



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:22 PM UTC

PDB ID : 8UW6 / pdb_00008uw6
Title : Acetylornithine deacetylase from Escherichia coli, di-zinc form.
Authors : Osipiuk, J.; Endres, M.; Kelley, E.; Becker, D.P.; Joachimiak, A.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2023-11-06
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

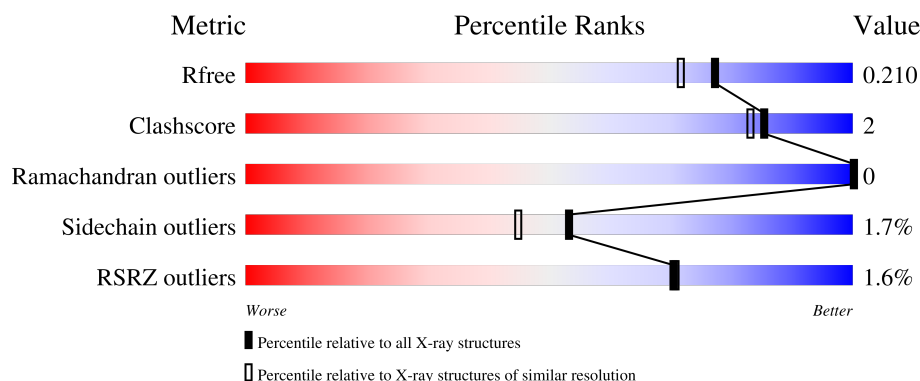
1 Overall quality at a glance

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	386	91% 7% ..
1	B	386	91% 8% ..
1	C	386	94% ..
1	D	386	4% 91% 7% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13422 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 Acetylornithine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	12	0
			3033	1933	520	567	13			
1	B	381	Total	C	N	O	S	0	17	0
			3083	1967	533	570	13			
1	C	380	Total	C	N	O	S	0	4	0
			2985	1898	517	557	13			
1	D	381	Total	C	N	O	S	0	9	0
			3020	1922	521	564	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	cloning artifact	UNP Q8X742
A	-1	ASN	-	cloning artifact	UNP Q8X742
A	0	ALA	-	cloning artifact	UNP Q8X742
B	-2	SER	-	cloning artifact	UNP Q8X742
B	-1	ASN	-	cloning artifact	UNP Q8X742
B	0	ALA	-	cloning artifact	UNP Q8X742
C	-2	SER	-	cloning artifact	UNP Q8X742
C	-1	ASN	-	cloning artifact	UNP Q8X742
C	0	ALA	-	cloning artifact	UNP Q8X742
D	-2	SER	-	cloning artifact	UNP Q8X742
D	-1	ASN	-	cloning artifact	UNP Q8X742
D	0	ALA	-	cloning artifact	UNP Q8X742

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

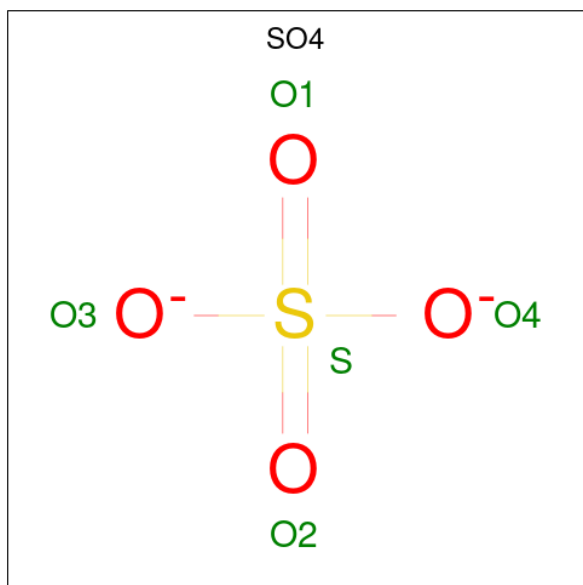
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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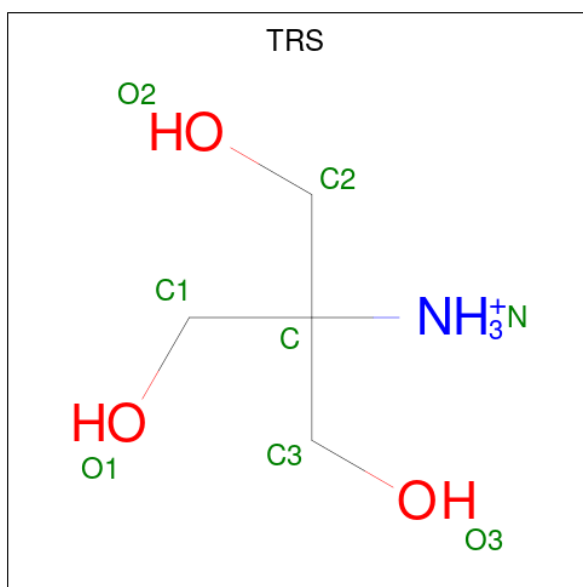
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	C	2	Total	Zn	0	0
			2	2		
2	D	3	Total	Zn	0	0
			3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



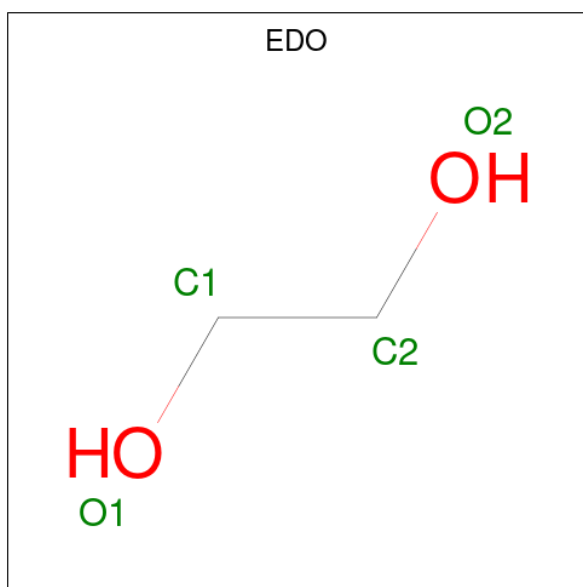
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	C	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

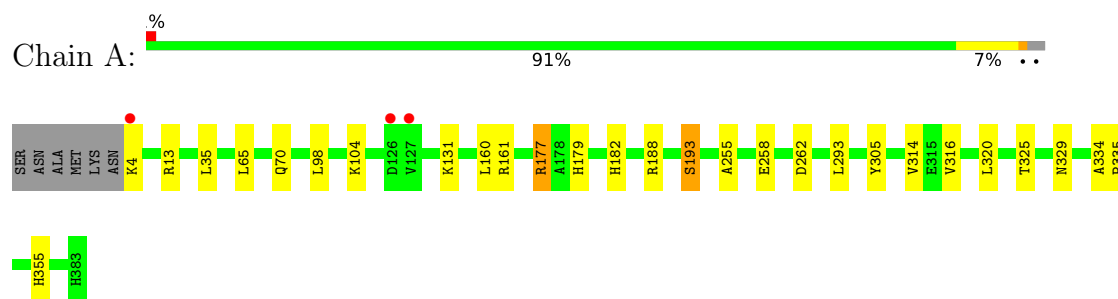
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	374	Total	O	0	0
			374	374		
6	B	269	Total	O	0	3
			269	269		
6	C	348	Total	O	0	0
			348	348		
6	D	219	Total	O	0	0
			219	219		

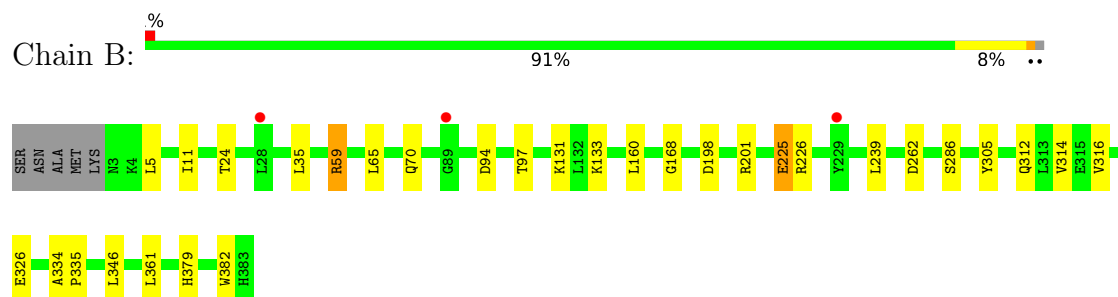
3 Residue-property plots [i](#)

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.

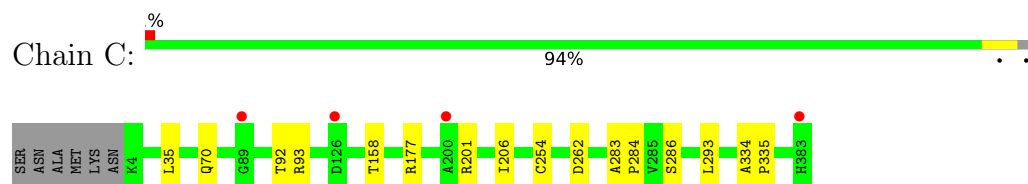
- Molecule 1: Acetylornithine deacetylase



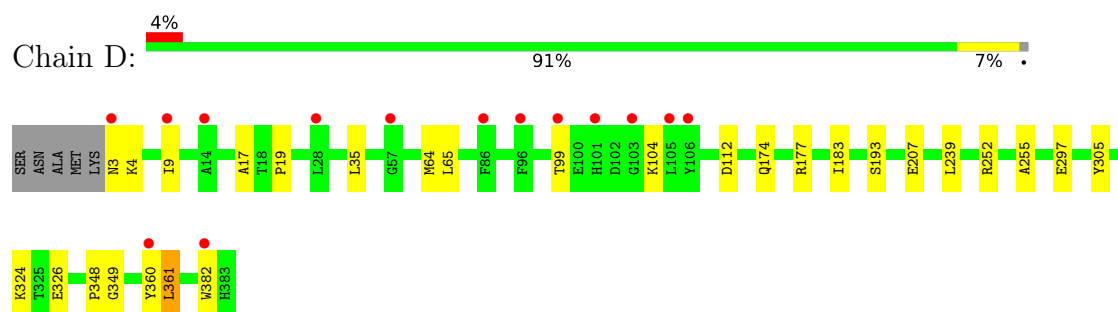
- Molecule 1: Acetylornithine deacetylase



- Molecule 1: Acetylornithine deacetylase



- Molecule 1: Acetylornithine deacetylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.40Å 126.32Å 123.41Å 90.00° 90.88° 90.00°	Depositor
Resolution (Å)	48.54 – 1.80 48.54 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.54-1.80) 97.6 (48.54-1.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.163 , 0.203 0.173 , 0.210	Depositor DCC
R_{free} test set	7260 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k 0.000 for -h,l,k 0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13422	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, ZN, TRS, 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	0.67	0/3147	0.97	4/4288 (0.1%)
1	B	0.62	0/3216	0.95	1/4380 (0.0%)
1	C	0.65	0/3075	0.99	2/4193 (0.0%)
1	D	0.64	1/3125 (0.0%)	0.96	1/4262 (0.0%)
All	All	0.64	1/12563 (0.0%)	0.97	8/17123 (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	2
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	112	ASP	CG-OD1	5.38	1.35	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	5.88	124.50	119.20
1	A	262	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	262	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	193	SER	N-CA-CB	5.49	117.95	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	HIS	CA-CB-CG	5.40	119.20	113.80
1	C	262	ASP	CA-CB-CG	5.25	117.85	112.60
1	D	297	GLU	CB-CA-C	5.20	118.31	109.53
1	C	92	THR	N-CA-C	-5.00	106.60	113.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	177	ARG	Sidechain
1	B	59[A]	ARG	Sidechain
1	B	59[B]	ARG	Sidechain
1	C	177	ARG	Sidechain
1	D	177	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	3033	0	3006	17	0
1	B	3083	0	3077	15	0
1	C	2985	0	2940	9	0
1	D	3020	0	2986	12	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
3	A	15	0	0	1	0
3	C	10	0	0	0	0
4	A	8	0	10	0	0
4	B	16	0	22	0	0
4	C	8	0	10	0	0
4	D	16	0	22	0	0
5	A	4	0	6	1	0
5	C	4	0	6	0	0
6	A	374	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	269	0	0	3	0
6	C	348	0	0	5	0
6	D	219	0	0	2	0
All	All	13422	0	12085	54	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 2.

All (54) 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:70:GLN:NE2	6:A:605:HOH:O	2.31	0.62
1:A:329:ASN:HB3	6:A:853:HOH:O	2.06	0.56
1:D:348:PRO:HB2	1:D:361:LEU:HD11	1.89	0.53
1:D:349:GLY:CA	1:D:361:LEU:HD12	2.39	0.52
1:D:349:GLY:HA3	1:D:361:LEU:HD12	1.92	0.52
1:A:70:GLN:HG2	6:A:639:HOH:O	2.10	0.50
1:D:104:LYS:HD3	1:D:360:TYR:CE1	2.46	0.50
1:B:65[A]:LEU:HD21	1:B:160:LEU:HD11	1.94	0.50
1:A:104:LYS:HD2	6:A:610:HOH:O	2.11	0.50
1:A:13[B]:ARG:HG3	1:A:98:LEU:HD23	1.95	0.49
1:C:206:ILE:HG13	1:C:254:CYS:SG	2.53	0.49
1:A:188:ARG:HE	1:A:258[B]:GLU:CD	2.21	0.48
1:B:133[B]:LYS:HE2	1:B:382:TRP:O	2.14	0.48
1:A:131[A]:LYS:NZ	6:A:618:HOH:O	2.45	0.48
3:A:507:SO4:O4	6:A:601:HOH:O	2.18	0.48
1:D:193:SER:HB2	1:D:255:ALA:HB2	1.96	0.47
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.97	0.47
1:B:24:THR:O	1:B:59[A]:ARG:NH2	2.41	0.47
1:B:133[B]:LYS:CE	1:B:382:TRP:O	2.62	0.47
1:A:320[A]:LEU:HG	6:A:740:HOH:O	2.14	0.46
1:C:93:ARG:HA	6:C:661:HOH:O	2.15	0.46
1:C:334:ALA:N	1:C:335:PRO:CD	2.79	0.46
1:D:17:ALA:O	1:D:19:PRO:HD3	2.16	0.45
1:D:324:LYS:HE2	1:D:326:GLU:OE2	2.16	0.45
1:D:252:ARG:HD3	6:D:781:HOH:O	2.16	0.45
1:B:326[B]:GLU:OE1	6:B:601:HOH:O	2.21	0.44
1:A:193:SER:HB2	1:A:255:ALA:HB2	1.99	0.44
1:C:158:THR:O	6:C:601:HOH:O	2.21	0.44
1:B:334:ALA:N	1:B:335:PRO:CD	2.81	0.43
1:D:239:LEU:C	1:D:239:LEU:HD23	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLY:HA2	1:B:346:LEU:O	2.18	0.43
1:B:225[A]:GLU:HG3	1:B:226:ARG:HG3	1.99	0.43
1:B:131:LYS:HE3	6:B:837:HOH:O	2.19	0.43
1:A:314:VAL:HG13	1:A:325:THR:CG2	2.49	0.43
1:B:239:LEU:C	1:B:239:LEU:HD23	2.43	0.43
1:C:293:LEU:C	1:C:293:LEU:HD23	2.45	0.42
1:A:355:HIS:CD2	1:A:355:HIS:N	2.88	0.42
1:C:70:GLN:HA	6:C:678:HOH:O	2.19	0.42
1:A:65:LEU:HD21	1:A:160:LEU:HD11	2.01	0.42
1:B:5:LEU:HG	1:B:11:ILE:HD11	2.00	0.42
1:A:182:HIS:ND1	5:A:506:EDO:H21	2.34	0.42
1:A:293:LEU:C	1:A:293:LEU:HD23	2.45	0.42
1:B:314:VAL:HG21	6:B:746:HOH:O	2.20	0.42
1:D:9:ILE:HD12	1:D:9:ILE:HA	1.93	0.42
1:D:64:MET:HG2	1:D:65:LEU:N	2.35	0.41
1:D:207:GLU:OE1	6:D:601:HOH:O	2.22	0.41
1:B:94:ASP:OD2	1:B:97:THR:OG1	2.38	0.41
1:B:198:ASP:OD2	1:B:201[B]:ARG:HD2	2.21	0.41
1:A:316:VAL:O	1:A:320[A]:LEU:HG	2.20	0.40
1:A:334:ALA:N	1:A:335:PRO:CD	2.84	0.40
1:C:93:ARG:CA	6:C:661:HOH:O	2.68	0.40
1:C:93:ARG:HB3	6:C:661:HOH:O	2.20	0.40
1:B:316:VAL:HG21	1:B:379[B]:HIS:CD2	2.57	0.40

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	390/386 (101%)	385 (99%)	5 (1%)	0	100	100
1	B	397/386 (103%)	392 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	382/386 (99%)	375 (98%)	7 (2%)	0	100	100
1	D	388/386 (100%)	379 (98%)	9 (2%)	0	100	100
All	All	1557/1544 (101%)	1531 (98%)	26 (2%)	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	331/324 (102%)	328 (99%)	3 (1%)	70	67
1	B	338/324 (104%)	329 (97%)	9 (3%)	39	27
1	C	323/324 (100%)	319 (99%)	4 (1%)	63	57
1	D	329/324 (102%)	319 (97%)	10 (3%)	36	24
All	All	1321/1296 (102%)	1295 (98%)	26 (2%)	53	38

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	35	LEU
1	A	305	TYR
1	B	35	LEU
1	B	70	GLN
1	B	225[A]	GLU
1	B	225[B]	GLU
1	B	286	SER
1	B	305	TYR
1	B	312[A]	GLN
1	B	312[B]	GLN
1	B	361	LEU
1	C	35	LEU
1	C	201	ARG

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Mol	Chain	Res	Type
1	C	286[A]	SER
1	C	286[B]	SER
1	D	3	ASN
1	D	4	LYS
1	D	35	LEU
1	D	99	THR
1	D	174[A]	GLN
1	D	174[B]	GLN
1	D	183	ILE
1	D	305	TYR
1	D	361	LEU
1	D	382	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	53	GLN
1	A	329	ASN
1	A	356	GLN
1	A	383	HIS
1	B	70	GLN
1	B	174	GLN
1	B	210	HIS
1	B	218	GLN
1	B	245	HIS
1	B	272	ASN
1	B	338	GLN
1	C	53	GLN
1	C	192	GLN
1	D	190	GLN
1	D	218	GLN
1	D	329	ASN

5.3.3 RNA ⓘ

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 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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	C	503	-	4,4,4	0.34	0	6,6,6	0.23	0
4	TRS	C	504	2	7,7,7	0.38	0	9,9,9	0.36	0
3	SO4	C	506	-	4,4,4	0.35	0	6,6,6	0.17	0
3	SO4	A	503	-	4,4,4	0.36	0	6,6,6	0.22	0
3	SO4	A	507	-	4,4,4	0.39	0	6,6,6	0.11	0
4	TRS	D	505	-	7,7,7	0.10	0	9,9,9	0.36	0
5	EDO	C	505	-	3,3,3	0.20	0	2,2,2	0.31	0
4	TRS	D	504	2	7,7,7	0.22	0	9,9,9	0.48	0
5	EDO	A	506	-	3,3,3	0.12	0	2,2,2	0.41	0
4	TRS	B	505	-	7,7,7	0.15	0	9,9,9	0.46	0
3	SO4	A	504	-	4,4,4	0.34	0	6,6,6	0.08	0
4	TRS	A	505	2	7,7,7	0.25	0	9,9,9	0.32	0
4	TRS	B	504	2	7,7,7	0.23	0	9,9,9	0.32	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
4	TRS	C	504	2	-	1/9/9/9	-
4	TRS	D	505	-	-	9/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	505	-	-	0/1/1/1	-
4	TRS	D	504	2	-	4/9/9/9	-
5	EDO	A	506	-	-	1/1/1/1	-
4	TRS	B	505	-	-	6/9/9/9	-
4	TRS	A	505	2	-	0/9/9/9	-
4	TRS	B	504	2	-	1/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	506	EDO	O1-C1-C2-O2
4	B	505	TRS	N-C-C1-O1
4	B	505	TRS	N-C-C3-O3
4	D	504	TRS	N-C-C3-O3
4	D	505	TRS	C2-C-C1-O1
4	D	505	TRS	N-C-C1-O1
4	D	505	TRS	C1-C-C3-O3
4	D	505	TRS	N-C-C3-O3
4	B	505	TRS	C2-C-C1-O1
4	B	505	TRS	C3-C-C1-O1
4	B	505	TRS	C1-C-C3-O3
4	B	505	TRS	C2-C-C3-O3
4	D	505	TRS	C3-C-C1-O1
4	D	505	TRS	C3-C-C2-O2
4	D	505	TRS	C2-C-C3-O3
4	D	504	TRS	C1-C-C3-O3
4	B	504	TRS	C3-C-C1-O1
4	C	504	TRS	C1-C-C3-O3
4	D	504	TRS	C3-C-C2-O2
4	D	504	TRS	N-C-C2-O2
4	D	505	TRS	C1-C-C2-O2
4	D	505	TRS	N-C-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	SO4	1	0
5	A	506	EDO	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	380/386 (98%)	-0.38	3 (0%) 82 83	9, 20, 39, 54	12 (3%)
1	B	381/386 (98%)	-0.16	3 (0%) 82 83	9, 24, 41, 63	17 (4%)
1	C	380/386 (98%)	-0.26	4 (1%) 78 78	12, 22, 42, 64	4 (1%)
1	D	381/386 (98%)	0.32	14 (3%) 45 45	15, 29, 57, 78	9 (2%)
All	All	1522/1544 (98%)	-0.12	24 (1%) 70 71	9, 24, 47, 78	42 (2%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	382	TRP	3.7
1	D	99	THR	3.6
1	D	103	GLY	3.4
1	B	229	TYR	3.0
1	A	127	VAL	2.9
1	D	9	ILE	2.5
1	D	105	LEU	2.5
1	A	126	ASP	2.4
1	D	3	ASN	2.4
1	C	126	ASP	2.4
1	D	106	TYR	2.4
1	B	28	LEU	2.3
1	D	28	LEU	2.3
1	D	360	TYR	2.3
1	C	383	HIS	2.3
1	D	57	GLY	2.3
1	D	86	PHE	2.2
1	D	96	PHE	2.2
1	B	89	GLY	2.2
1	C	200	ALA	2.2
1	D	101	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	4	LYS	2.1
1	C	89	GLY	2.1
1	D	14	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TRS	D	505	8/8	0.80	0.14	23,26,29,29	8
5	EDO	C	505	4/4	0.81	0.16	37,42,44,51	0
5	EDO	A	506	4/4	0.84	0.12	44,44,48,53	0
4	TRS	C	504	8/8	0.91	0.10	12,19,22,24	0
3	SO4	C	503	5/5	0.91	0.10	35,37,38,38	5
4	TRS	A	505	8/8	0.91	0.10	12,16,18,18	8
4	TRS	B	505	8/8	0.91	0.10	25,32,35,35	0
4	TRS	D	504	8/8	0.92	0.09	26,31,32,36	0
2	ZN	D	503	1/1	0.93	0.08	43,43,43,43	0
3	SO4	C	506	5/5	0.93	0.08	40,43,44,49	5
3	SO4	A	504	5/5	0.93	0.07	44,46,49,50	5
3	SO4	A	507	5/5	0.94	0.07	37,46,47,49	0
4	TRS	B	504	8/8	0.94	0.09	17,24,25,27	8
3	SO4	A	503	5/5	0.97	0.06	25,28,30,31	5
2	ZN	D	502	1/1	0.98	0.03	26,26,26,26	1
2	ZN	D	501	1/1	1.00	0.02	25,25,25,25	0
2	ZN	A	501	1/1	1.00	0.01	13,13,13,13	0
2	ZN	A	502	1/1	1.00	0.01	17,17,17,17	1
2	ZN	B	501	1/1	1.00	0.01	18,18,18,18	0
2	ZN	B	502	1/1	1.00	0.02	22,22,22,22	1

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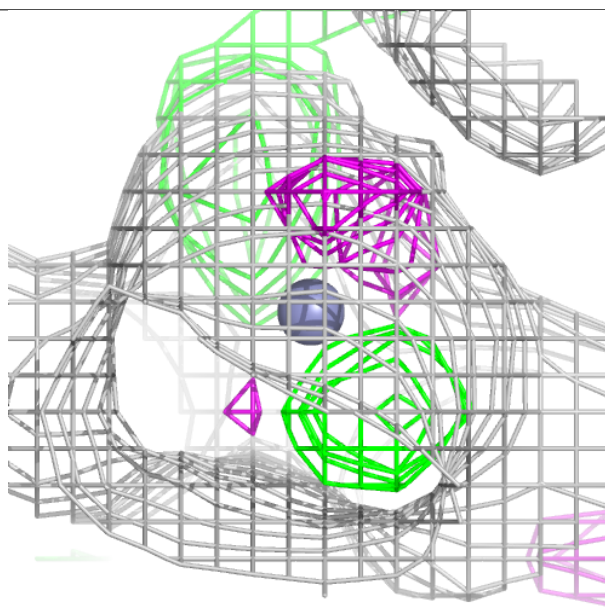
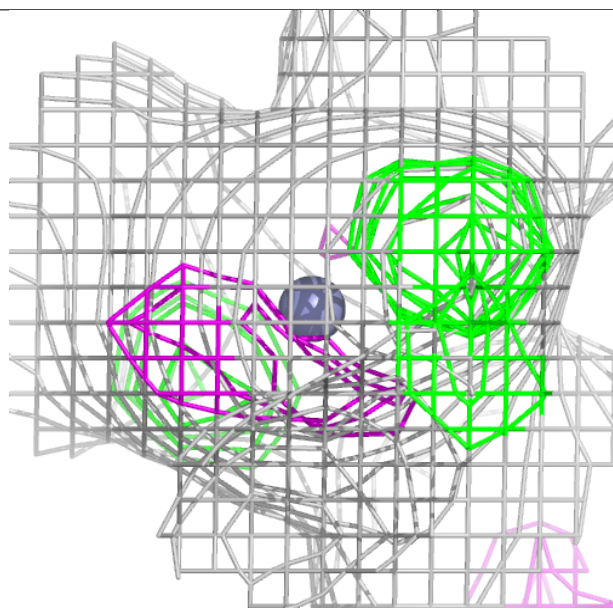
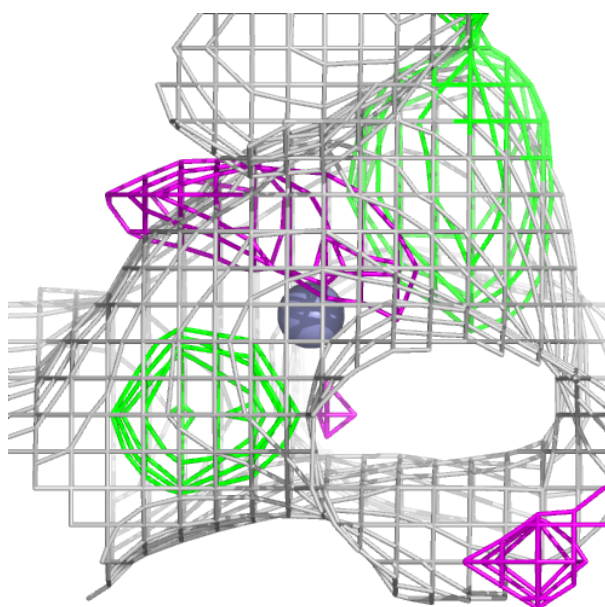
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	503	1/1	1.00	0.02	21,21,21,21	0
2	ZN	C	501	1/1	1.00	0.01	14,14,14,14	0
2	ZN	C	502	1/1	1.00	0.02	19,19,19,19	1

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.

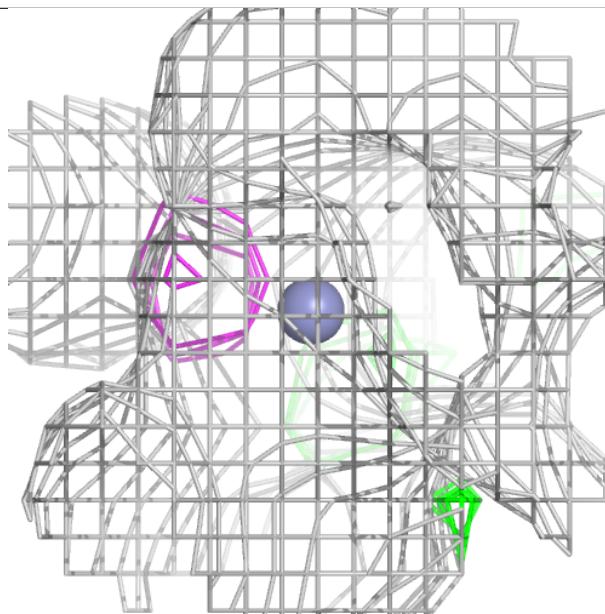
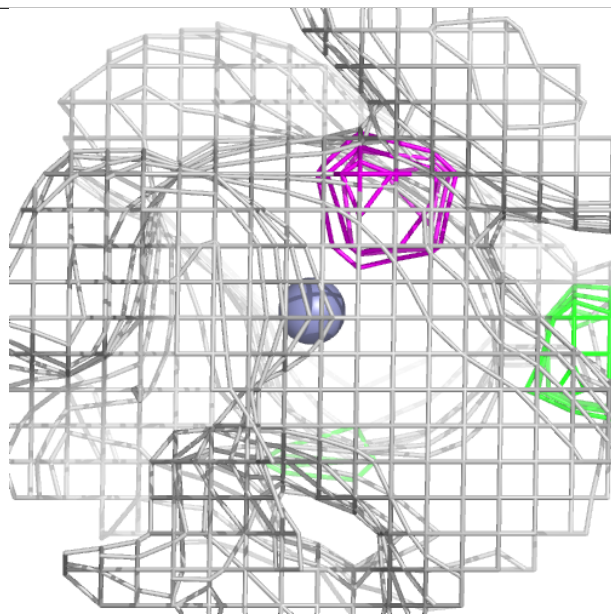
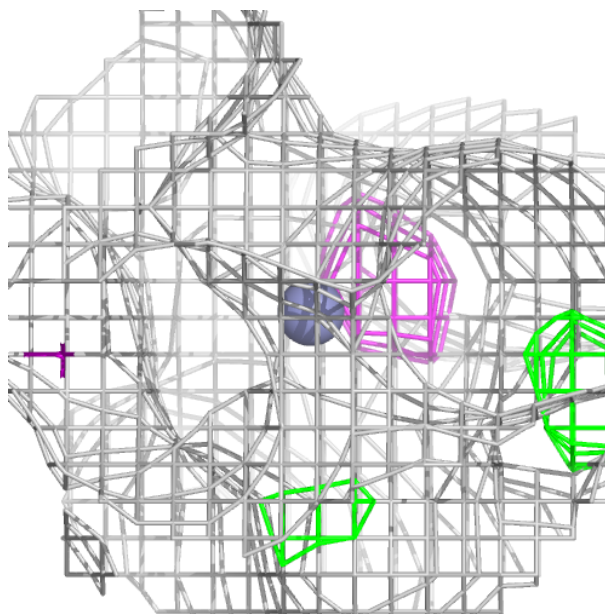
Electron density around ZN D 503:

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



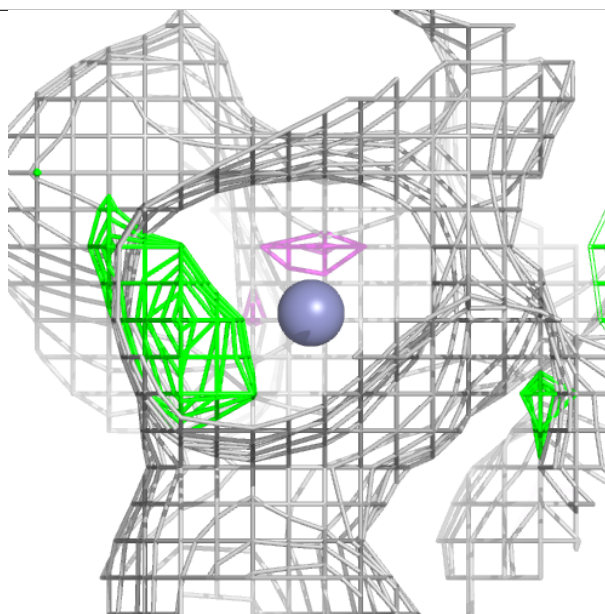
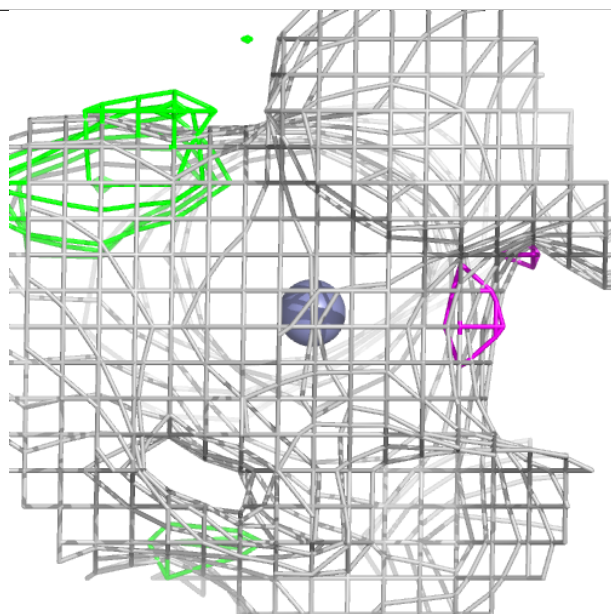
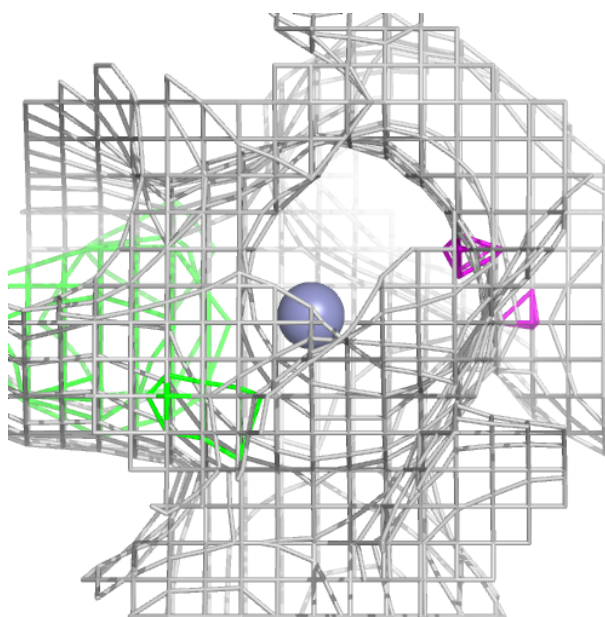
Electron density around ZN D 502:

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



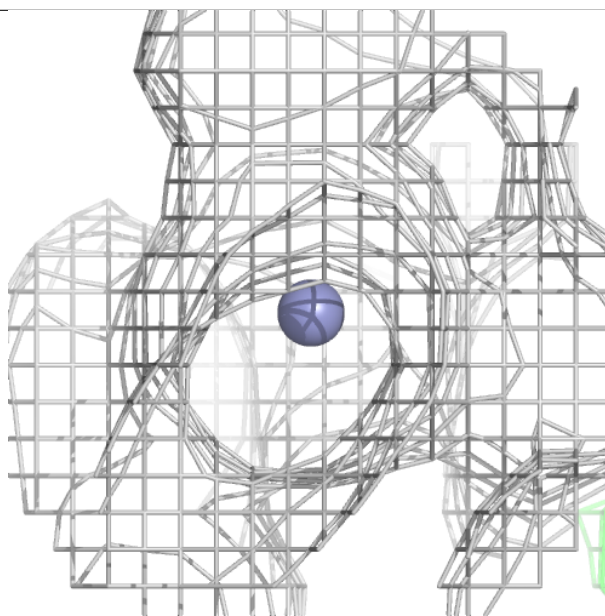
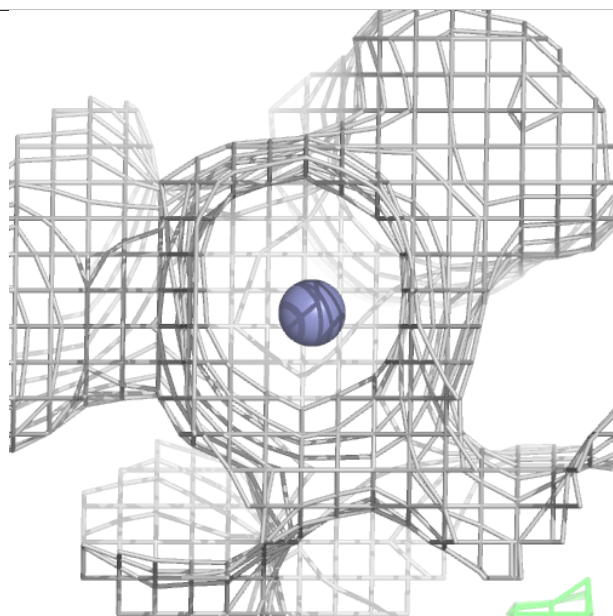
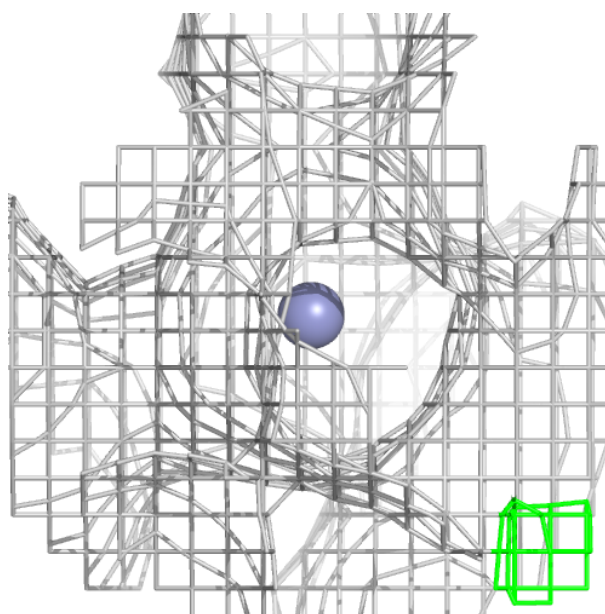
Electron density around ZN D 501:

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and green (positive)



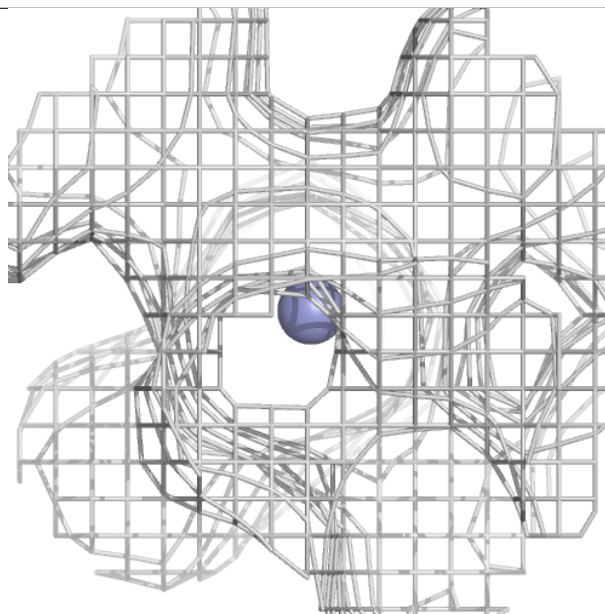
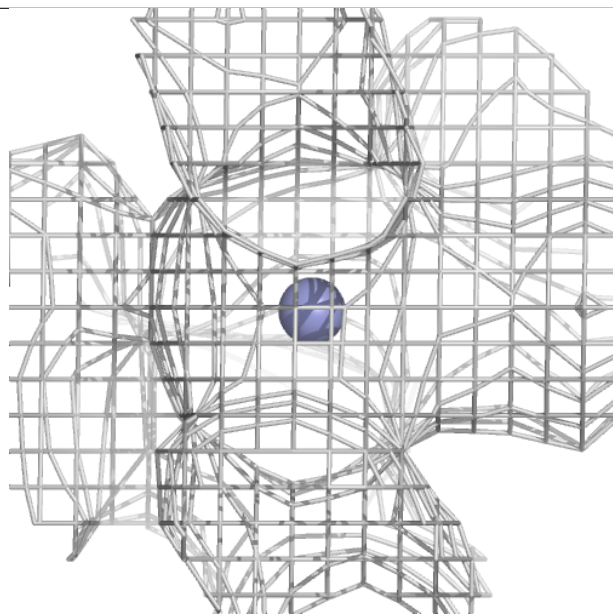
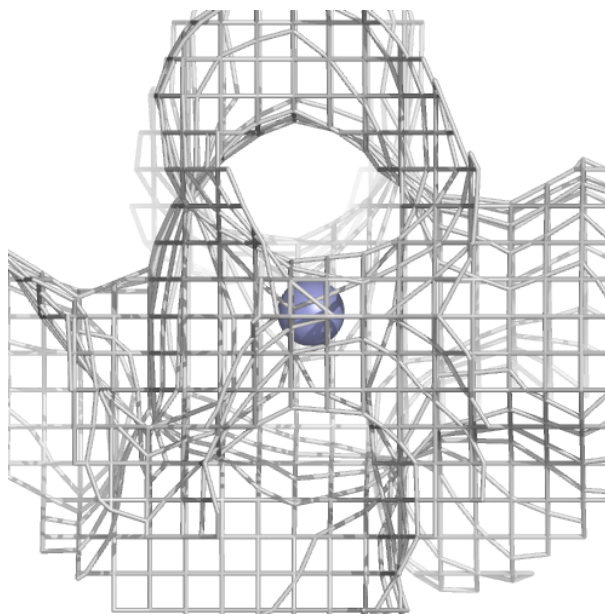
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



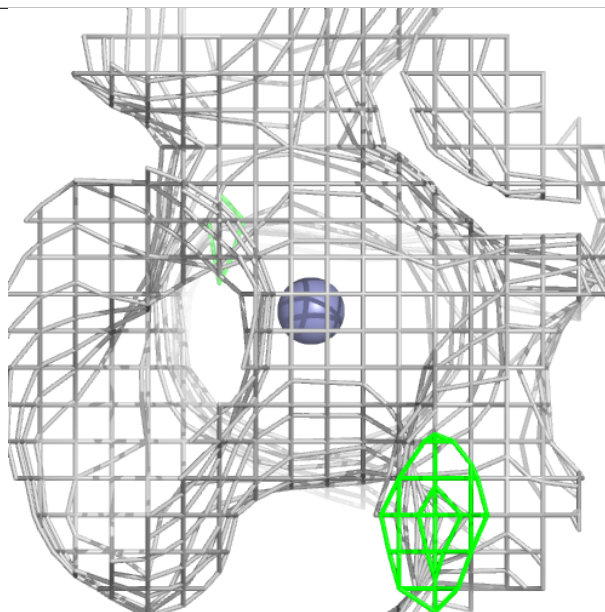
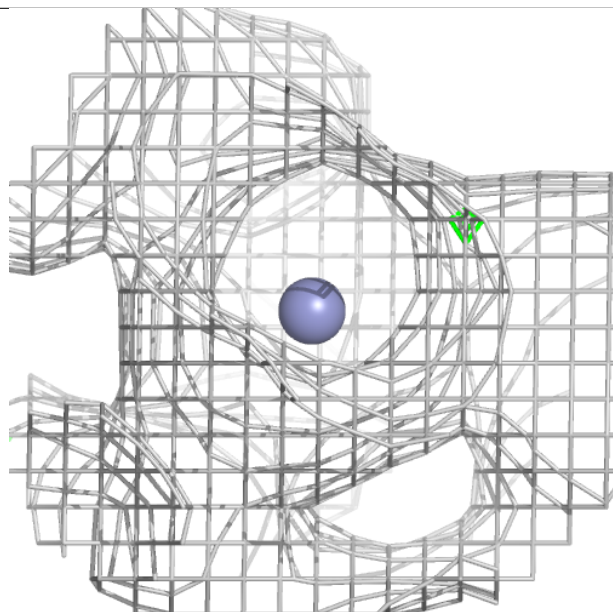
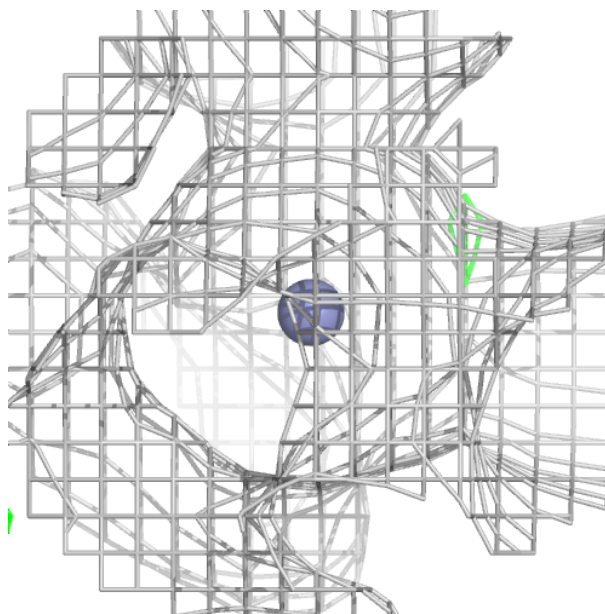
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and green (positive)



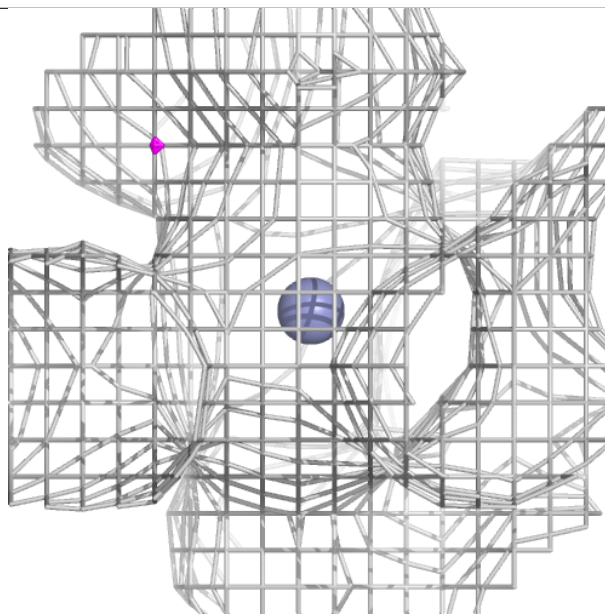
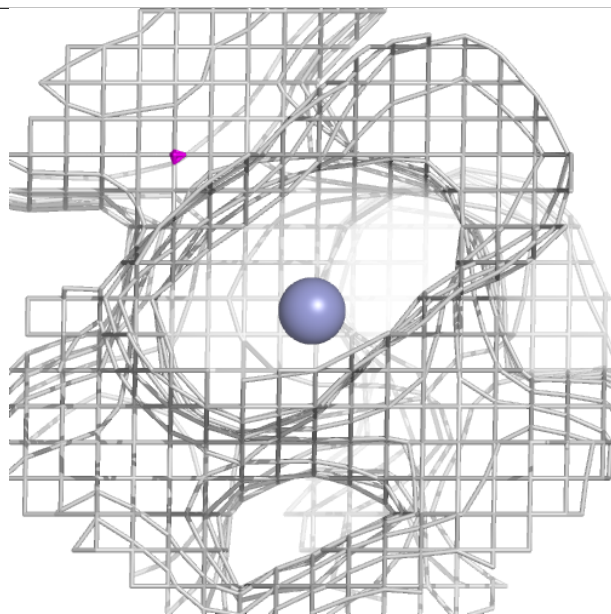
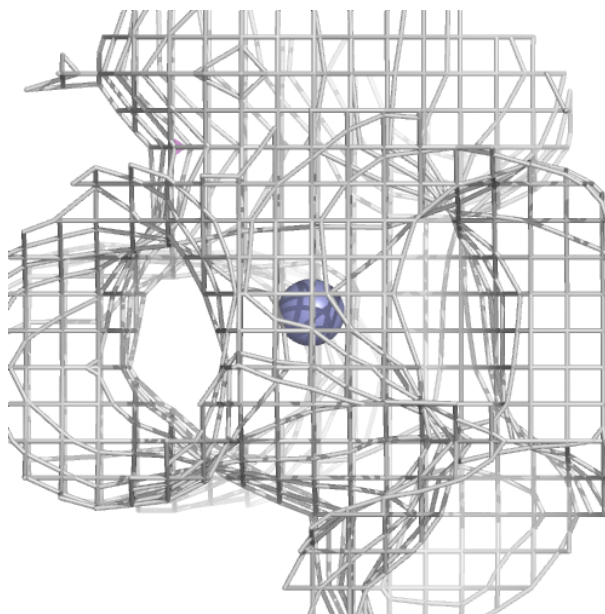
Electron density around ZN B 501:

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



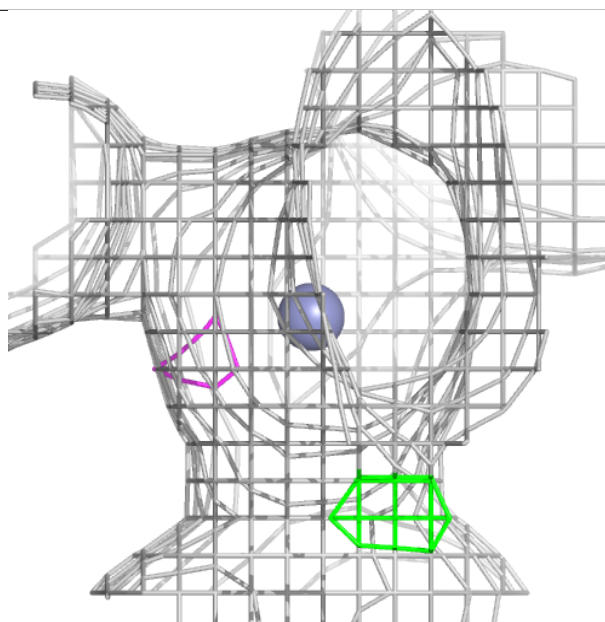
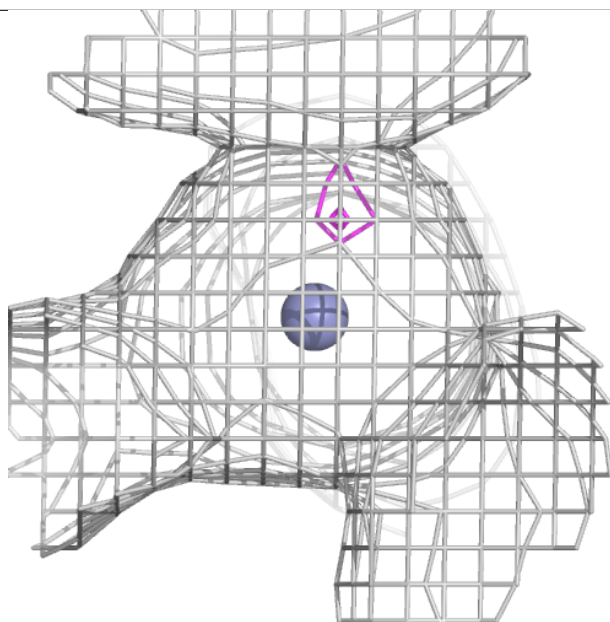
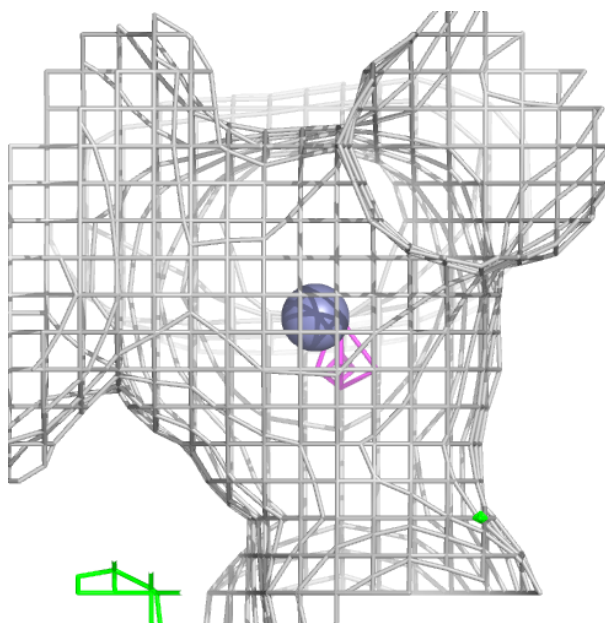
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



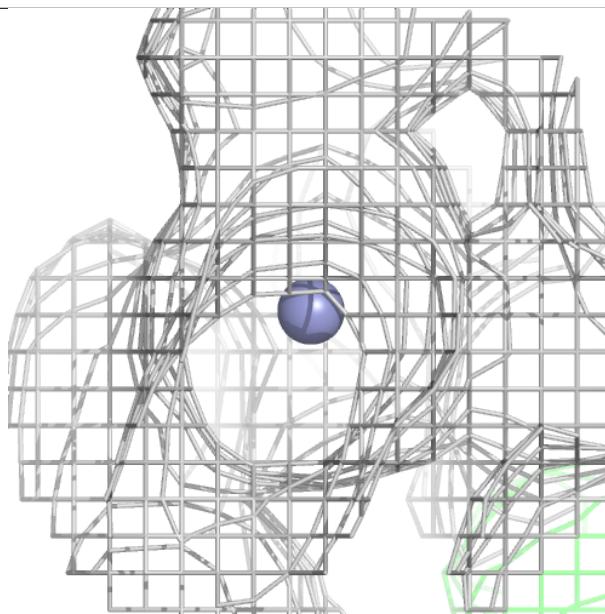
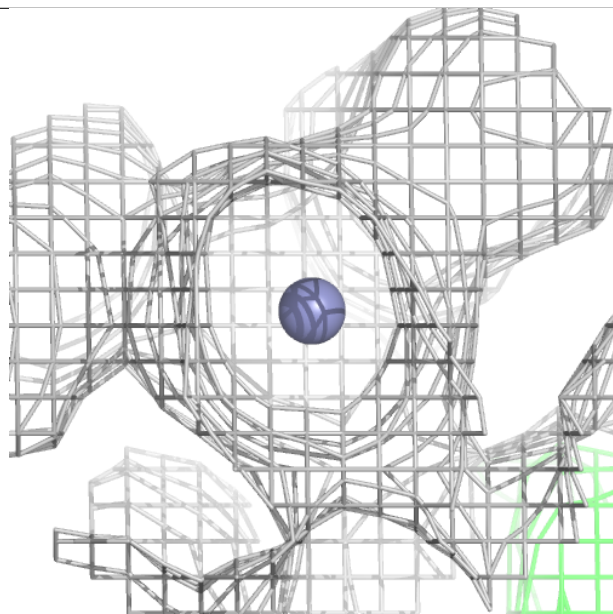
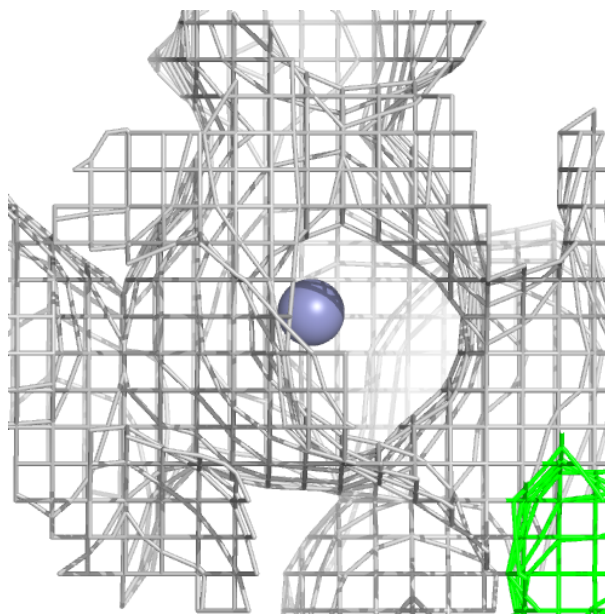
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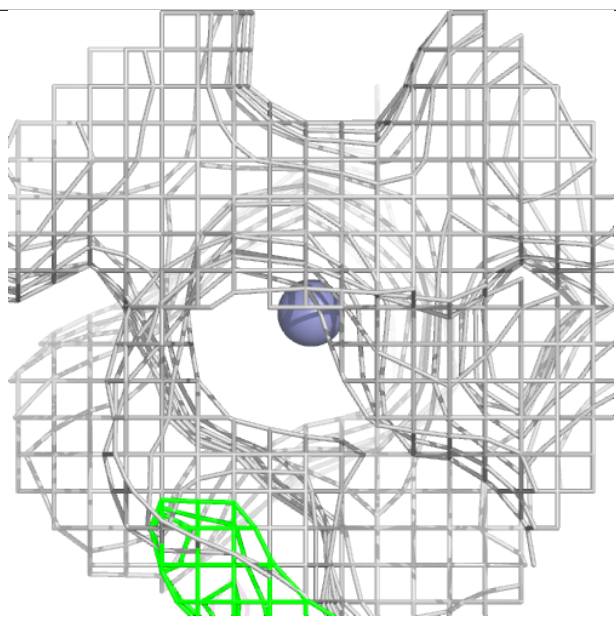
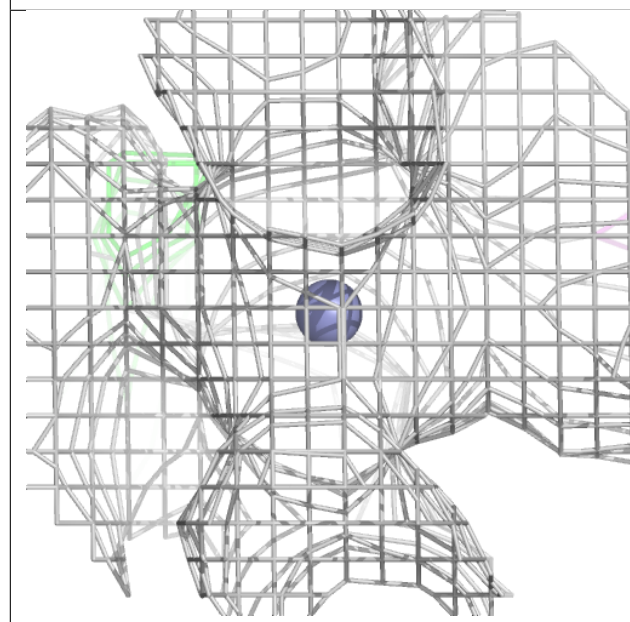
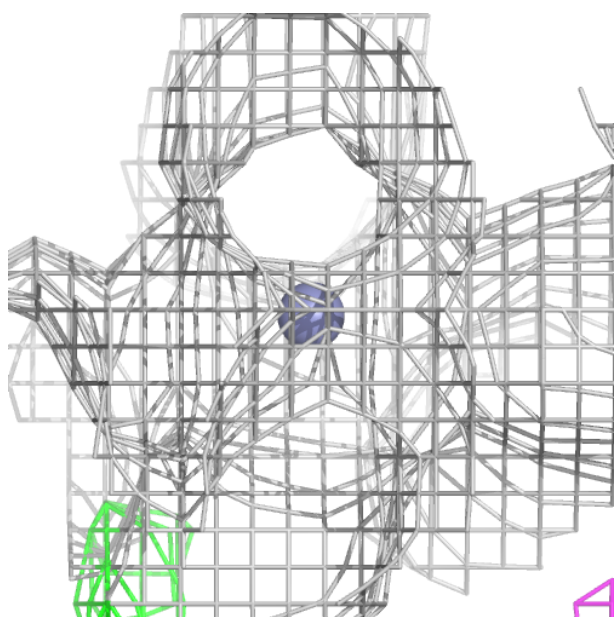
Electron density around ZN C 501:

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and green (positive)



Electron density around ZN C 502:

$2mF_o-DF_c$ (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.