



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 09:32 PM UTC

PDB ID : 9TI2 / pdb\_00009ti2  
Title : Crystal structure of the zinc-containing Phosphotriesterase dPTE2-H55(pi)MH  
Authors : Manser, B.P.; Deliz Liang, A.  
Deposited on : 2025-12-04  
Resolution : 1.69 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](mailto: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>.

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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

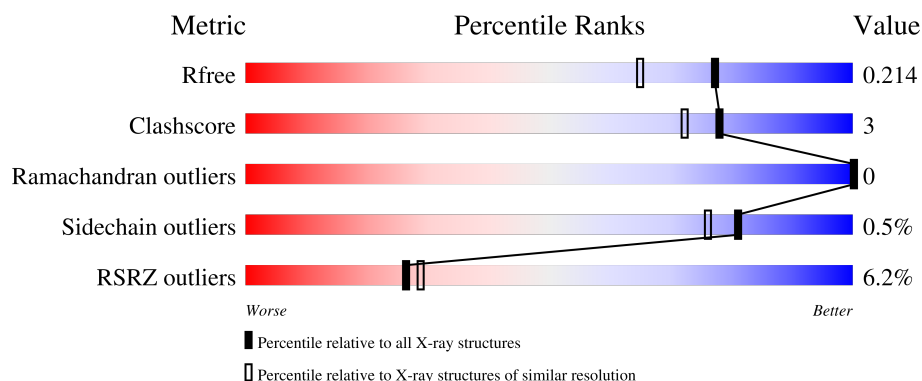
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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  $\geq 3$ , 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	342	<div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	B	342	<div> <div>88%</div> <div>8%</div> <div>5%</div> </div>
1	C	342	<div> <div>4%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	D	342	<div> <div>4%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	E	342	<div> <div>3%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	342	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	406	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30693 atoms, of which 14863 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	329	Total	C	H	N	O	S	0	0	0
			5019	1595	2486	445	485	8			
1	B	326	Total	C	H	N	O	S	0	0	0
			4982	1583	2469	442	480	8			
1	C	325	Total	C	H	N	O	S	0	0	0
			4958	1577	2456	438	479	8			
1	D	327	Total	C	H	N	O	S	0	0	0
			5001	1589	2480	443	481	8			
1	E	326	Total	C	H	N	O	S	0	0	0
			4982	1583	2469	442	480	8			
1	F	323	Total	C	H	N	O	S	0	0	0
			4918	1567	2431	436	476	8			

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P0A434
A	2	ASN	-	expression tag	UNP P0A434
A	3	ILE	-	expression tag	UNP P0A434
A	4	GLY	-	expression tag	UNP P0A434
A	5	SER	-	expression tag	UNP P0A434
A	6	GLY	-	expression tag	UNP P0A434
A	7	ILE	-	expression tag	UNP P0A434
A	8	THR	-	expression tag	UNP P0A434
A	9	ASN	-	expression tag	UNP P0A434
A	10	SER	-	expression tag	UNP P0A434
A	31	MET	THR	engineered mutation	UNP P0A434
A	54	ASP	LYS	engineered mutation	UNP P0A434
A	88	GLU	SER	engineered mutation	UNP P0A434
A	95	GLU	ARG	engineered mutation	UNP P0A434
A	159	ARG	LEU	engineered mutation	UNP P0A434
A	162	ARG	LYS	engineered mutation	UNP P0A434
A	180	ASP	ALA	engineered mutation	UNP P0A434

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Chain	Residue	Modelled	Actual	Comment	Reference
A	191	ASP	ALA	engineered mutation	UNP P0A434
A	199	ASP	SER	engineered mutation	UNP P0A434
A	215	ASP	SER	engineered mutation	UNP P0A434
A	246	ALA	SER	engineered mutation	UNP P0A434
A	251	LEU	ILE	engineered mutation	UNP P0A434
A	270	ALA	MET	engineered mutation	UNP P0A434
A	271	ASP	LYS	engineered mutation	UNP P0A434
A	320	ASP	GLN	engineered mutation	UNP P0A434
A	324	GLU	ALA	engineered mutation	UNP P0A434
A	325	THR	GLY	engineered mutation	UNP P0A434
A	327	MET	THR	engineered mutation	UNP P0A434
A	329	ASP	THR	engineered mutation	UNP P0A434
B	1	SER	-	expression tag	UNP P0A434
B	2	ASN	-	expression tag	UNP P0A434
B	3	ILE	-	expression tag	UNP P0A434
B	4	GLY	-	expression tag	UNP P0A434
B	5	SER	-	expression tag	UNP P0A434
B	6	GLY	-	expression tag	UNP P0A434
B	7	ILE	-	expression tag	UNP P0A434
B	8	THR	-	expression tag	UNP P0A434
B	9	ASN	-	expression tag	UNP P0A434
B	10	SER	-	expression tag	UNP P0A434
B	31	MET	THR	engineered mutation	UNP P0A434
B	54	ASP	LYS	engineered mutation	UNP P0A434
B	88	GLU	SER	engineered mutation	UNP P0A434
B	95	GLU	ARG	engineered mutation	UNP P0A434
B	159	ARG	LEU	engineered mutation	UNP P0A434
B	162	ARG	LYS	engineered mutation	UNP P0A434
B	180	ASP	ALA	engineered mutation	UNP P0A434
B	191	ASP	ALA	engineered mutation	UNP P0A434
B	199	ASP	SER	engineered mutation	UNP P0A434
B	215	ASP	SER	engineered mutation	UNP P0A434
B	246	ALA	SER	engineered mutation	UNP P0A434
B	251	LEU	ILE	engineered mutation	UNP P0A434
B	270	ALA	MET	engineered mutation	UNP P0A434
B	271	ASP	LYS	engineered mutation	UNP P0A434
B	320	ASP	GLN	engineered mutation	UNP P0A434
B	324	GLU	ALA	engineered mutation	UNP P0A434
B	325	THR	GLY	engineered mutation	UNP P0A434
B	327	MET	THR	engineered mutation	UNP P0A434
B	329	ASP	THR	engineered mutation	UNP P0A434
C	1	SER	-	expression tag	UNP P0A434

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ASN	-	expression tag	UNP P0A434
C	3	ILE	-	expression tag	UNP P0A434
C	4	GLY	-	expression tag	UNP P0A434
C	5	SER	-	expression tag	UNP P0A434
C	6	GLY	-	expression tag	UNP P0A434
C	7	ILE	-	expression tag	UNP P0A434
C	8	THR	-	expression tag	UNP P0A434
C	9	ASN	-	expression tag	UNP P0A434
C	10	SER	-	expression tag	UNP P0A434
C	31	MET	THR	engineered mutation	UNP P0A434
C	54	ASP	LYS	engineered mutation	UNP P0A434
C	88	GLU	SER	engineered mutation	UNP P0A434
C	95	GLU	ARG	engineered mutation	UNP P0A434
C	159	ARG	LEU	engineered mutation	UNP P0A434
C	162	ARG	LYS	engineered mutation	UNP P0A434
C	180	ASP	ALA	engineered mutation	UNP P0A434
C	191	ASP	ALA	engineered mutation	UNP P0A434
C	199	ASP	SER	engineered mutation	UNP P0A434
C	215	ASP	SER	engineered mutation	UNP P0A434
C	246	ALA	SER	engineered mutation	UNP P0A434
C	251	LEU	ILE	engineered mutation	UNP P0A434
C	270	ALA	MET	engineered mutation	UNP P0A434
C	271	ASP	LYS	engineered mutation	UNP P0A434
C	320	ASP	GLN	engineered mutation	UNP P0A434
C	324	GLU	ALA	engineered mutation	UNP P0A434
C	325	THR	GLY	engineered mutation	UNP P0A434
C	327	MET	THR	engineered mutation	UNP P0A434
C	329	ASP	THR	engineered mutation	UNP P0A434
D	1	SER	-	expression tag	UNP P0A434
D	2	ASN	-	expression tag	UNP P0A434
D	3	ILE	-	expression tag	UNP P0A434
D	4	GLY	-	expression tag	UNP P0A434
D	5	SER	-	expression tag	UNP P0A434
D	6	GLY	-	expression tag	UNP P0A434
D	7	ILE	-	expression tag	UNP P0A434
D	8	THR	-	expression tag	UNP P0A434
D	9	ASN	-	expression tag	UNP P0A434
D	10	SER	-	expression tag	UNP P0A434
D	31	MET	THR	engineered mutation	UNP P0A434
D	54	ASP	LYS	engineered mutation	UNP P0A434
D	88	GLU	SER	engineered mutation	UNP P0A434
D	95	GLU	ARG	engineered mutation	UNP P0A434

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Chain	Residue	Modelled	Actual	Comment	Reference
D	159	ARG	LEU	engineered mutation	UNP P0A434
D	162	ARG	LYS	engineered mutation	UNP P0A434
D	180	ASP	ALA	engineered mutation	UNP P0A434
D	191	ASP	ALA	engineered mutation	UNP P0A434
D	199	ASP	SER	engineered mutation	UNP P0A434
D	215	ASP	SER	engineered mutation	UNP P0A434
D	246	ALA	SER	engineered mutation	UNP P0A434
D	251	LEU	ILE	engineered mutation	UNP P0A434
D	270	ALA	MET	engineered mutation	UNP P0A434
D	271	ASP	LYS	engineered mutation	UNP P0A434
D	320	ASP	GLN	engineered mutation	UNP P0A434
D	324	GLU	ALA	engineered mutation	UNP P0A434
D	325	THR	GLY	engineered mutation	UNP P0A434
D	327	MET	THR	engineered mutation	UNP P0A434
D	329	ASP	THR	engineered mutation	UNP P0A434
E	1	SER	-	expression tag	UNP P0A434
E	2	ASN	-	expression tag	UNP P0A434
E	3	ILE	-	expression tag	UNP P0A434
E	4	GLY	-	expression tag	UNP P0A434
E	5	SER	-	expression tag	UNP P0A434
E	6	GLY	-	expression tag	UNP P0A434
E	7	ILE	-	expression tag	UNP P0A434
E	8	THR	-	expression tag	UNP P0A434
E	9	ASN	-	expression tag	UNP P0A434
E	10	SER	-	expression tag	UNP P0A434
E	31	MET	THR	engineered mutation	UNP P0A434
E	54	ASP	LYS	engineered mutation	UNP P0A434
E	88	GLU	SER	engineered mutation	UNP P0A434
E	95	GLU	ARG	engineered mutation	UNP P0A434
E	159	ARG	LEU	engineered mutation	UNP P0A434
E	162	ARG	LYS	engineered mutation	UNP P0A434
E	180	ASP	ALA	engineered mutation	UNP P0A434
E	191	ASP	ALA	engineered mutation	UNP P0A434
E	199	ASP	SER	engineered mutation	UNP P0A434
E	215	ASP	SER	engineered mutation	UNP P0A434
E	246	ALA	SER	engineered mutation	UNP P0A434
E	251	LEU	ILE	engineered mutation	UNP P0A434
E	270	ALA	MET	engineered mutation	UNP P0A434
E	271	ASP	LYS	engineered mutation	UNP P0A434
E	320	ASP	GLN	engineered mutation	UNP P0A434
E	324	GLU	ALA	engineered mutation	UNP P0A434
E	325	THR	GLY	engineered mutation	UNP P0A434

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Chain	Residue	Modelled	Actual	Comment	Reference
E	327	MET	THR	engineered mutation	UNP P0A434
E	329	ASP	THR	engineered mutation	UNP P0A434
F	1	SER	-	expression tag	UNP P0A434
F	2	ASN	-	expression tag	UNP P0A434
F	3	ILE	-	expression tag	UNP P0A434
F	4	GLY	-	expression tag	UNP P0A434
F	5	SER	-	expression tag	UNP P0A434
F	6	GLY	-	expression tag	UNP P0A434
F	7	ILE	-	expression tag	UNP P0A434
F	8	THR	-	expression tag	UNP P0A434
F	9	ASN	-	expression tag	UNP P0A434
F	10	SER	-	expression tag	UNP P0A434
F	31	MET	THR	engineered mutation	UNP P0A434
F	54	ASP	LYS	engineered mutation	UNP P0A434
F	88	GLU	SER	engineered mutation	UNP P0A434
F	95	GLU	ARG	engineered mutation	UNP P0A434
F	159	ARG	LEU	engineered mutation	UNP P0A434
F	162	ARG	LYS	engineered mutation	UNP P0A434
F	180	ASP	ALA	engineered mutation	UNP P0A434
F	191	ASP	ALA	engineered mutation	UNP P0A434
F	199	ASP	SER	engineered mutation	UNP P0A434
F	215	ASP	SER	engineered mutation	UNP P0A434
F	246	ALA	SER	engineered mutation	UNP P0A434
F	251	LEU	ILE	engineered mutation	UNP P0A434
F	270	ALA	MET	engineered mutation	UNP P0A434
F	271	ASP	LYS	engineered mutation	UNP P0A434
F	320	ASP	GLN	engineered mutation	UNP P0A434
F	324	GLU	ALA	engineered mutation	UNP P0A434
F	325	THR	GLY	engineered mutation	UNP P0A434
F	327	MET	THR	engineered mutation	UNP P0A434
F	329	ASP	THR	engineered mutation	UNP P0A434

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0

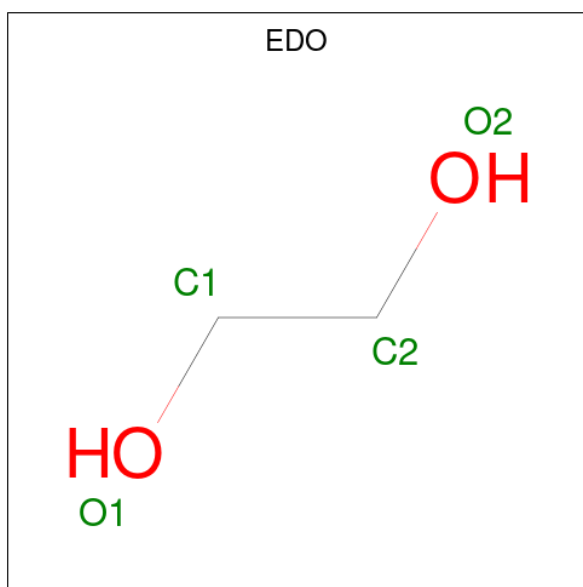
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

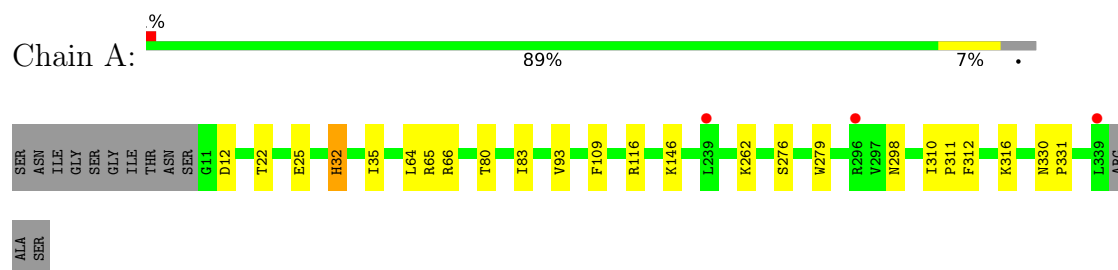
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total	O	0	0
			170	170		
4	B	212	Total	O	0	0
			212	212		
4	C	78	Total	O	0	0
			78	78		
4	D	112	Total	O	0	0
			112	112		
4	E	84	Total	O	0	0
			84	84		
4	F	45	Total	O	0	0
			45	45		

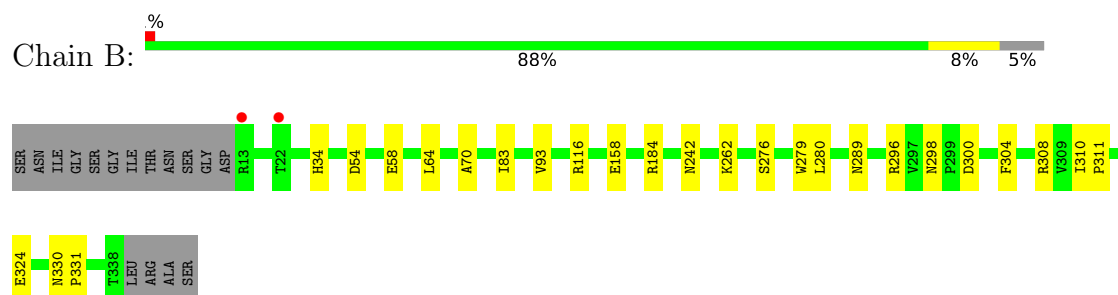
### 3 Residue-property plots [i](#)

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.

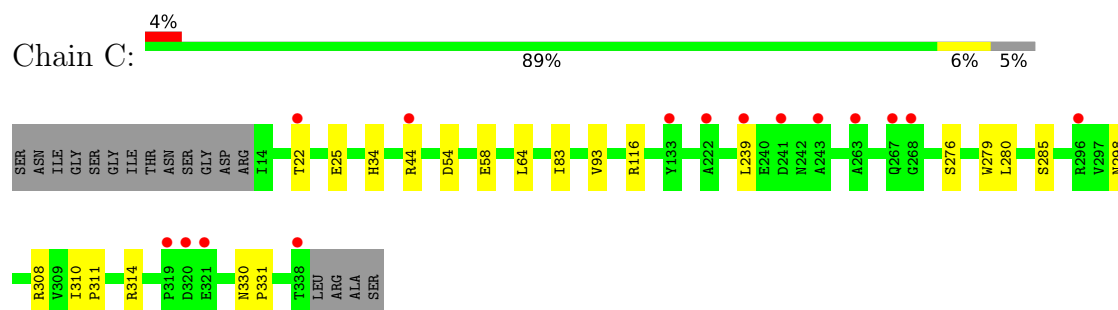
#### • Molecule 1: Parathion hydrolase



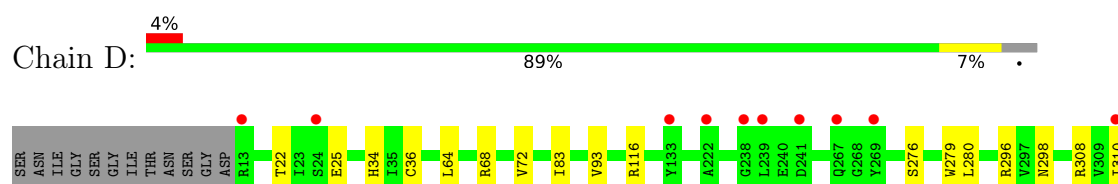
#### • Molecule 1: Parathion hydrolase

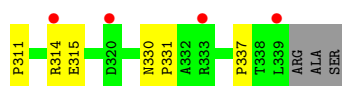


#### • Molecule 1: Parathion hydrolase

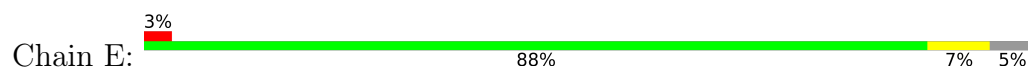


#### • Molecule 1: Parathion hydrolase

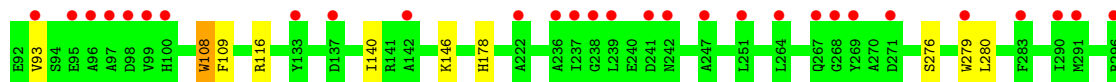
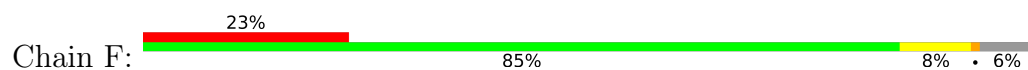




● Molecule 1: Parathion hydrolase



● Molecule 1: Parathion hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	442.55Å 57.93Å 84.46Å 90.00° 100.88° 90.00°	Depositor
Resolution (Å)	19.90 – 1.69 19.90 – 1.69	Depositor EDS
% Data completeness (in resolution range)	59.3 (19.90-1.69) 59.3 (19.90-1.69)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.204 , 0.216 0.202 , 0.214	Depositor DCC
$R_{free}$ test set	7003 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h-2*k,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30693	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0994e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, MHS, ZN, EDO

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	0.43	0/2555	0.66	2/3470 (0.1%)
1	B	0.49	0/2535	0.70	0/3443
1	C	0.47	0/2524	0.70	0/3429
1	D	0.53	0/2543	0.76	1/3454 (0.0%)
1	E	0.42	0/2535	0.65	0/3443
1	F	0.47	0/2509	0.74	2/3408 (0.1%)
All	All	0.47	0/15201	0.70	5/20647 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	3
1	D	0	4
1	E	0	2
1	F	0	3
All	All	0	16

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ILE	N-CA-C	-6.11	105.11	111.58
1	A	109	PHE	CA-CB-CG	5.65	119.45	113.80
1	D	337	PRO	CB-CA-C	5.16	118.42	111.71
1	F	108	TRP	CA-C-O	-5.07	115.27	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	69	ALA	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	B	116	ARG	Sidechain
1	B	184	ARG	Sidechain
1	B	296	ARG	Sidechain
1	C	44	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2533	2486	2504	14	0
1	B	2513	2469	2486	18	0
1	C	2502	2456	2473	12	0
1	D	2521	2480	2497	9	0
1	E	2513	2469	2486	11	1
1	F	2487	2431	2455	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	B	28	42	42	9	0
3	C	12	18	18	1	0
3	D	8	12	12	0	0
4	A	170	0	0	3	0
4	B	212	0	0	6	3
4	C	78	0	0	1	1
4	D	112	0	0	1	3
4	E	84	0	0	0	1
4	F	45	0	0	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15830	14863	14973	83	5

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 83 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:262:LYS:HE2	4:A:633:HOH:O	1.59	1.01
1:F:16:THR:HG22	1:F:19:GLY:O	1.64	0.96
3:B:404:EDO:O1	4:B:501:HOH:O	1.85	0.93
1:F:67:ALA:HB2	4:F:502:HOH:O	1.75	0.86
1:B:70:ALA:O	4:B:503:HOH:O	2.06	0.73

All (5) 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)
4:B:678:HOH:O	4:D:589:HOH:O[4_446]	1.77	0.43
4:D:581:HOH:O	4:E:511:HOH:O[1_565]	1.80	0.40
4:B:614:HOH:O	4:C:563:HOH:O[4_455]	1.97	0.23
4:B:678:HOH:O	4:D:606:HOH:O[4_446]	2.07	0.13
1:E:262:LYS:HZ1	4:F:505:HOH:O[2_556]	1.54	0.06

## 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	325/342 (95%)	316 (97%)	9 (3%)	0	100	100
1	B	322/342 (94%)	311 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	321/342 (94%)	311 (97%)	10 (3%)	0	100	100
1	D	323/342 (94%)	312 (97%)	11 (3%)	0	100	100
1	E	322/342 (94%)	313 (97%)	9 (3%)	0	100	100
1	F	319/342 (93%)	310 (97%)	9 (3%)	0	100	100
All	All	1932/2052 (94%)	1873 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	264/274 (96%)	263 (100%)	1 (0%)	84	80
1	B	262/274 (96%)	261 (100%)	1 (0%)	84	80
1	C	261/274 (95%)	260 (100%)	1 (0%)	84	80
1	D	263/274 (96%)	261 (99%)	2 (1%)	73	65
1	E	262/274 (96%)	261 (100%)	1 (0%)	84	80
1	F	259/274 (94%)	257 (99%)	2 (1%)	73	65
All	All	1571/1644 (96%)	1563 (100%)	8 (0%)	81	76

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	276	SER
1	F	24	SER
1	D	315	GLU
1	D	276	SER
1	E	276	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MHS	C	32	1,2	10,11,12	0.78	0	5,14,16	0.50	0
1	KCX	F	146	1,2	10,11,12	0.44	0	6,12,14	0.67	0
1	KCX	C	146	1,2	10,11,12	0.44	0	6,12,14	0.62	0
1	MHS	B	32	1,2	10,11,12	0.79	0	5,14,16	0.46	0
1	KCX	A	146	1,2	10,11,12	0.29	0	6,12,14	0.48	0
1	MHS	F	32	1,2	10,11,12	0.78	0	5,14,16	0.51	0
1	MHS	E	32	1,2	10,11,12	0.78	0	5,14,16	0.51	0
1	MHS	D	32	1,2	10,11,12	0.78	0	5,14,16	0.52	0
1	KCX	B	146	1,2	10,11,12	0.64	0	6,12,14	0.92	0
1	KCX	D	146	1,2	10,11,12	0.42	0	6,12,14	0.68	0
1	KCX	E	146	1,2	10,11,12	0.43	0	6,12,14	0.60	0
1	MHS	A	32	1,2	10,11,12	1.19	1 (10%)	5,14,16	1.02	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
1	MHS	C	32	1,2	-	3/5/6/8	0/1/1/1
1	KCX	F	146	1,2	-	1/9/10/12	-
1	KCX	C	146	1,2	-	0/9/10/12	-
1	MHS	B	32	1,2	-	3/5/6/8	0/1/1/1
1	KCX	A	146	1,2	-	2/9/10/12	-
1	MHS	F	32	1,2	-	3/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MHS	E	32	1,2	-	3/5/6/8	0/1/1/1
1	MHS	D	32	1,2	-	3/5/6/8	0/1/1/1
1	KCX	B	146	1,2	-	1/9/10/12	-
1	KCX	D	146	1,2	-	0/9/10/12	-
1	KCX	E	146	1,2	-	0/9/10/12	-
1	MHS	A	32	1,2	-	3/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	MHS	CD2-CG	-2.30	1.33	1.36

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	32	MHS	O-C-CA-CB
1	A	32	MHS	CA-CB-CG-ND1
1	B	32	MHS	O-C-CA-CB
1	B	32	MHS	CA-CB-CG-ND1
1	C	32	MHS	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	146	KCX	1	0
1	A	146	KCX	1	0
1	F	32	MHS	1	0
1	E	146	KCX	1	0
1	A	32	MHS	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	EDO	B	405	-	3,3,3	0.13	0	2,2,2	0.10	0
3	EDO	B	401	-	3,3,3	0.11	0	2,2,2	0.19	0
3	EDO	B	402	-	3,3,3	0.20	0	2,2,2	0.10	0
3	EDO	D	402	-	3,3,3	0.13	0	2,2,2	0.06	0
3	EDO	B	407	-	3,3,3	0.30	0	2,2,2	0.25	0
3	EDO	B	404	-	3,3,3	0.18	0	2,2,2	0.04	0
3	EDO	B	403	-	3,3,3	0.15	0	2,2,2	0.05	0
3	EDO	C	402	-	3,3,3	0.09	0	2,2,2	0.11	0
3	EDO	D	401	-	3,3,3	0.18	0	2,2,2	0.09	0
3	EDO	C	403	-	3,3,3	0.10	0	2,2,2	0.02	0
3	EDO	C	401	-	3,3,3	0.14	0	2,2,2	0.06	0
3	EDO	B	406	-	3,3,3	0.10	0	2,2,2	0.09	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	EDO	B	405	-	-	1/1/1/1	-
3	EDO	B	401	-	-	0/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	D	402	-	-	0/1/1/1	-
3	EDO	B	407	-	-	0/1/1/1	-
3	EDO	B	404	-	-	1/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
3	EDO	D	401	-	-	0/1/1/1	-
3	EDO	C	403	-	-	0/1/1/1	-
3	EDO	C	401	-	-	0/1/1/1	-
3	EDO	B	406	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	EDO	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2
3	B	406	EDO	O1-C1-C2-O2
3	B	405	EDO	O1-C1-C2-O2
3	B	402	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	EDO	1	0
3	B	404	EDO	3	0
3	B	403	EDO	1	0
3	C	402	EDO	1	0
3	B	406	EDO	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	327/342 (95%)	-0.46	3 (0%) 81 83	9, 18, 33, 58	0
1	B	324/342 (94%)	-0.35	2 (0%) 85 88	8, 15, 27, 46	0
1	C	323/342 (94%)	0.50	15 (4%) 37 41	17, 33, 45, 61	0
1	D	325/342 (95%)	0.17	14 (4%) 40 44	15, 25, 40, 61	0
1	E	324/342 (94%)	0.27	10 (3%) 51 55	17, 30, 46, 74	0
1	F	321/342 (93%)	1.32	77 (23%) 2 2	26, 45, 65, 81	0
All	All	1944/2052 (94%)	0.24	121 (6%) 26 29	8, 27, 52, 81	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	239	LEU	5.6
1	F	69	ALA	5.1
1	F	239	LEU	4.8
1	F	97	ALA	4.3
1	F	99	VAL	4.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	F	146	12/13	0.88	0.11	28,31,35,37	0
1	KCX	E	146	12/13	0.89	0.10	17,19,25,31	0
1	KCX	D	146	12/13	0.89	0.08	14,17,20,21	0
1	KCX	C	146	12/13	0.90	0.09	22,24,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MHS	F	32	11/12	0.91	0.12	37,38,40,40	0
1	MHS	C	32	11/12	0.93	0.09	19,20,24,25	0
1	MHS	A	32	11/12	0.93	0.07	9,12,14,14	0
1	KCX	B	146	12/13	0.93	0.06	6,8,12,13	0
1	KCX	A	146	12/13	0.94	0.07	8,9,13,15	0
1	MHS	D	32	11/12	0.96	0.06	11,14,15,15	0
1	MHS	B	32	11/12	0.96	0.05	5,7,8,9	0
1	MHS	E	32	11/12	0.96	0.06	18,20,22,23	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	405	4/4	0.75	0.18	32,38,43,48	0
3	EDO	D	402	4/4	0.78	0.15	24,29,33,37	0
3	EDO	B	404	4/4	0.81	0.20	26,31,38,43	0
3	EDO	C	401	4/4	0.82	0.18	30,36,41,41	0
3	EDO	B	406	4/4	0.84	0.15	26,38,42,47	0
3	EDO	B	407	4/4	0.84	0.16	26,31,37,37	0
3	EDO	C	402	4/4	0.89	0.10	27,33,37,37	0
3	EDO	C	403	4/4	0.90	0.12	20,31,38,38	0
3	EDO	B	401	4/4	0.91	0.09	21,28,34,34	0
3	EDO	B	402	4/4	0.92	0.09	18,23,28,28	0
3	EDO	B	403	4/4	0.93	0.07	20,26,28,31	0
2	ZN	B	409	1/1	0.93	0.05	15,15,15,15	0
3	EDO	D	401	4/4	0.93	0.11	18,23,32,32	0
2	ZN	C	404	1/1	0.93	0.04	18,18,18,18	0
2	ZN	F	402	1/1	0.95	0.05	26,26,26,26	0
2	ZN	D	403	1/1	0.97	0.03	16,16,16,16	0
2	ZN	F	401	1/1	0.97	0.04	24,24,24,24	0
2	ZN	A	401	1/1	0.97	0.04	14,14,14,14	0
2	ZN	D	404	1/1	0.98	0.03	19,19,19,19	0
2	ZN	E	402	1/1	0.98	0.03	21,21,21,21	0

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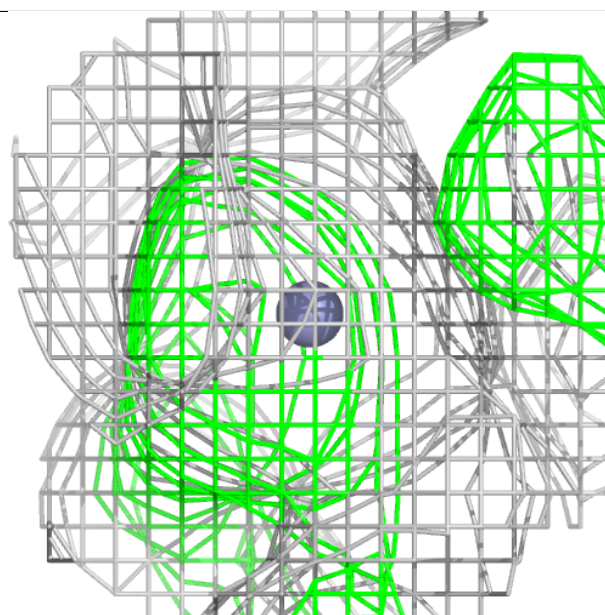
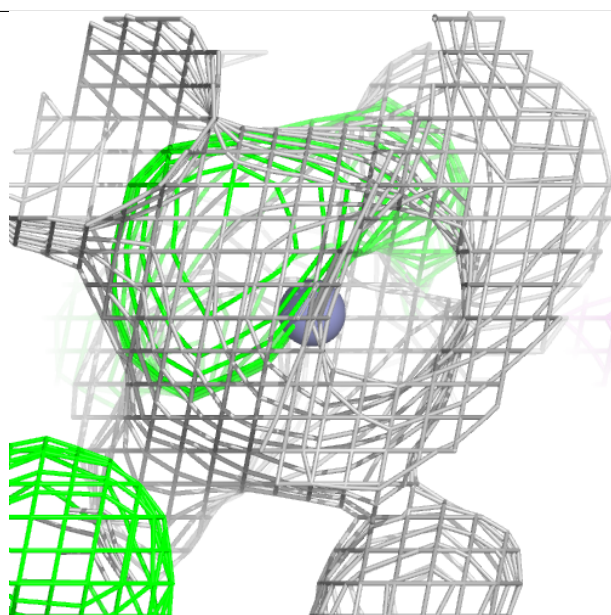
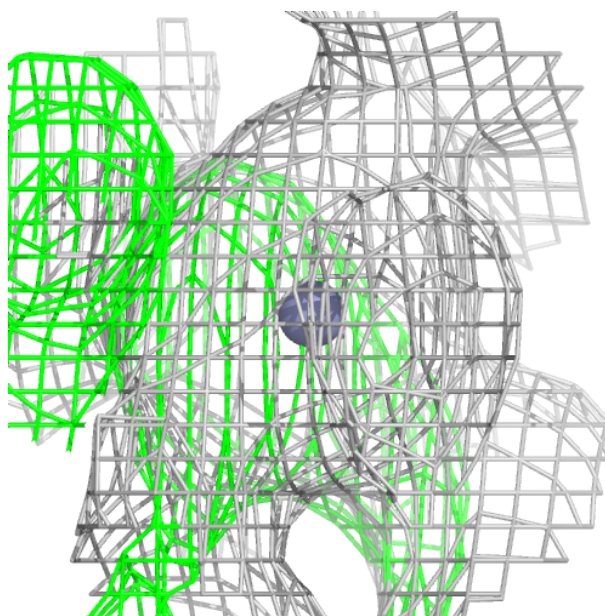
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	E	401	1/1	0.99	0.02	19,19,19,19	0
2	ZN	C	405	1/1	0.99	0.02	18,18,18,18	0
2	ZN	A	402	1/1	0.99	0.03	17,17,17,17	0
2	ZN	B	408	1/1	0.99	0.03	11,11,11,11	0

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 ZN B 409:**

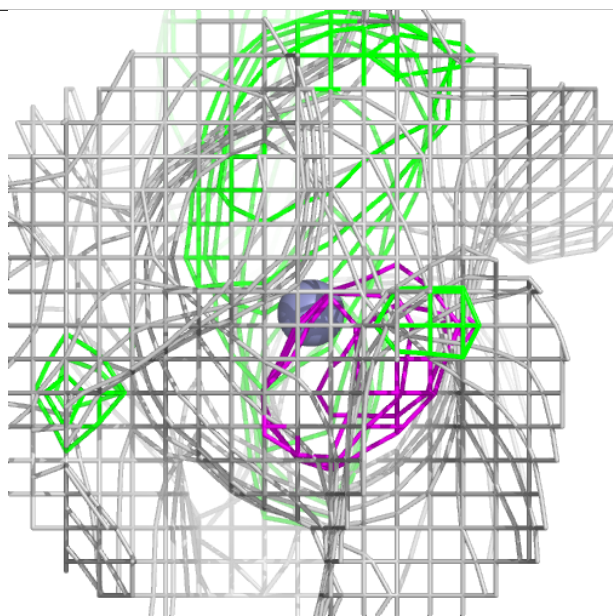
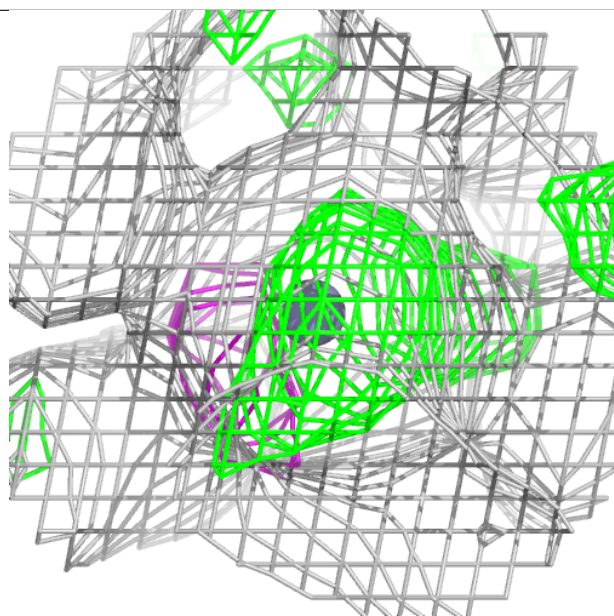
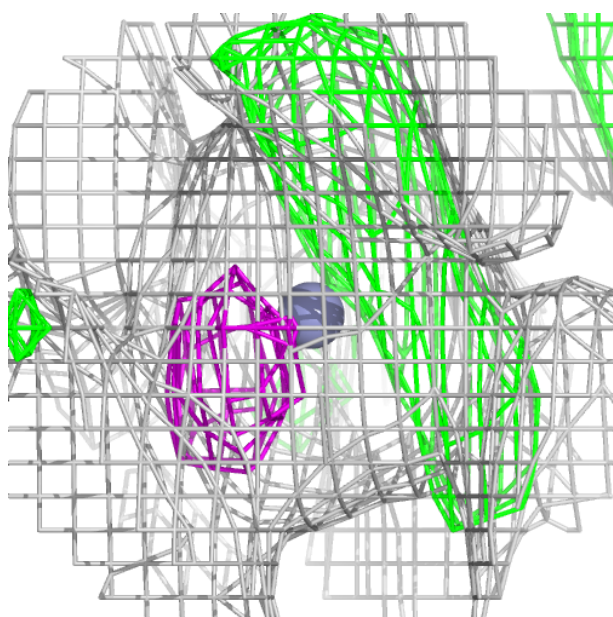
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mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





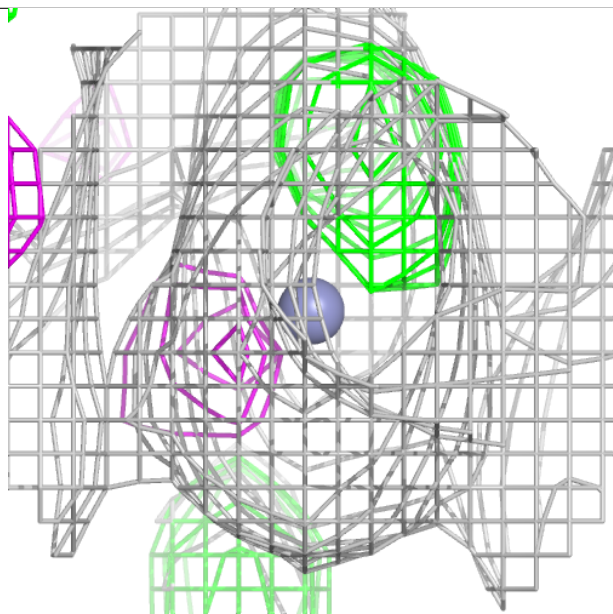
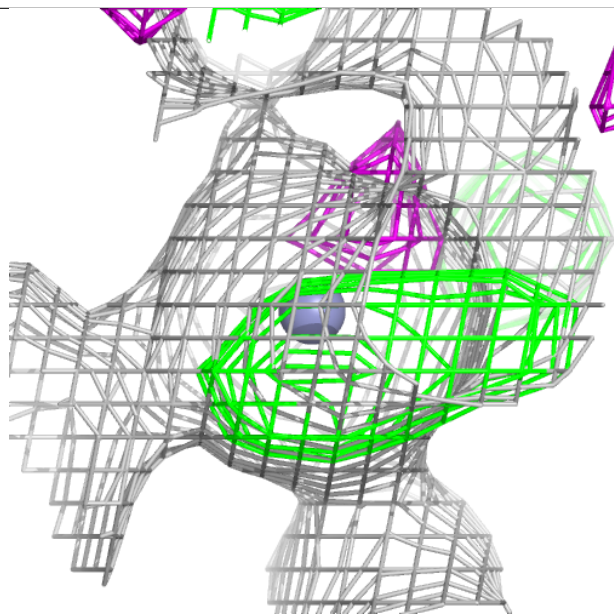
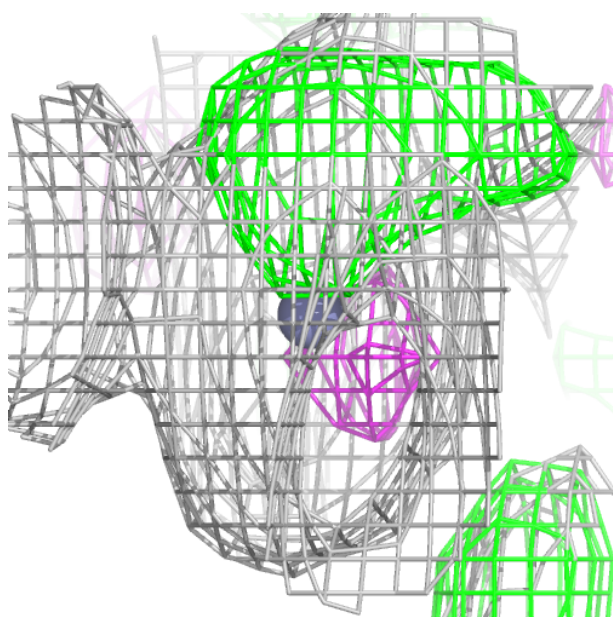
**Electron density around ZN C 404:**

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



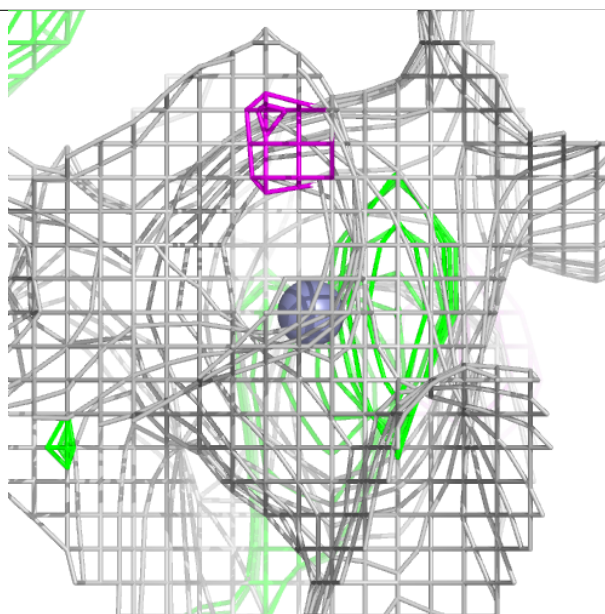
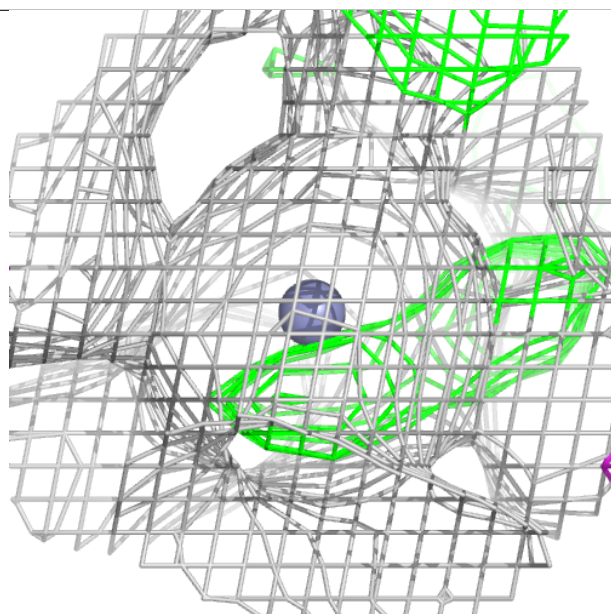
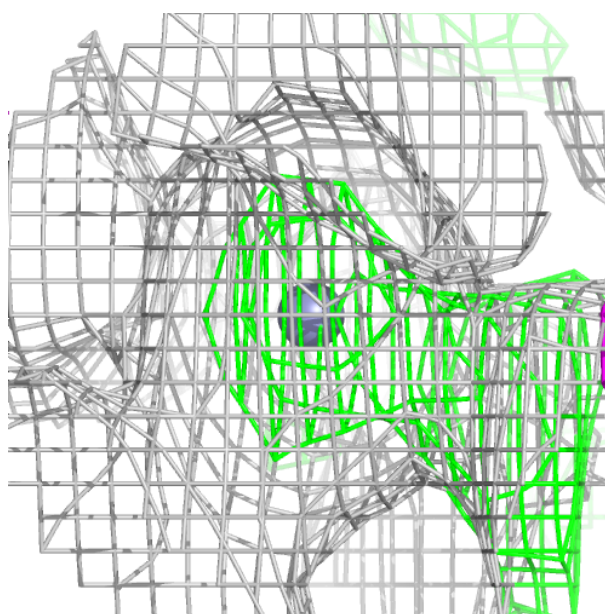
**Electron density around ZN F 402:**

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



**Electron density around ZN D 403:**

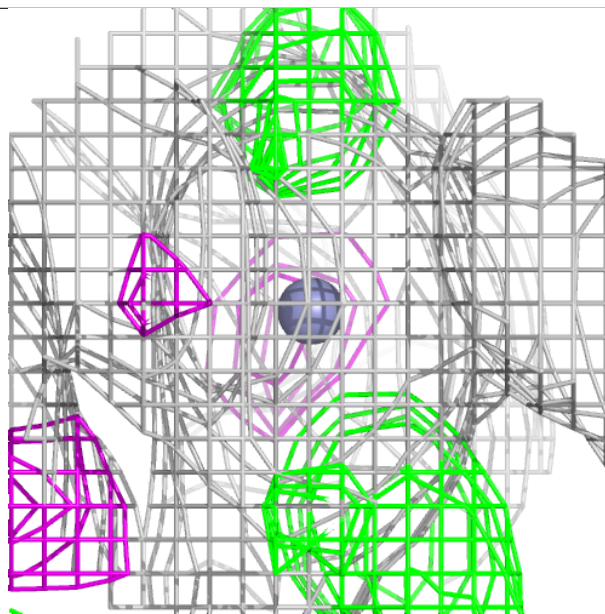
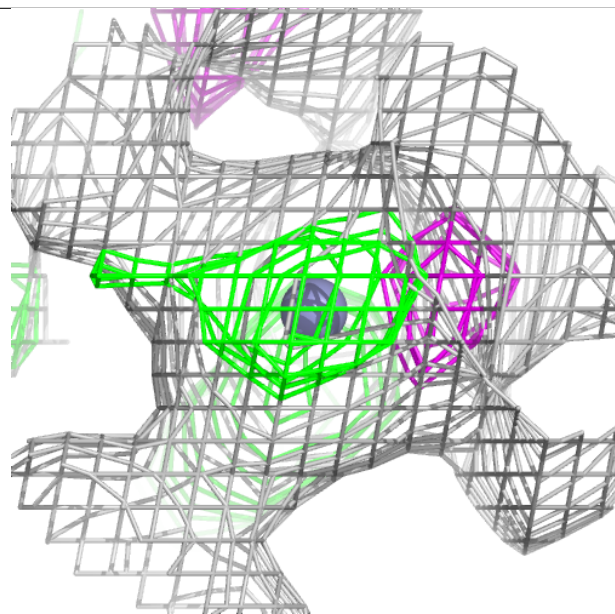
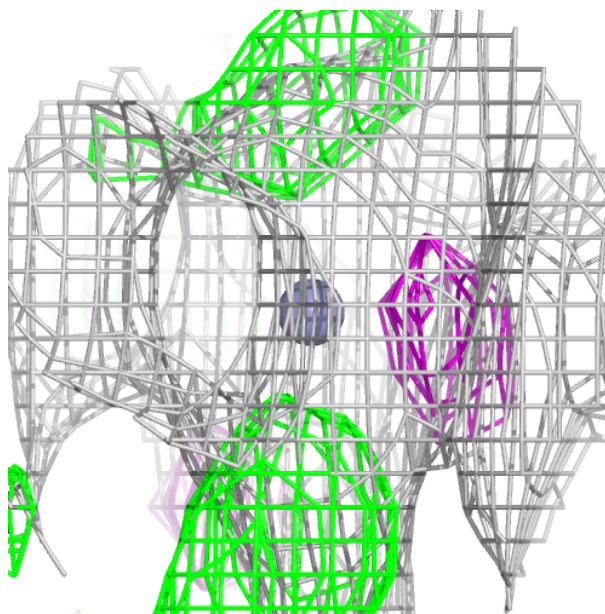
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





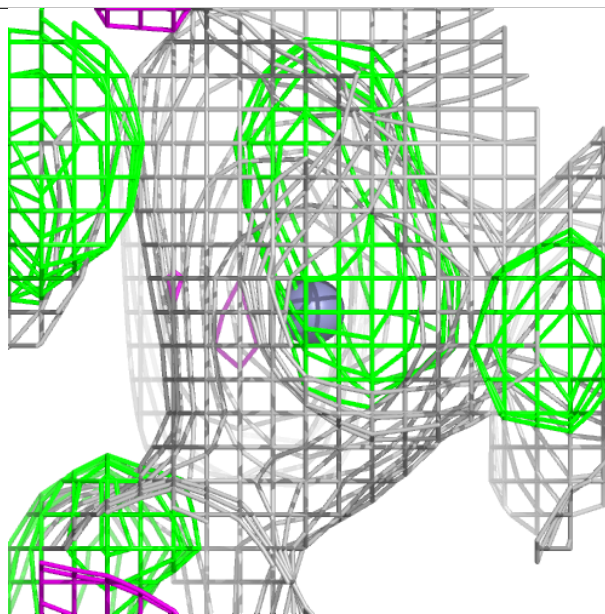
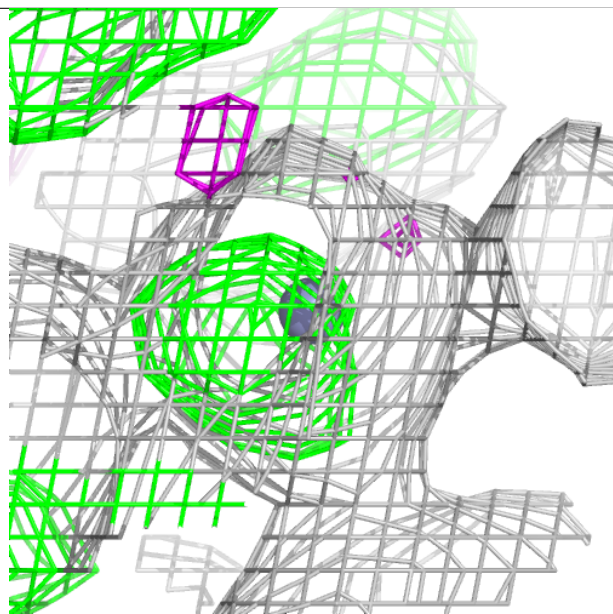
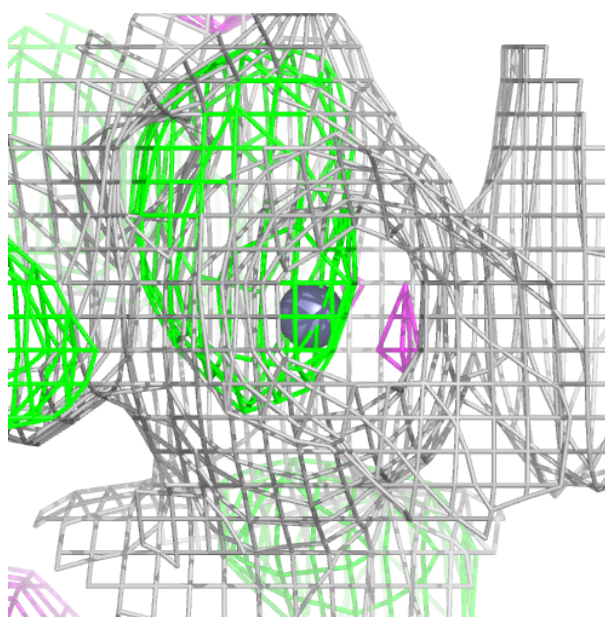
**Electron density around ZN F 401:**

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



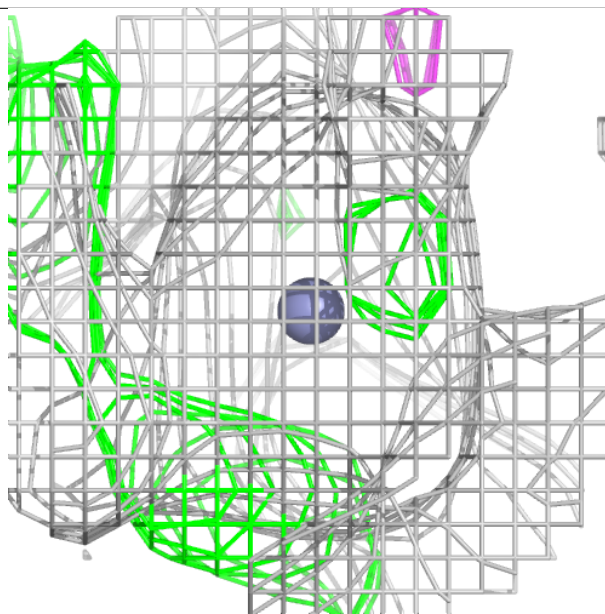
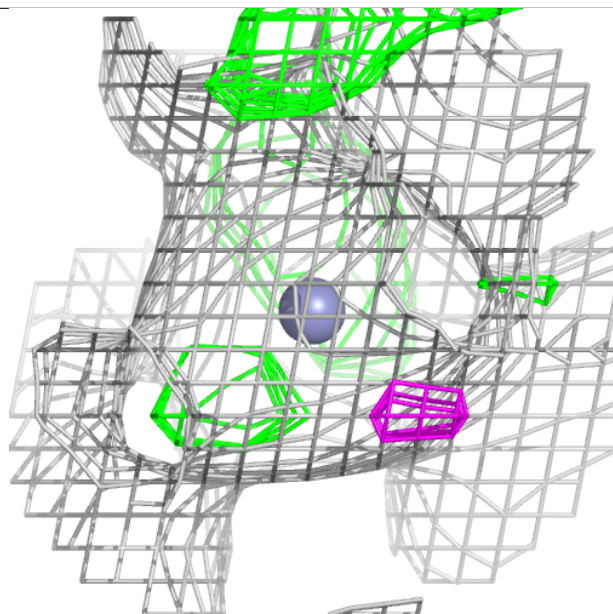
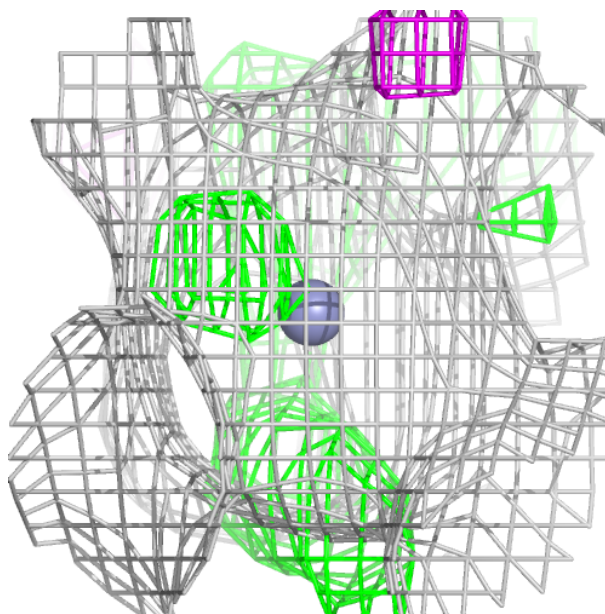
**Electron density around ZN A 401:**

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



**Electron density around ZN D 404:**

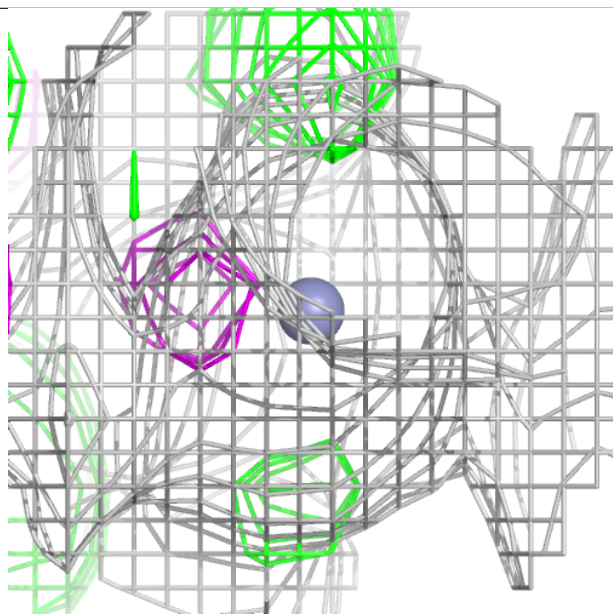
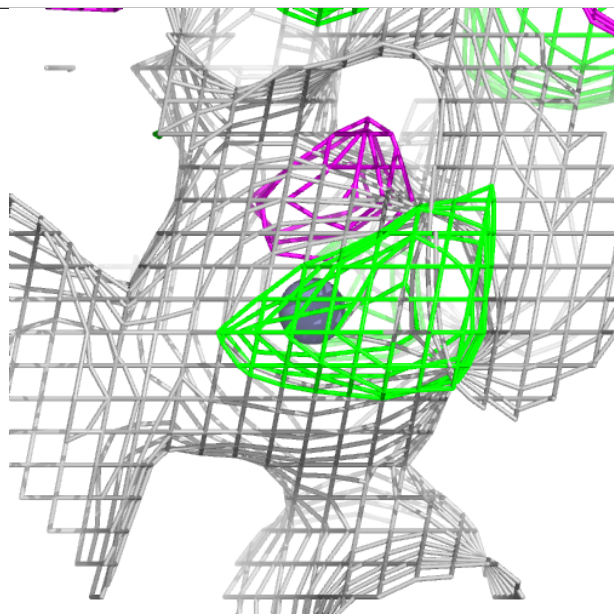
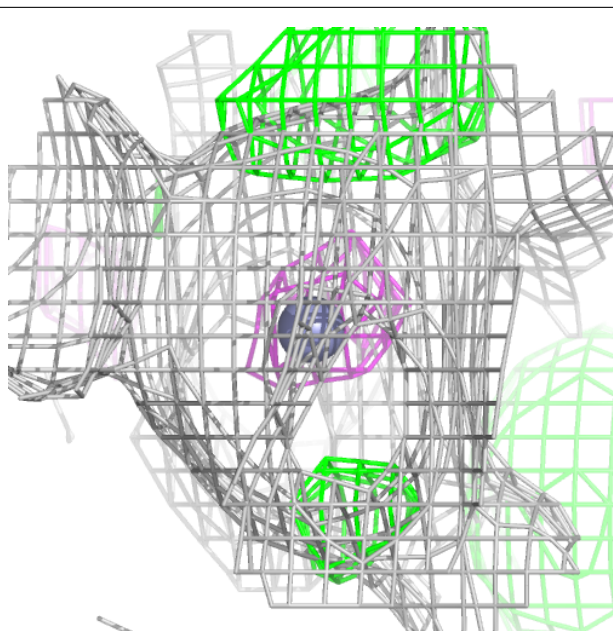
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





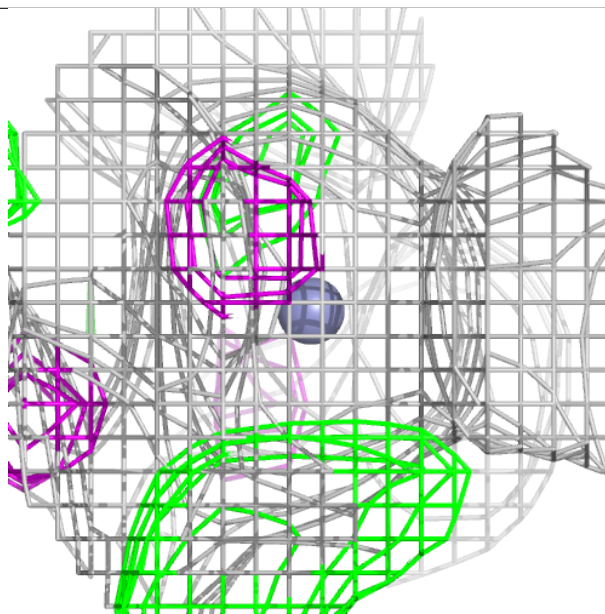
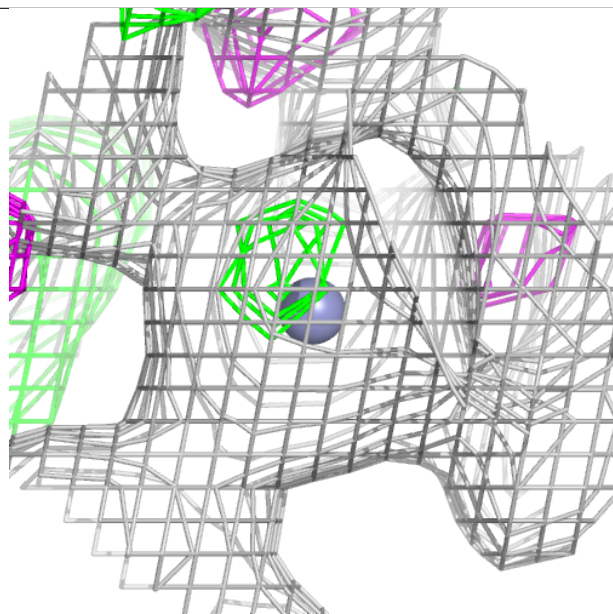
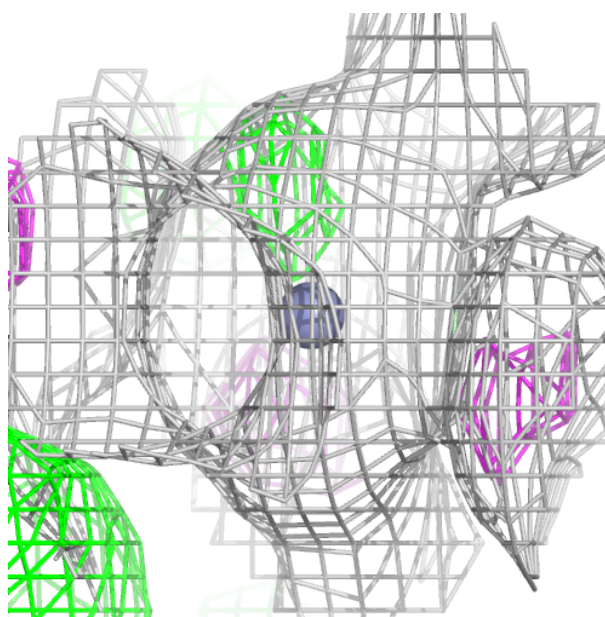
**Electron density around ZN E 402:**

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



**Electron density around ZN E 401:**

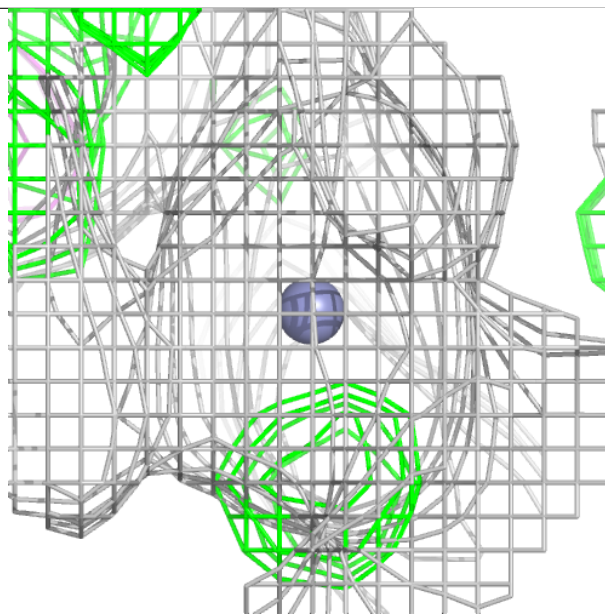
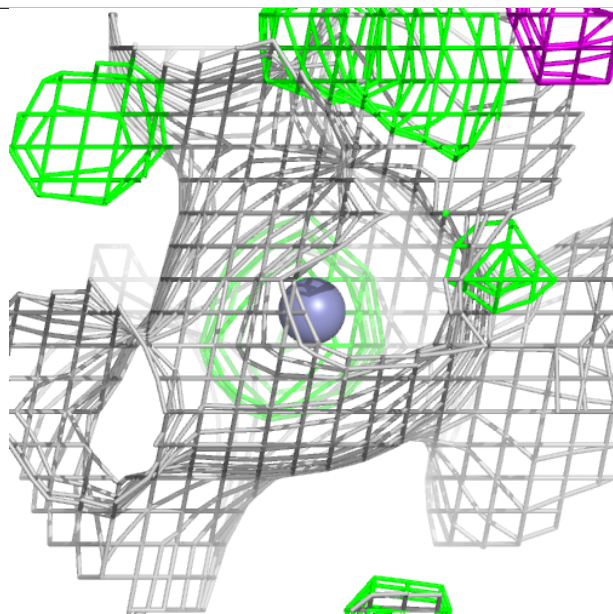
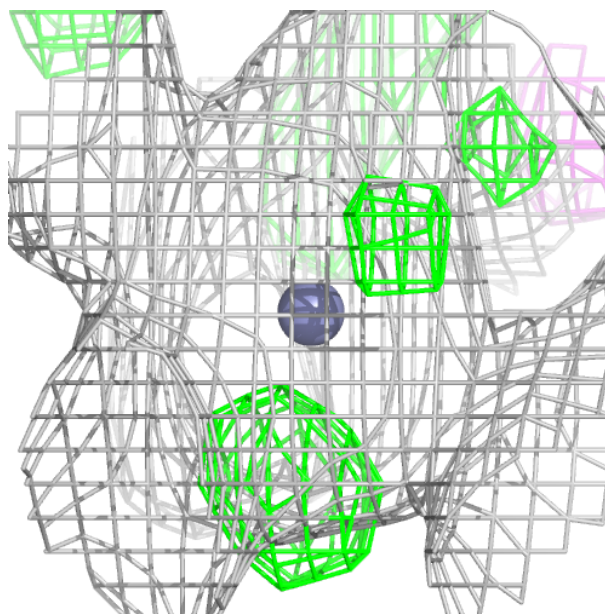
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





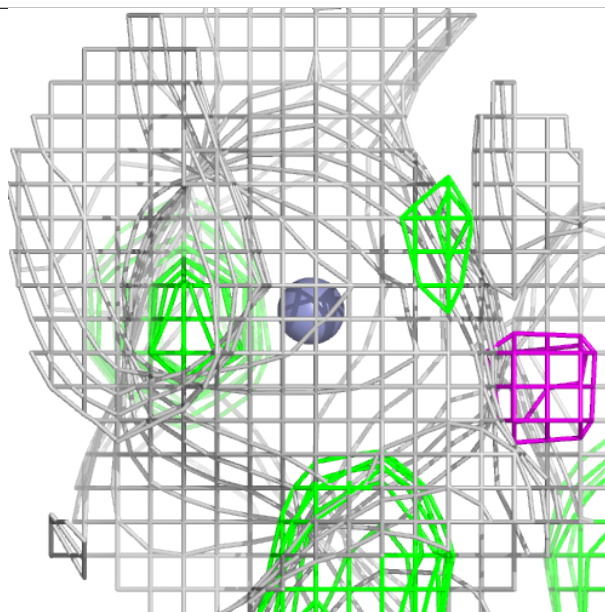
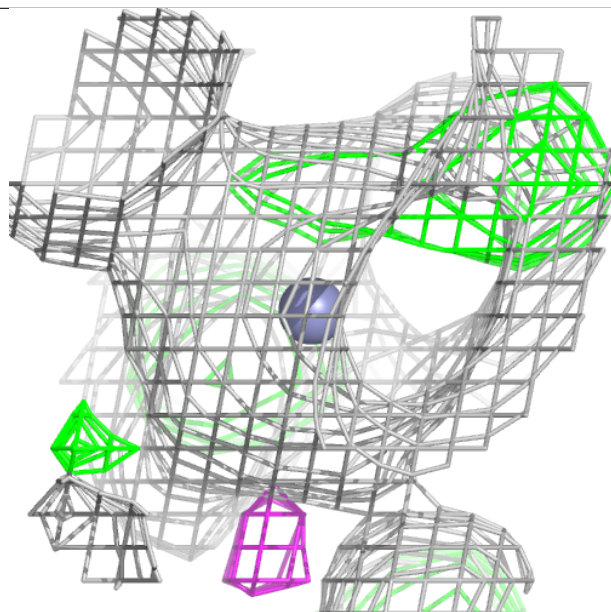
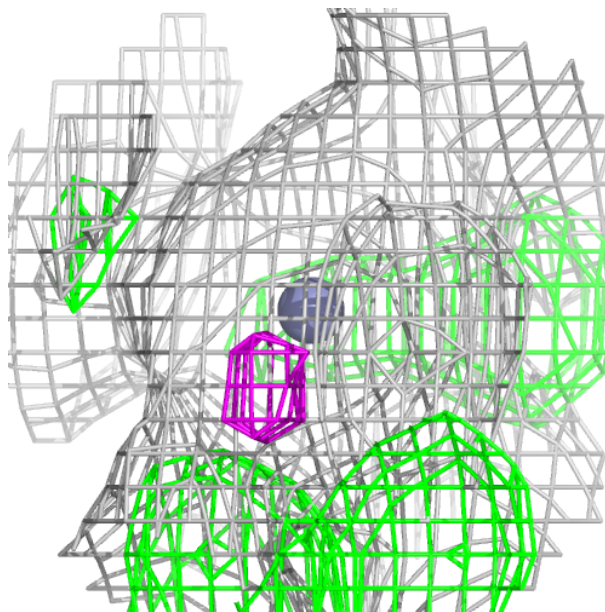
**Electron density around ZN C 405:**

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



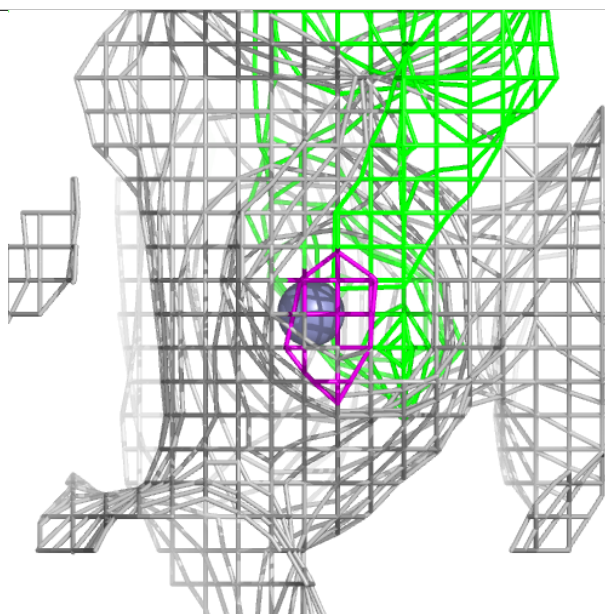
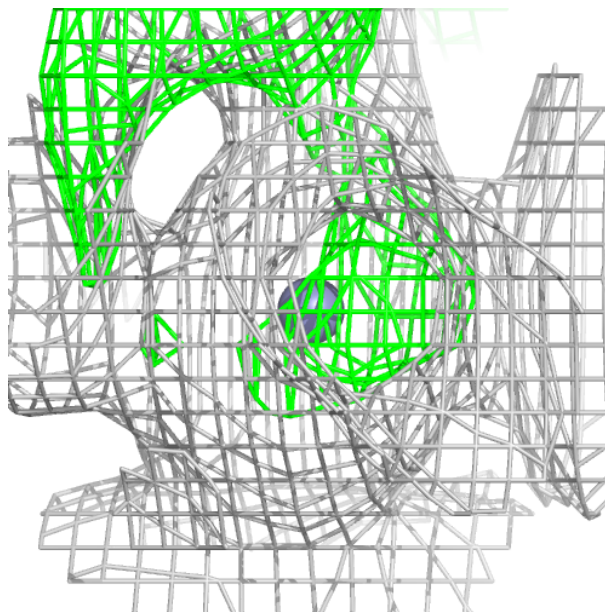
**Electron density around ZN A 402:**

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



**Electron density around ZN B 408:**

$2mF_o-DF_c$  (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.