	B	215	Total 215	O 215	0	0
6	C	253	Total 253	O 253	0	0

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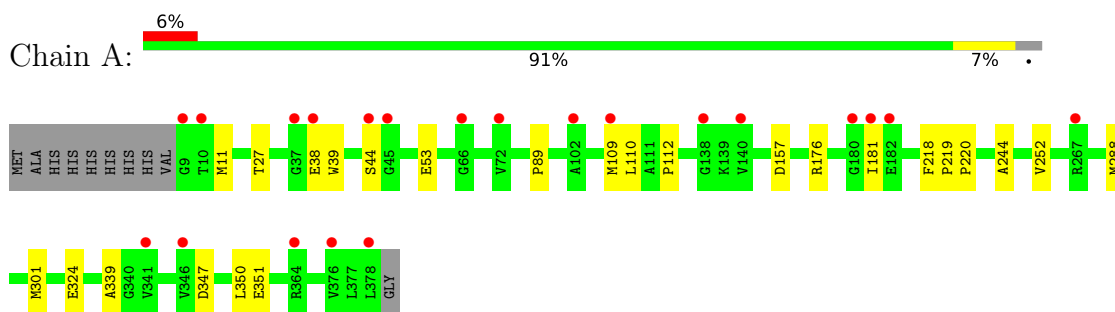
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	264	Total 264	O 264	0	0
6	E	308	Total 308	O 308	0	0
6	F	327	Total 327	O 327	0	0
6	G	252	Total 252	O 252	0	0
6	H	228	Total 228	O 228	0	0

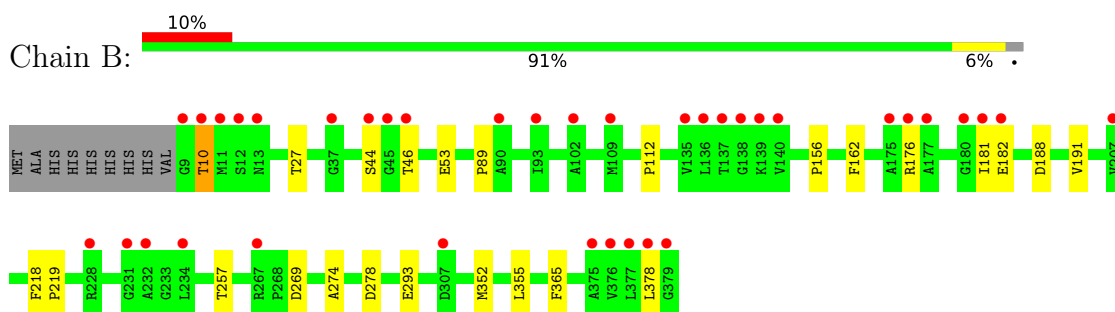
3 Residue-property plots

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.

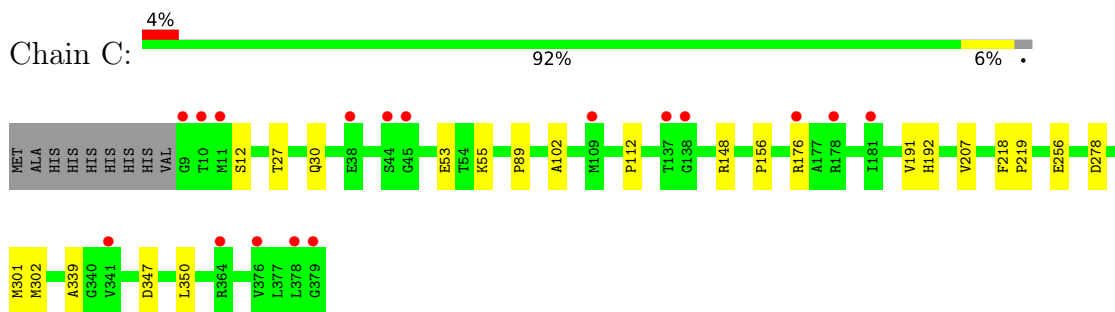
- Molecule 1: Propanil hydrolase



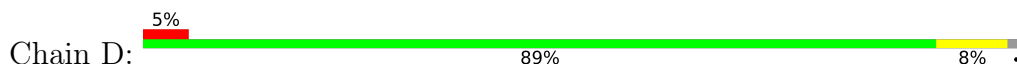
- Molecule 1: Propanil hydrolase

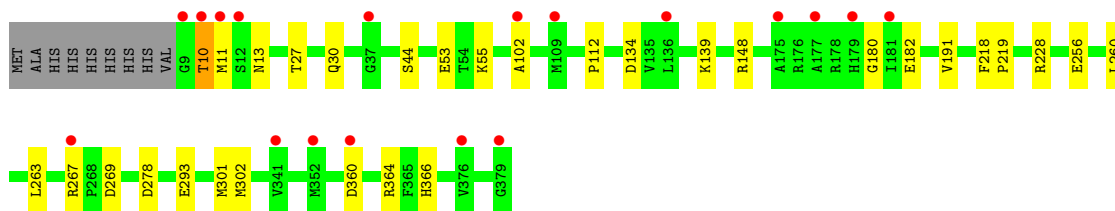


- Molecule 1: Propanil hydrolase

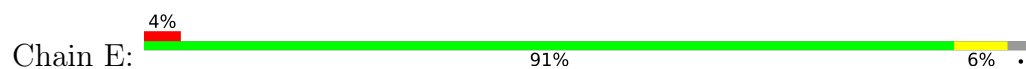


- Molecule 1: Propanil hydrolase

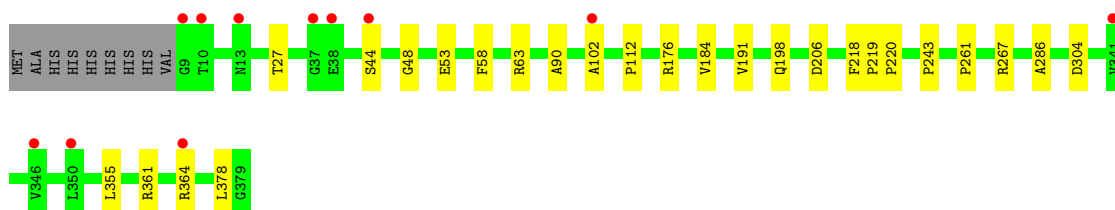




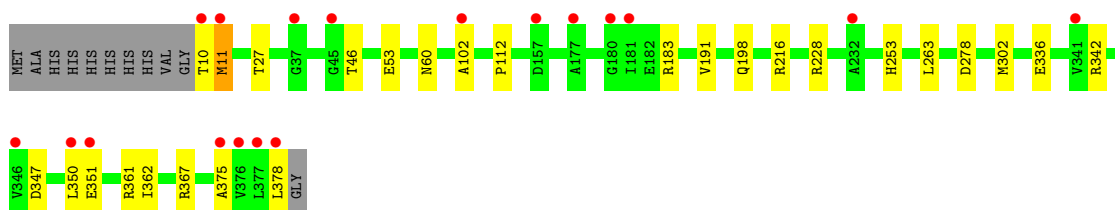
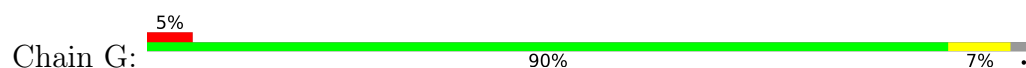
• Molecule 1: Propanil hydrolase



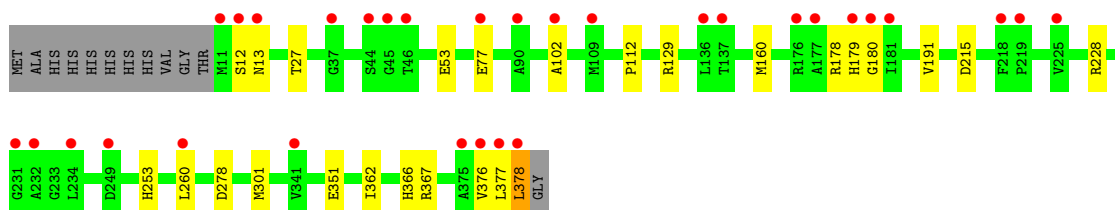
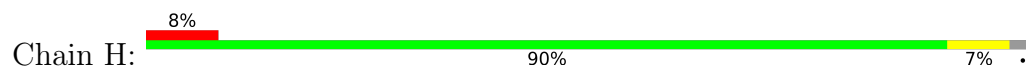
• Molecule 1: Propanil hydrolase



• Molecule 1: Propanil hydrolase



• Molecule 1: Propanil hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.86Å 103.70Å 104.50Å 113.60° 93.00° 120.61°	Depositor
Resolution (Å)	44.56 – 1.48 44.56 – 1.48	Depositor EDS
% Data completeness (in resolution range)	91.1 (44.56-1.48) 91.1 (44.56-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.173 , 0.199 0.176 , 0.202	Depositor DCC
R_{free} test set	24854 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-h-k-l 0.005 for -h-k-l,l,k 0.064 for l,-h-k-l,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	25009	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: ZN, BGC, K, ACT

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	0.26	0/2948	0.48	0/4009
1	B	0.23	0/2931	0.46	1/3984 (0.0%)
1	C	0.24	0/2898	0.49	0/3942
1	D	0.23	0/2917	0.46	0/3966
1	E	0.27	0/2917	0.50	0/3966
1	F	0.26	0/2920	0.50	0/3970
1	G	0.24	0/2931	0.50	0/3984
1	H	0.24	0/2886	0.48	0/3926
All	All	0.25	0/23348	0.49	1/31747 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	THR	N-CA-C	5.03	121.50	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2861	0	2789	19	0
1	B	2856	0	2783	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2829	0	2747	16	0
1	D	2842	0	2767	19	0
1	E	2839	0	2765	18	0
1	F	2845	0	2771	27	0
1	G	2850	0	2787	21	0
1	H	2817	0	2736	20	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
3	A	12	0	12	0	0
3	B	12	0	12	0	0
3	C	24	0	24	2	0
3	E	24	0	24	0	0
3	F	12	0	12	3	0
3	G	12	0	12	2	0
3	H	12	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	267	0	0	7	3
6	B	215	0	0	5	0
6	C	253	0	0	4	1
6	D	264	0	0	7	5
6	E	308	0	0	9	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	327	0	0	17	4
6	G	252	0	0	10	3
6	H	228	0	0	9	6
All	All	25009	0	22277	156	12

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 3.

The worst 5 of 156 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:D:267:ARG:NH2	6:D:501:HOH:O	1.96	0.98
1:F:364:ARG:NH2	6:F:501:HOH:O	2.07	0.88
1:F:361:ARG:O	6:F:501:HOH:O	1.90	0.87
1:F:53:GLU:OE2	6:F:502:HOH:O	1.95	0.85
1:B:176:ARG:NH1	1:B:181:ILE:O	2.11	0.84

The worst 5 of 12 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)
6:A:594:HOH:O	6:F:502:HOH:O[1_566]	1.79	0.41
6:D:722:HOH:O	6:H:586:HOH:O[1_454]	1.84	0.36
6:A:565:HOH:O	6:F:735:HOH:O[1_566]	1.85	0.35
6:E:529:HOH:O	6:G:547:HOH:O[1_665]	2.00	0.20
6:D:504:HOH:O	6:H:503:HOH:O[1_454]	2.01	0.19

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	374/380 (98%)	365 (98%)	9 (2%)	0	100	100
1	B	372/380 (98%)	359 (96%)	12 (3%)	1 (0%)	36	17
1	C	369/380 (97%)	360 (98%)	8 (2%)	1 (0%)	36	17
1	D	371/380 (98%)	358 (96%)	10 (3%)	3 (1%)	16	3
1	E	370/380 (97%)	361 (98%)	9 (2%)	0	100	100
1	F	371/380 (98%)	360 (97%)	10 (3%)	1 (0%)	36	17
1	G	371/380 (98%)	360 (97%)	9 (2%)	2 (0%)	24	8
1	H	366/380 (96%)	352 (96%)	11 (3%)	3 (1%)	16	3
All	All	2964/3040 (98%)	2875 (97%)	78 (3%)	11 (0%)	30	11

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	THR
1	G	11	MET
1	H	377	LEU
1	D	180	GLY
1	F	102	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	299/301 (99%)	299 (100%)	0	100	100
1	B	296/301 (98%)	296 (100%)	0	100	100
1	C	292/301 (97%)	292 (100%)	0	100	100
1	D	295/301 (98%)	294 (100%)	1 (0%)	86	75
1	E	295/301 (98%)	295 (100%)	0	100	100
1	F	295/301 (98%)	294 (100%)	1 (0%)	86	75
1	G	297/301 (99%)	297 (100%)	0	100	100
1	H	292/301 (97%)	291 (100%)	1 (0%)	86	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2361/2408 (98%)	2358 (100%)	3 (0%)	88	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	44	SER
1	F	58	PHE
1	H	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	60	ASN
1	E	239	ASN
1	E	237	ASN
1	F	13	ASN
1	B	239	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 16 are monoatomic - leaving 17 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	$\# Z > 2$
2	ACT	G	401	4	3,3,3	1.10	0	3,3,3	1.24	0
3	BGC	B	402	-	12,12,12	0.53	0	17,17,17	0.80	0
3	BGC	F	402	-	12,12,12	0.48	0	17,17,17	1.43	2 (11%)
2	ACT	H	401	4	3,3,3	1.12	0	3,3,3	1.19	0
2	ACT	F	401	4	3,3,3	1.24	0	3,3,3	0.68	0
2	ACT	B	401	4	3,3,3	1.21	0	3,3,3	1.00	0
3	BGC	E	403	-	12,12,12	0.43	0	17,17,17	0.79	0
2	ACT	A	401	4	3,3,3	1.16	0	3,3,3	1.10	0
3	BGC	C	402	-	12,12,12	0.77	0	17,17,17	1.32	1 (5%)
3	BGC	A	402	-	12,12,12	0.58	0	17,17,17	0.84	0
3	BGC	H	402	-	12,12,12	0.53	0	17,17,17	1.21	2 (11%)
2	ACT	E	401	4	3,3,3	1.25	0	3,3,3	0.67	0
2	ACT	D	401	4	3,3,3	1.20	0	3,3,3	0.94	0
3	BGC	G	402	-	12,12,12	0.63	0	17,17,17	1.29	1 (5%)
2	ACT	C	401	4	3,3,3	1.14	0	3,3,3	1.35	0
3	BGC	E	402	-	12,12,12	0.57	0	17,17,17	1.15	1 (5%)
3	BGC	C	403	-	12,12,12	0.55	0	17,17,17	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	B	402	-	-	0/2/22/22	0/1/1/1
3	BGC	F	402	-	-	2/2/22/22	0/1/1/1
3	BGC	E	403	-	-	0/2/22/22	0/1/1/1
3	BGC	C	402	-	-	2/2/22/22	0/1/1/1
3	BGC	A	402	-	-	0/2/22/22	0/1/1/1
3	BGC	H	402	-	-	2/2/22/22	0/1/1/1
3	BGC	G	402	-	-	2/2/22/22	0/1/1/1
3	BGC	E	402	-	-	0/2/22/22	0/1/1/1
3	BGC	C	403	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	BGC	C3-C4-C5	-3.24	104.36	110.23
3	H	402	BGC	C1-C2-C3	-2.82	104.61	110.36
3	E	402	BGC	C3-C4-C5	-2.68	105.37	110.23
3	F	402	BGC	C4-C3-C2	-2.29	106.81	110.83
3	H	402	BGC	O3-C3-C2	2.26	115.69	110.38

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	402	BGC	O5-C5-C6-O6
3	G	402	BGC	O5-C5-C6-O6
3	G	402	BGC	C4-C5-C6-O6
3	C	402	BGC	O5-C5-C6-O6
3	F	402	BGC	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	BGC	3	0
3	C	402	BGC	2	0
3	G	402	BGC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	370/380 (97%)	0.52	21 (5%)	29	32	12, 27, 43, 79	6 (1%)
1	B	371/380 (97%)	0.88	37 (9%)	12	13	14, 30, 49, 78	3 (0%)
1	C	371/380 (97%)	0.50	17 (4%)	37	41	19, 27, 43, 85	0
1	D	371/380 (97%)	0.54	18 (4%)	35	38	15, 27, 44, 73	2 (0%)
1	E	369/380 (97%)	0.26	14 (3%)	44	48	14, 24, 38, 67	3 (0%)
1	F	371/380 (97%)	0.26	11 (2%)	52	57	15, 23, 39, 75	2 (0%)
1	G	369/380 (97%)	0.54	18 (4%)	35	38	14, 27, 43, 63	4 (1%)
1	H	368/380 (96%)	0.71	31 (8%)	17	18	19, 29, 46, 64	0
All	All	2960/3040 (97%)	0.53	167 (5%)	30	32	12, 27, 44, 85	20 (0%)

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	THR	6.3
1	D	10	THR	5.3
1	D	9	GLY	5.2
1	G	10	THR	5.1
1	H	378	LEU	4.8

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 ⓘ

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.

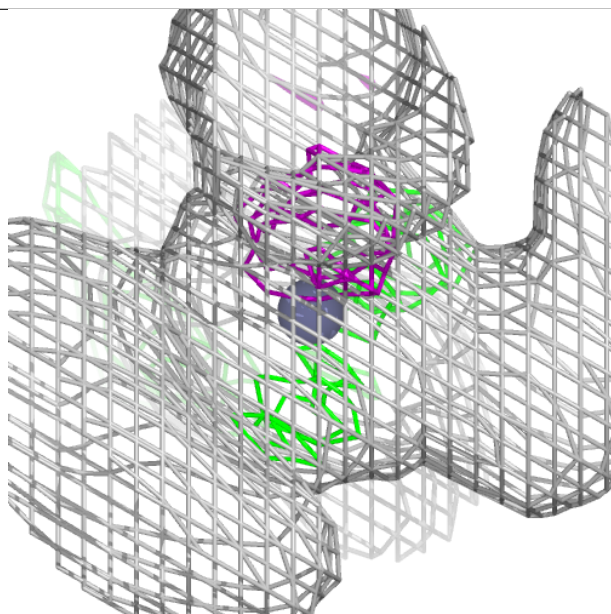
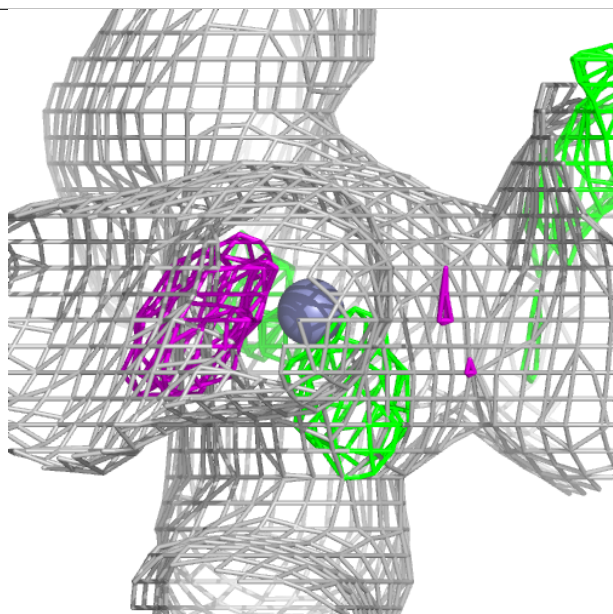
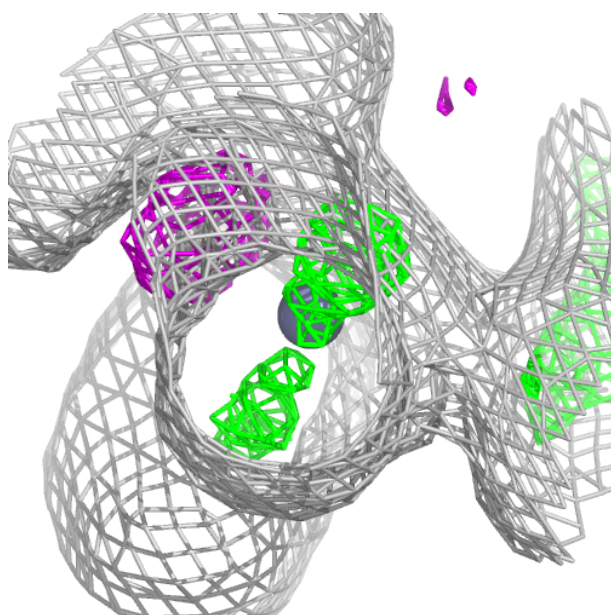
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	G	402	12/12	0.74	0.15	33,50,62,63	0
3	BGC	B	402	12/12	0.76	0.27	26,31,41,42	12
3	BGC	F	402	12/12	0.77	0.14	26,46,56,61	0
3	BGC	E	402	12/12	0.78	0.30	24,32,39,39	12
3	BGC	C	402	12/12	0.79	0.29	27,31,46,47	12
3	BGC	A	402	12/12	0.82	0.29	24,30,36,41	12
3	BGC	C	403	12/12	0.84	0.15	31,37,44,49	12
3	BGC	H	402	12/12	0.84	0.12	38,47,54,54	0
3	BGC	E	403	12/12	0.87	0.13	28,45,58,72	0
2	ACT	H	401	4/4	0.95	0.07	26,26,27,28	0
2	ACT	B	401	4/4	0.95	0.08	25,27,28,30	0
2	ACT	D	401	4/4	0.96	0.07	25,25,26,26	0
2	ACT	E	401	4/4	0.96	0.10	20,21,21,23	0
5	K	H	404	1/1	0.96	0.10	27,27,27,27	1
2	ACT	G	401	4/4	0.97	0.07	25,27,28,29	0
2	ACT	A	401	4/4	0.97	0.09	23,23,24,24	0
2	ACT	C	401	4/4	0.97	0.07	20,21,21,21	4
5	K	B	404	1/1	0.97	0.06	23,23,23,23	1
2	ACT	F	401	4/4	0.97	0.07	20,21,21,23	0
5	K	G	404	1/1	0.98	0.06	25,25,25,25	1
4	ZN	G	403	1/1	0.99	0.03	20,20,20,20	1
4	ZN	H	403	1/1	0.99	0.03	22,22,22,22	1
5	K	A	404	1/1	0.99	0.05	23,23,23,23	0
4	ZN	B	403	1/1	0.99	0.04	22,22,22,22	1
5	K	C	405	1/1	0.99	0.03	21,21,21,21	1
5	K	D	403	1/1	0.99	0.05	21,21,21,21	1
4	ZN	D	402	1/1	0.99	0.04	21,21,21,21	1
4	ZN	F	403	1/1	0.99	0.02	19,19,19,19	1
4	ZN	C	404	1/1	1.00	0.01	21,21,21,21	1
5	K	E	405	1/1	1.00	0.04	20,20,20,20	0
5	K	F	404	1/1	1.00	0.06	21,21,21,21	0
4	ZN	A	403	1/1	1.00	0.01	20,20,20,20	1
4	ZN	E	404	1/1	1.00	0.01	18,18,18,18	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.

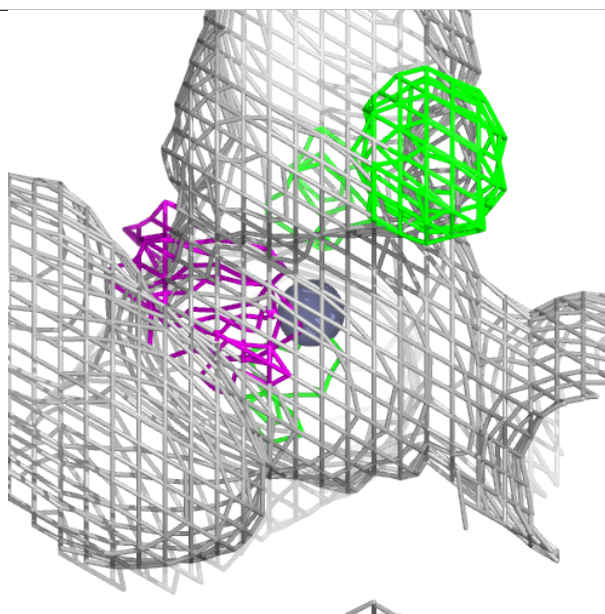
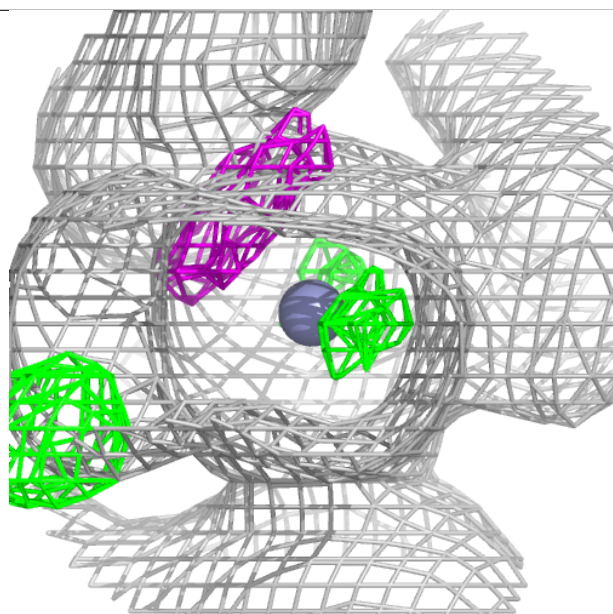
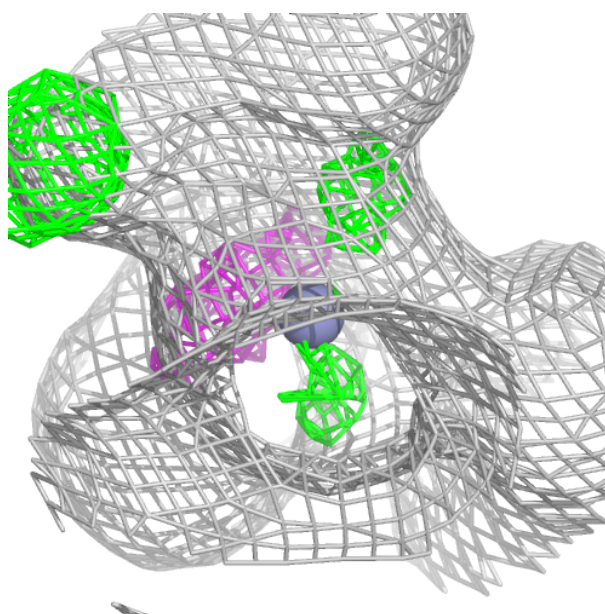
Electron density around ZN G 403:

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and green (positive)



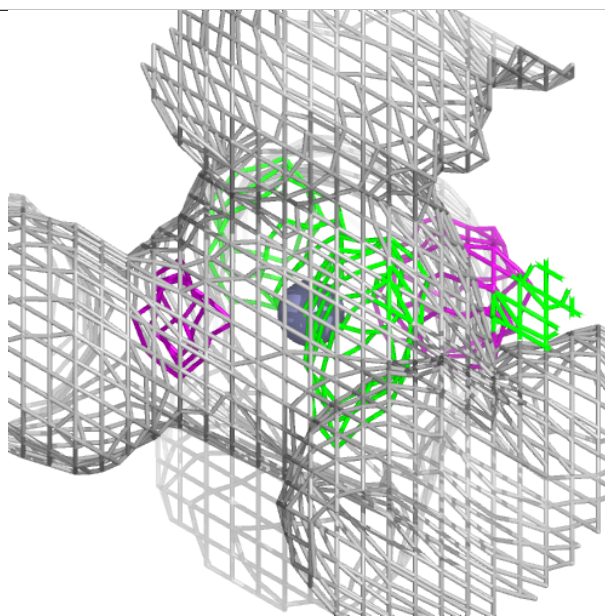
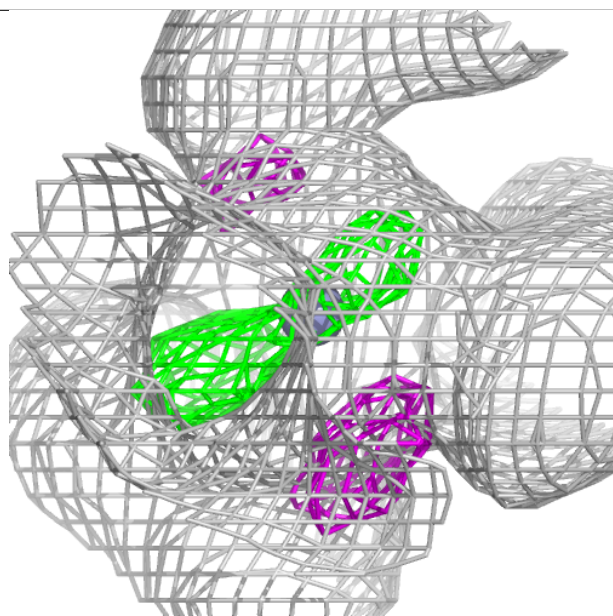
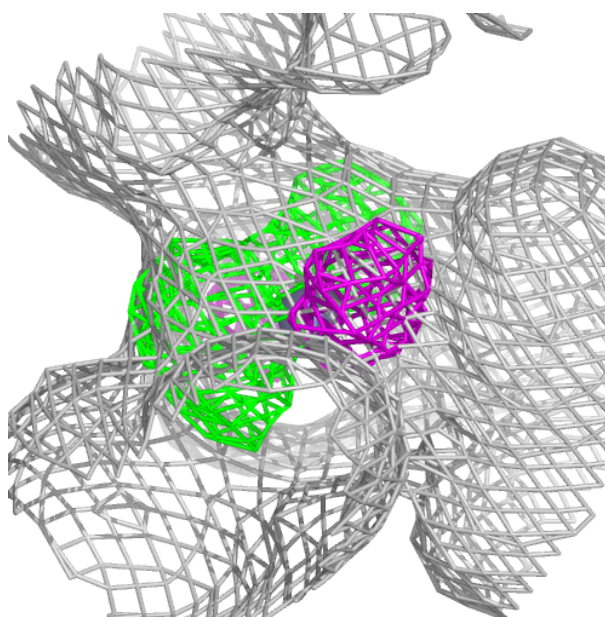
Electron density around ZN H 403:

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



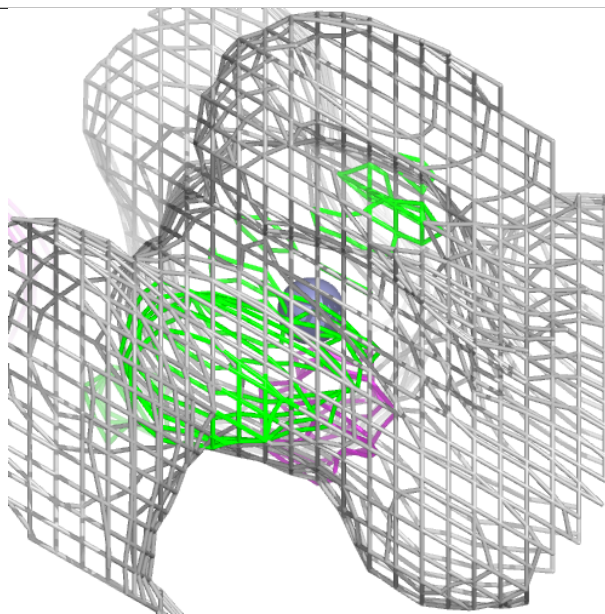
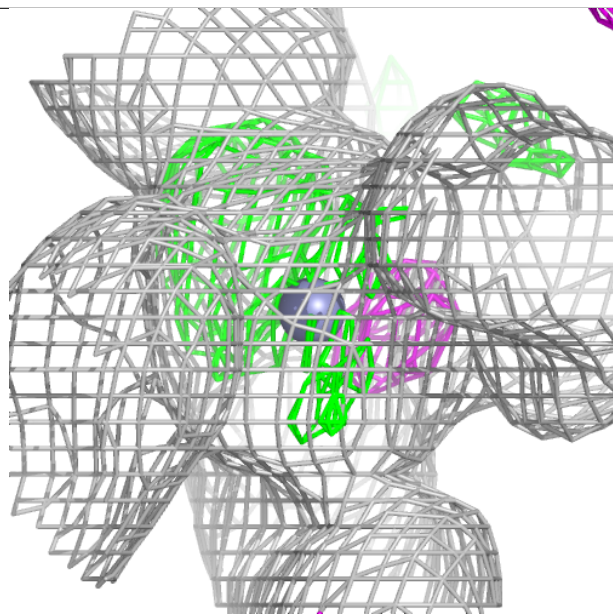
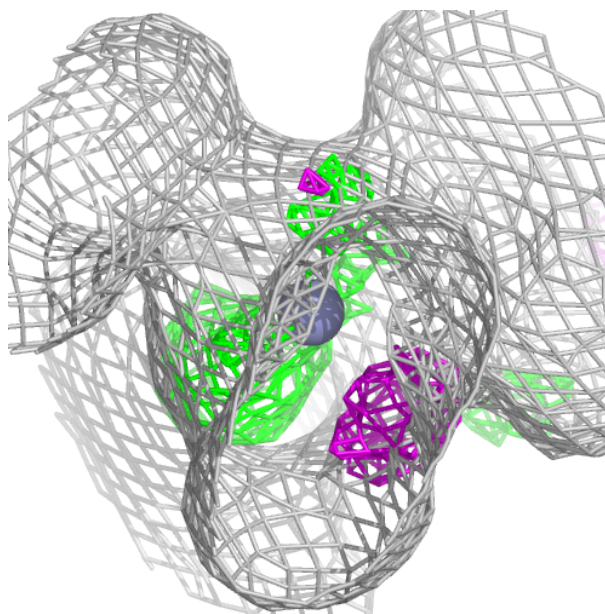
Electron density around ZN B 403:

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and green (positive)



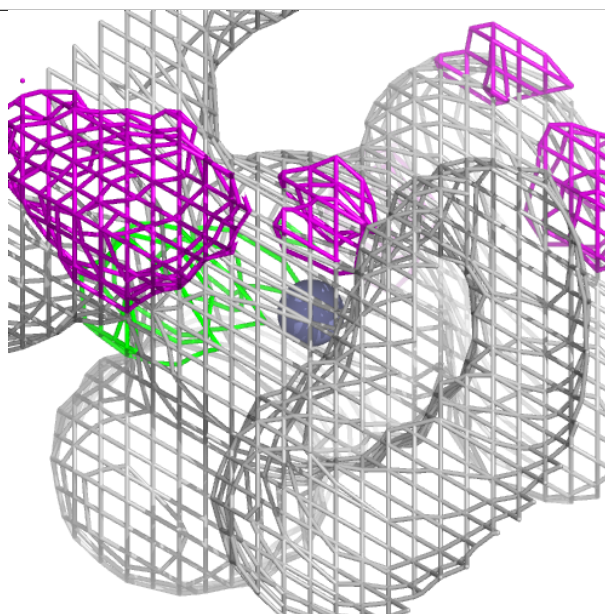
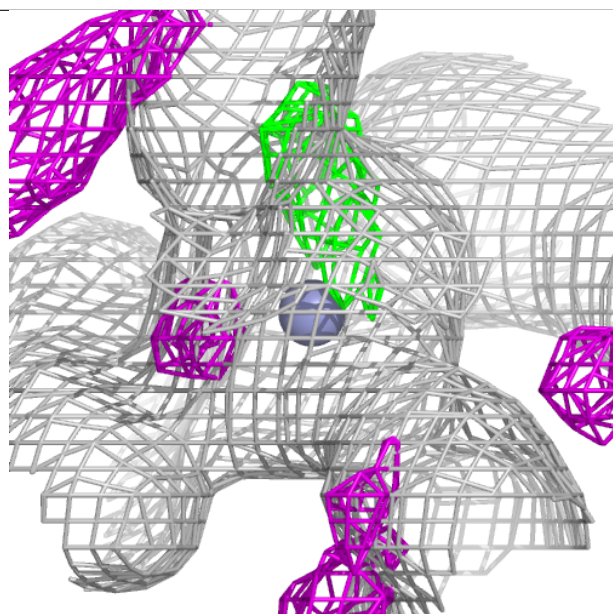
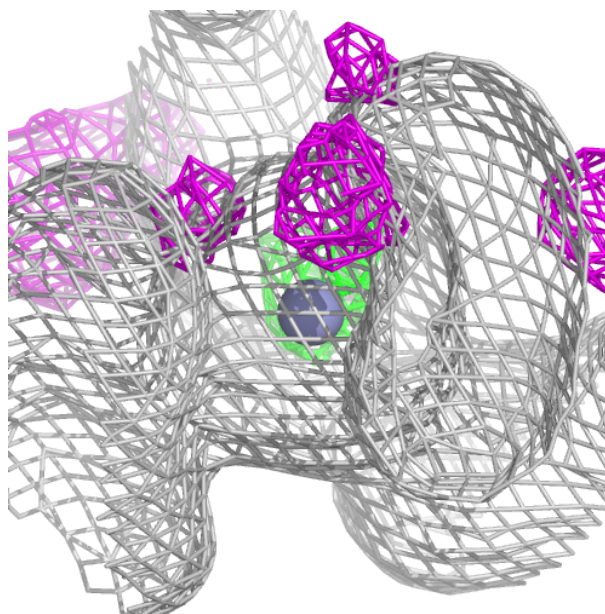
Electron density around ZN D 402:

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and green (positive)



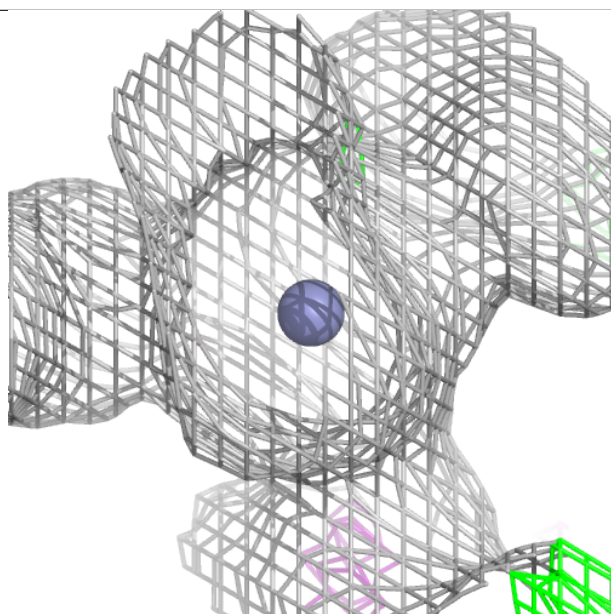
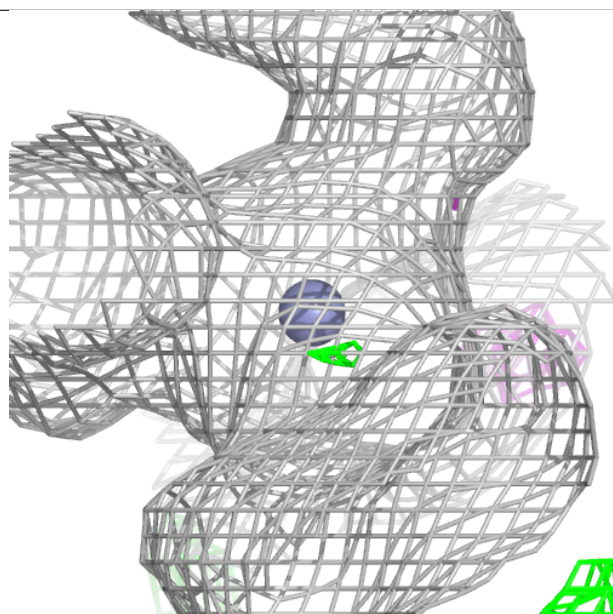
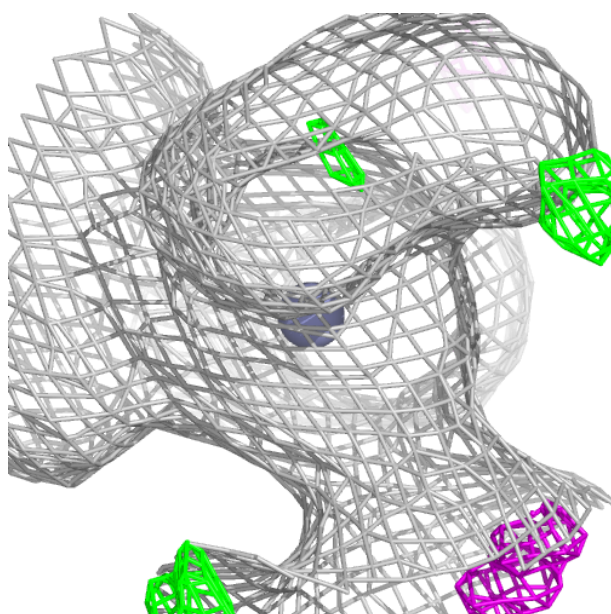
Electron density around ZN F 403:

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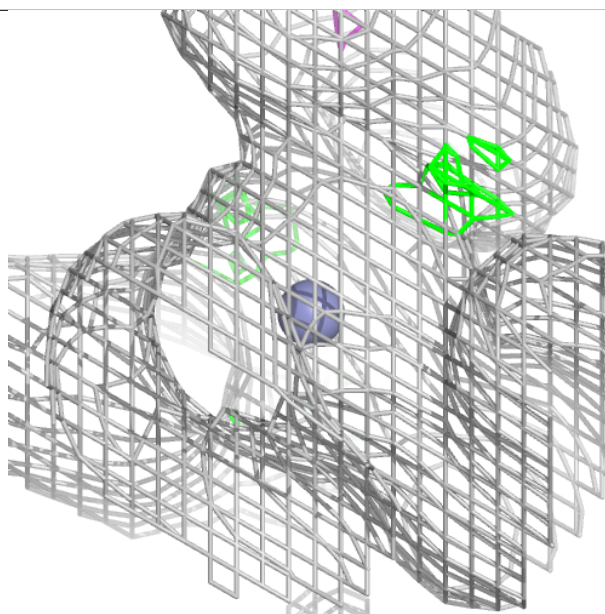
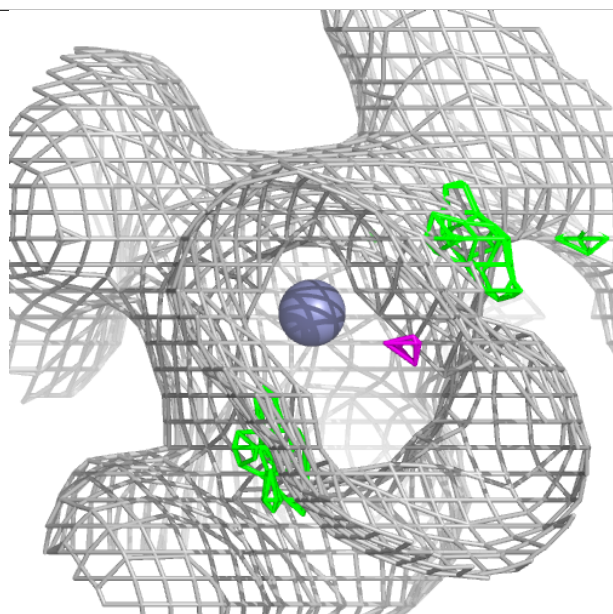
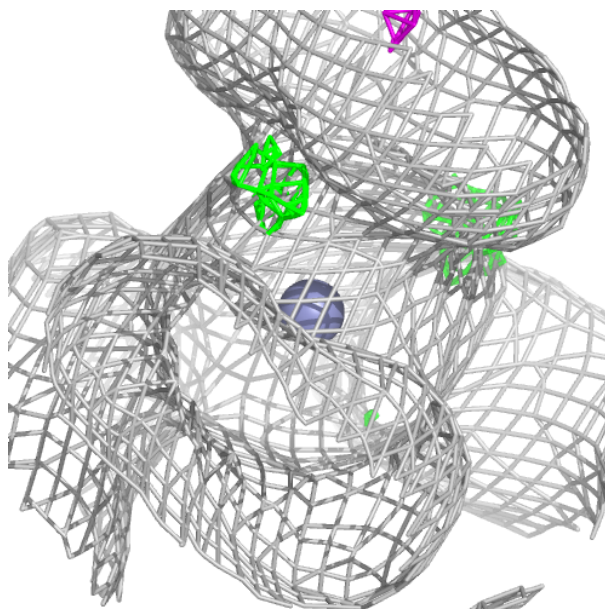
Electron density around ZN C 404:

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and green (positive)



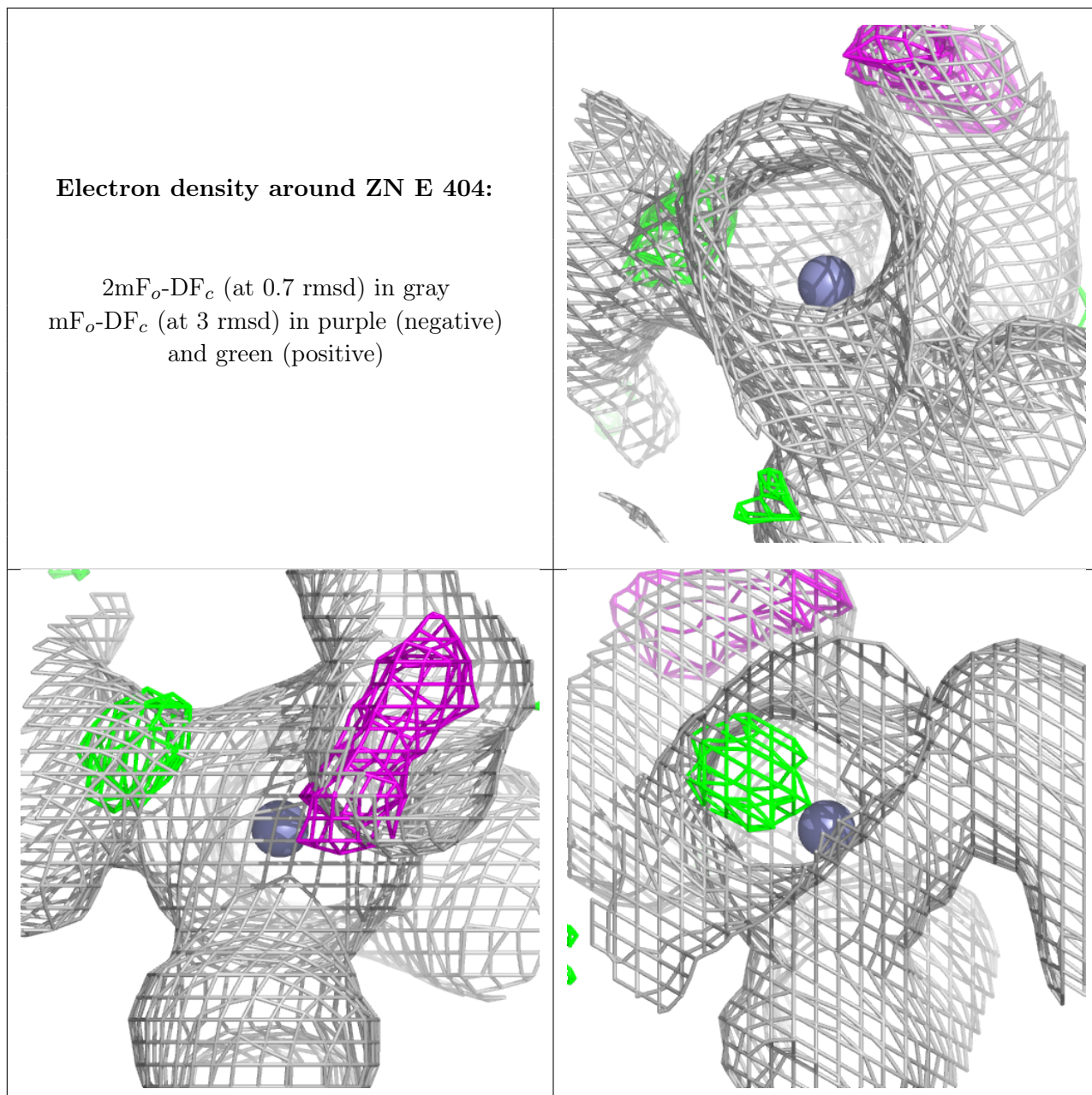
Electron density around ZN A 403:

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and green (positive)



Electron density around ZN E 404:

$2mF_o-DF_c$ (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.