



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:12 PM UTC

PDB ID : 7NE9 / pdb_00007ne9
Title : A single sensor controls large variations in zinc quotas in a marine cyanobacterium
Authors : Fulop, V.
Deposited on : 2021-02-03
Resolution : 2.10 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

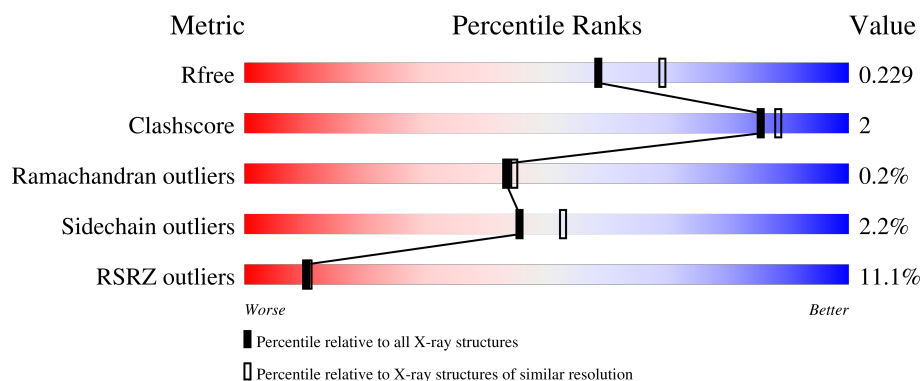
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	AAA	134	9% 84% 5% 10%
1	BBB	134	10% 85% • 10%
1	CCC	134	10% 82% 5% • 12%
1	DDD	134	10% 82% 7% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3865 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.

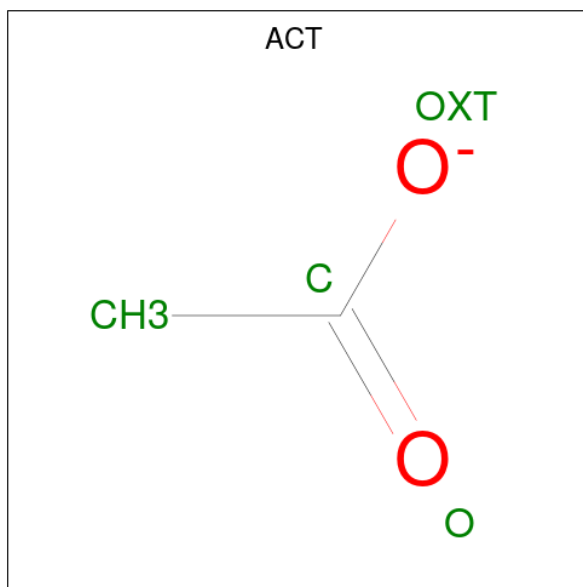
- Molecule 1 is a protein called Ferric uptake regulator family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	120	Total	C	N	O	S	0	0	0
			931	574	175	173	9			
1	BBB	120	Total	C	N	O	S	0	0	0
			931	574	175	173	9			
1	CCC	118	Total	C	N	O	S	0	0	0
			919	566	173	171	9			
1	DDD	120	Total	C	N	O	S	0	0	0
			931	574	175	173	9			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	2	Total	Zn	0	0
			2	2		
2	BBB	3	Total	Zn	0	0
			3	3		
2	CCC	2	Total	Zn	0	0
			2	2		
2	DDD	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			4	2	2		

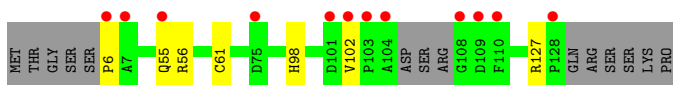
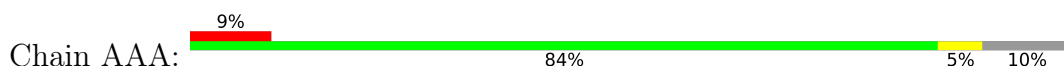
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	37	Total	O	0	0
			37	37		
4	BBB	33	Total	O	0	0
			33	33		
4	CCC	32	Total	O	0	0
			32	32		
4	DDD	38	Total	O	0	0
			38	38		

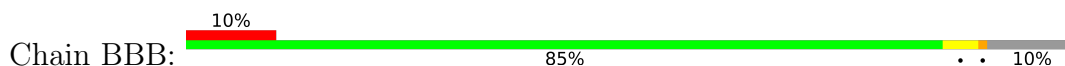
3 Residue-property plots [i](#)

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.

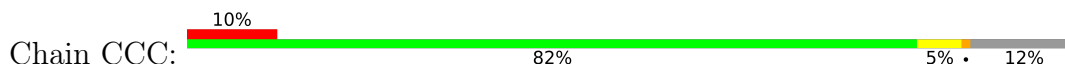
- Molecule 1: Ferric uptake regulator family



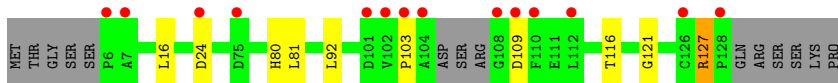
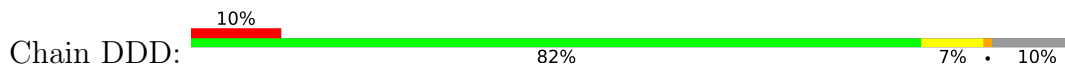
- Molecule 1: Ferric uptake regulator family



- Molecule 1: Ferric uptake regulator family



- Molecule 1: Ferric uptake regulator family



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.25Å 129.25Å 77.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.62 – 2.10 64.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.62-2.10) 99.9 (64.62-2.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.194 , 0.218 0.209 , 0.229	Depositor DCC
R_{free} test set	1650 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3865	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: ACT, ZN

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	AAA	1.01	0/949	1.25	0/1284
1	BBB	1.02	0/949	1.30	0/1284
1	CCC	1.04	0/936	1.30	1/1265 (0.1%)
1	DDD	1.02	1/949 (0.1%)	1.31	0/1284
All	All	1.02	1/3783 (0.0%)	1.29	1/5117 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	80	HIS	CE1-NE2	5.53	1.38	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	75	ASP	CA-CB-CG	6.66	119.26	112.60

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	AAA	931	0	893	3	0
1	BBB	931	0	893	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	919	0	881	7	0
1	DDD	931	0	893	6	0
2	AAA	2	0	0	0	0
2	BBB	3	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	2	0	0	0	0
3	BBB	4	0	3	0	0
4	AAA	37	0	0	2	0
4	BBB	33	0	0	1	0
4	CCC	32	0	0	3	0
4	DDD	38	0	0	0	0
All	All	3865	0	3563	16	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 (16) 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:CCC:116:THR:HG22	4:CCC:328:HOH:O	1.58	1.03
1:AAA:61:CYS:SG	4:AAA:336:HOH:O	2.32	0.87
4:CCC:328:HOH:O	1:DDD:116:THR:HG22	1.96	0.65
1:CCC:65:PRO:HD2	4:CCC:331:HOH:O	2.02	0.59
1:CCC:124:SER:HB3	1:DDD:109:ASP:HB3	1.88	0.54
1:CCC:111:GLU:HB2	1:DDD:127:ARG:HH21	1.73	0.53
1:BBB:51:ARG:NH1	4:BBB:301:HOH:O	2.43	0.50
1:AAA:6:PRO:O	1:AAA:56:ARG:NH2	2.41	0.48
1:BBB:81:LEU:CD1	1:BBB:92:LEU:HD21	2.44	0.48
1:CCC:81:LEU:CD1	1:CCC:92:LEU:HD21	2.47	0.44
1:AAA:98:HIS:HD2	4:AAA:301:HOH:O	2.00	0.44
1:BBB:102:VAL:CG1	1:BBB:112:LEU:HD22	2.48	0.43
1:CCC:81:LEU:HD13	1:CCC:92:LEU:HD21	1.99	0.43
1:DDD:16:LEU:HD23	1:DDD:16:LEU:HA	1.91	0.43
1:CCC:111:GLU:O	1:DDD:121:GLY:HA3	2.19	0.42
1:DDD:81:LEU:CD1	1:DDD:92:LEU:HD21	2.51	0.41

There are no symmetry-related clashes.

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	AAA	116/134 (87%)	111 (96%)	5 (4%)	0	100	100
1	BBB	116/134 (87%)	113 (97%)	3 (3%)	0	100	100
1	CCC	114/134 (85%)	111 (97%)	3 (3%)	0	100	100
1	DDD	116/134 (87%)	112 (97%)	3 (3%)	1 (1%)	14	10
All	All	462/536 (86%)	447 (97%)	14 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	103	PRO

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	AAA	101/114 (89%)	98 (97%)	3 (3%)	36	41
1	BBB	101/114 (89%)	99 (98%)	2 (2%)	48	56
1	CCC	100/114 (88%)	98 (98%)	2 (2%)	48	56
1	DDD	101/114 (89%)	99 (98%)	2 (2%)	48	56
All	All	403/456 (88%)	394 (98%)	9 (2%)	45	53

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	55	GLN
1	AAA	102	VAL
1	AAA	127	ARG
1	BBB	24	ASP
1	BBB	102	VAL
1	CCC	75	ASP
1	CCC	102	VAL
1	DDD	24	ASP
1	DDD	127	ARG

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

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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	ACT	BBB	204	-	3,3,3	1.45	0	3,3,3	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

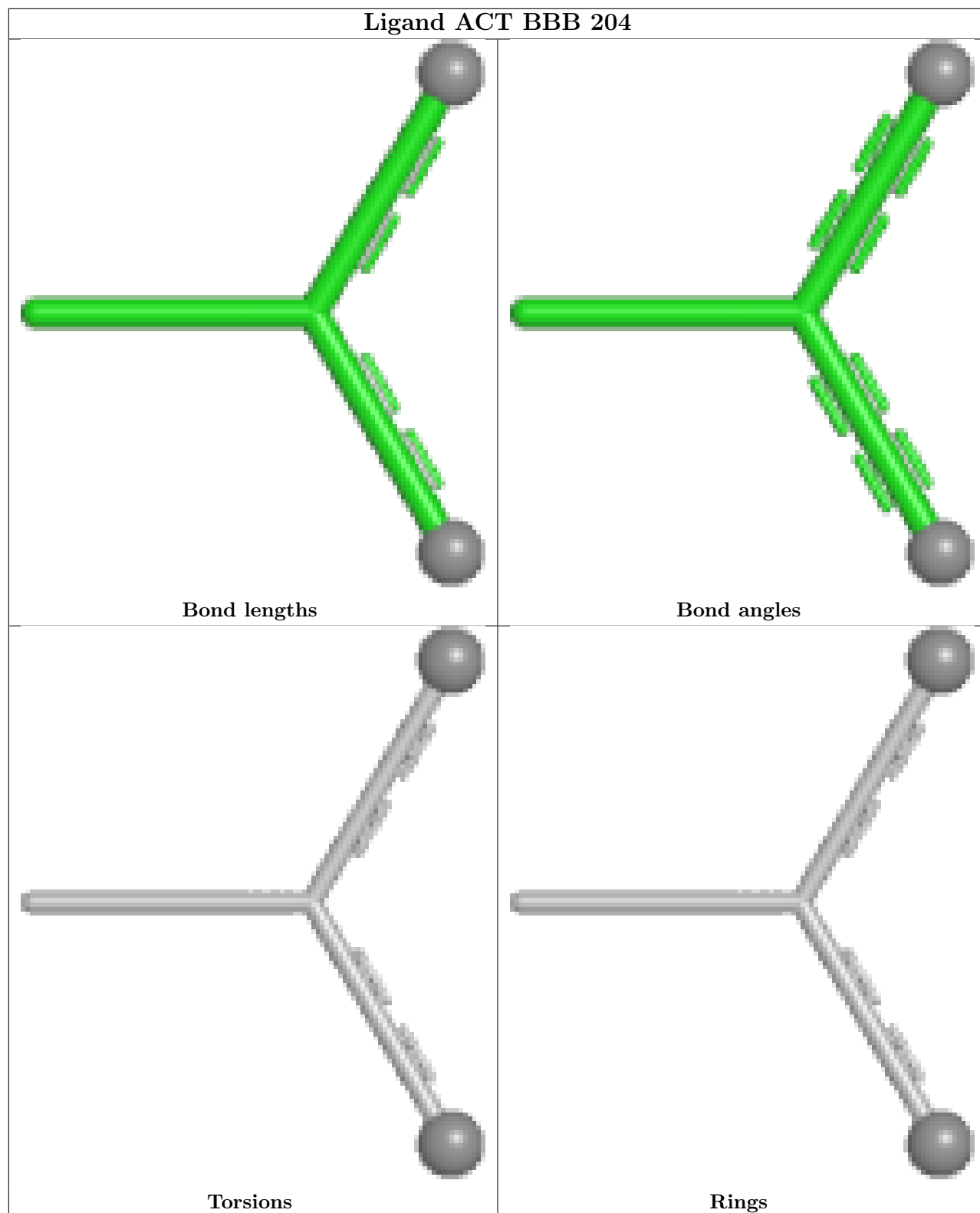
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	AAA	120/134 (89%)	0.61	12 (10%)	12 13	31, 43, 95, 110	0
1	BBB	120/134 (89%)	0.61	13 (10%)	11 11	33, 45, 96, 103	0
1	CCC	118/134 (88%)	0.74	14 (11%)	9 9	35, 50, 80, 123	0
1	DDD	120/134 (89%)	0.68	14 (11%)	9 9	34, 46, 96, 117	0
All	All	478/536 (89%)	0.66	53 (11%)	10 10	31, 47, 95, 123	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	102	VAL	8.7
1	AAA	104	ALA	7.3
1	BBB	108	GLY	6.5
1	BBB	128	PRO	6.3
1	DDD	104	ALA	6.2
1	DDD	128	PRO	6.2
1	CCC	108	GLY	6.0
1	DDD	103	PRO	5.8
1	CCC	128	PRO	5.6
1	AAA	102	VAL	5.3
1	BBB	104	ALA	5.0
1	AAA	6	PRO	5.0
1	DDD	6	PRO	5.0
1	DDD	102	VAL	4.9
1	BBB	102	VAL	4.9
1	CCC	6	PRO	4.7
1	DDD	108	GLY	4.5
1	BBB	6	PRO	4.4
1	BBB	103	PRO	4.4
1	AAA	128	PRO	4.2
1	AAA	108	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	103	PRO	4.1
1	AAA	110	PHE	3.9
1	DDD	110	PHE	3.9
1	DDD	7	ALA	3.9
1	BBB	127	ARG	3.9
1	CCC	68	GLU	3.6
1	CCC	7	ALA	3.6
1	CCC	109	ASP	3.5
1	DDD	109	ASP	3.4
1	AAA	75	ASP	3.3
1	AAA	109	ASP	3.1
1	BBB	110	PHE	2.8
1	DDD	112	LEU	2.6
1	BBB	33	ARG	2.6
1	DDD	126	CYS	2.5
1	CCC	110	PHE	2.5
1	BBB	75	ASP	2.5
1	CCC	36	ASP	2.4
1	AAA	55	GLN	2.3
1	BBB	7	ALA	2.3
1	BBB	52	GLN	2.3
1	AAA	101	ASP	2.2
1	CCC	101	ASP	2.2
1	CCC	88	THR	2.2
1	AAA	7	ALA	2.2
1	DDD	75	ASP	2.2
1	BBB	109	ASP	2.1
1	CCC	93	ASP	2.1
1	DDD	24	ASP	2.1
1	CCC	24	ASP	2.1
1	DDD	101	ASP	2.1
1	CCC	94	HIS	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

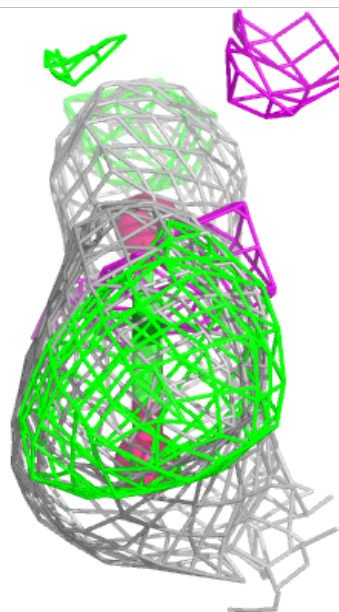
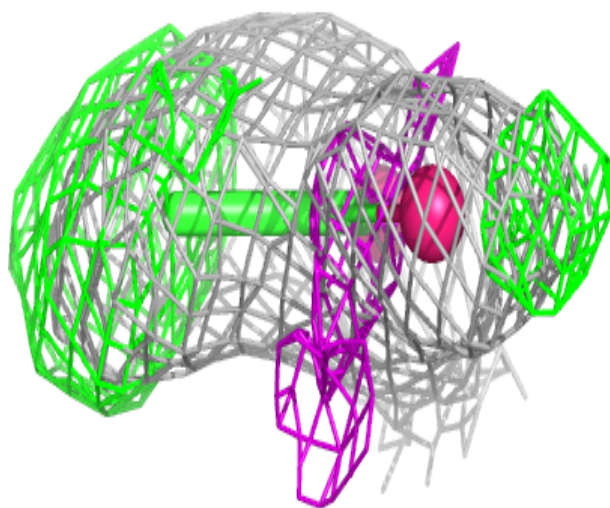
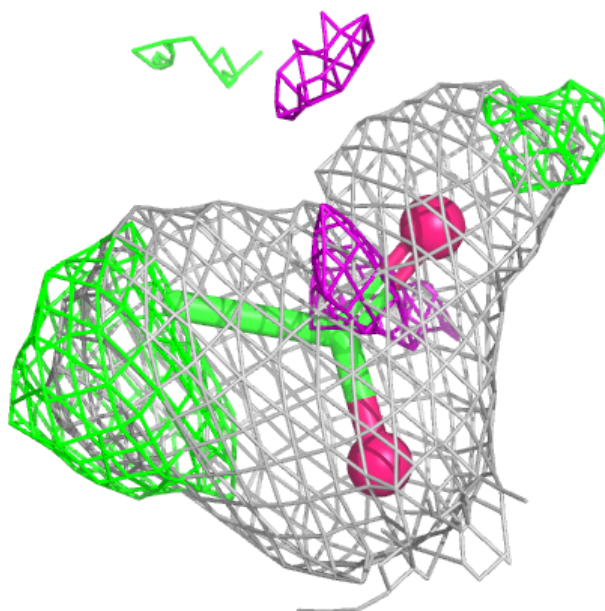
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	BBB	204	4/4	0.70	0.28	51,56,58,64	0
2	ZN	BBB	201	1/1	0.96	0.04	33,33,33,33	0
2	ZN	AAA	201	1/1	0.96	0.05	33,33,33,33	0
2	ZN	DDD	201	1/1	0.97	0.05	34,34,34,34	0
2	ZN	DDD	202	1/1	0.97	0.07	52,52,52,52	0
2	ZN	CCC	201	1/1	0.97	0.05	38,38,38,38	0
2	ZN	BBB	202	1/1	0.98	0.08	53,53,53,53	0
2	ZN	BBB	203	1/1	0.98	0.04	40,40,40,40	0
2	ZN	AAA	202	1/1	0.98	0.07	57,57,57,57	0
2	ZN	CCC	202	1/1	0.99	0.05	45,45,45,45	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.

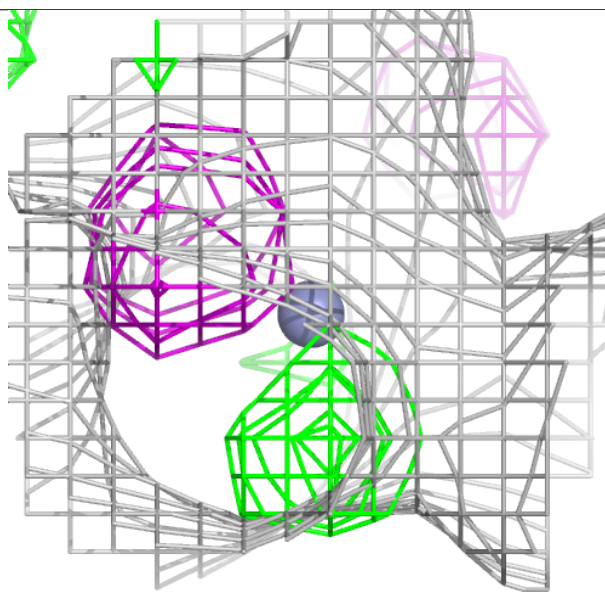
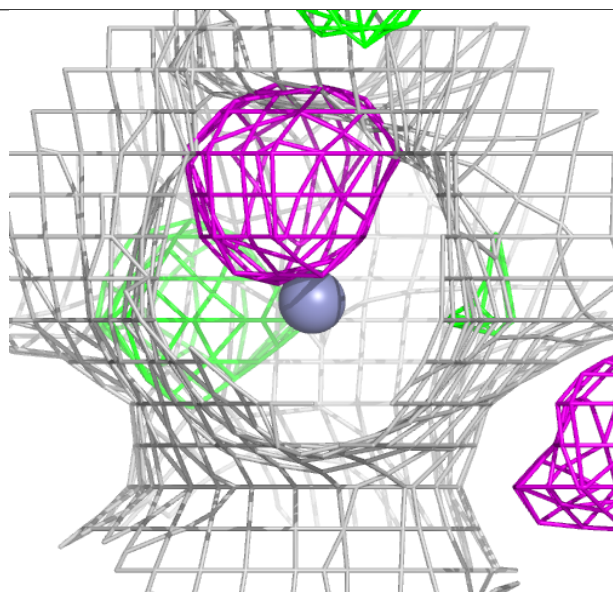
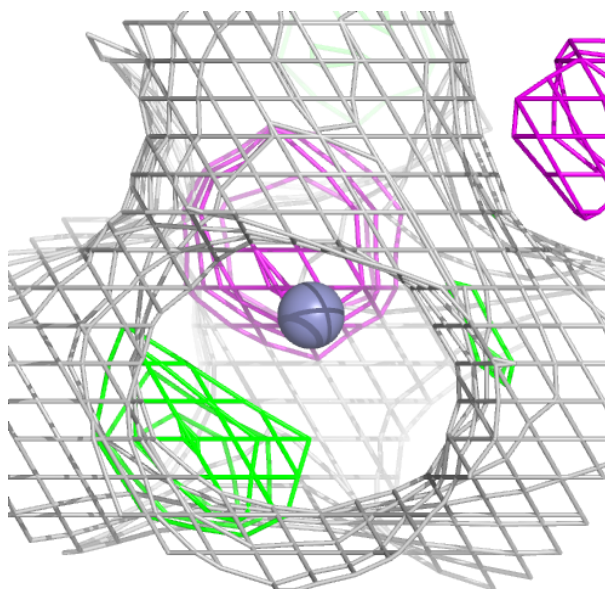
Electron density around ACT BBB 204:

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



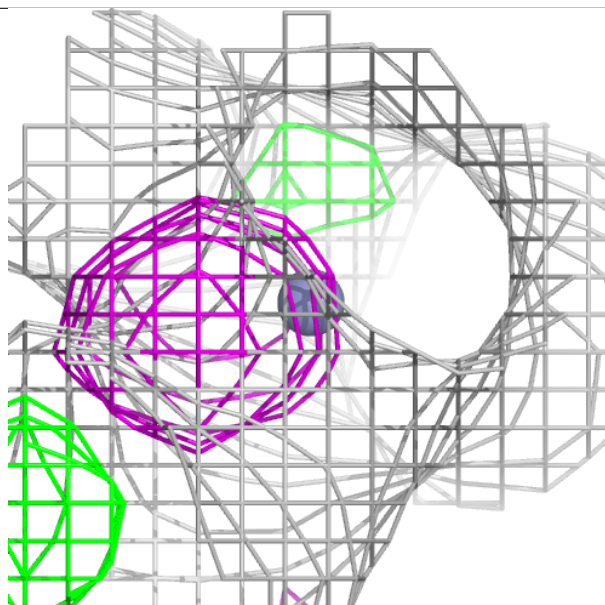
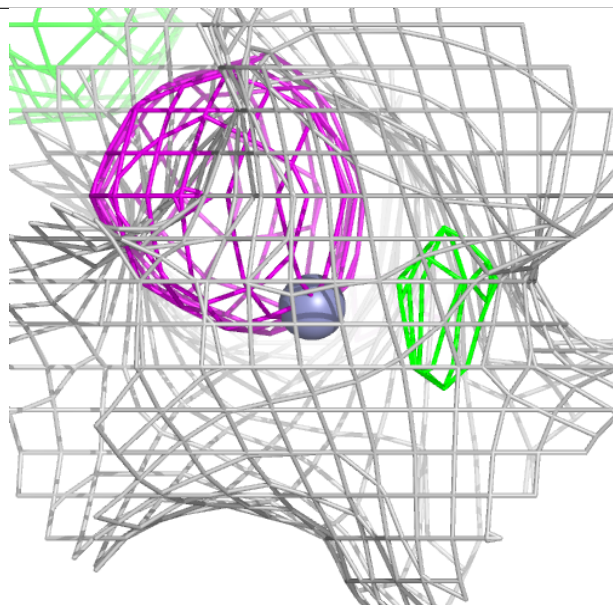
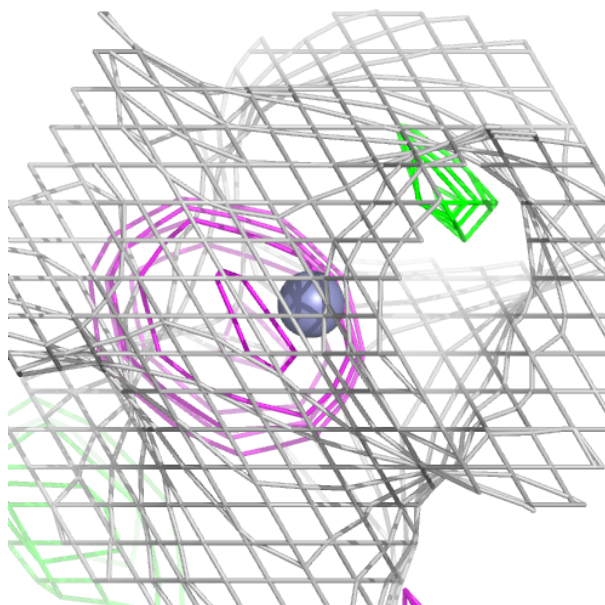
Electron density around ZN BBB 201:

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



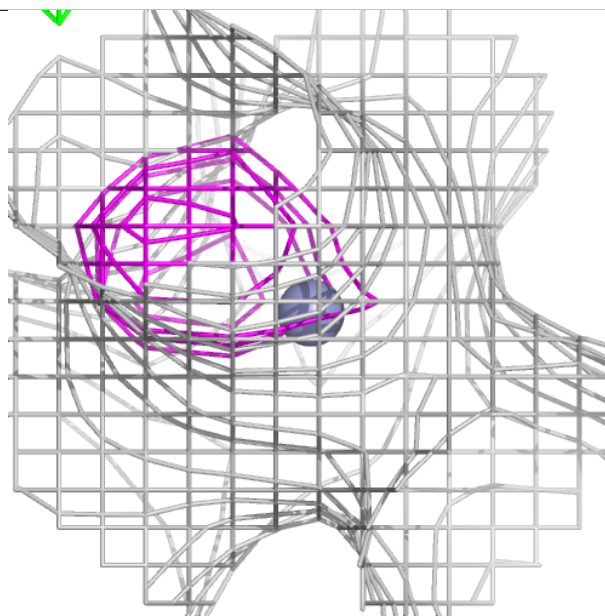
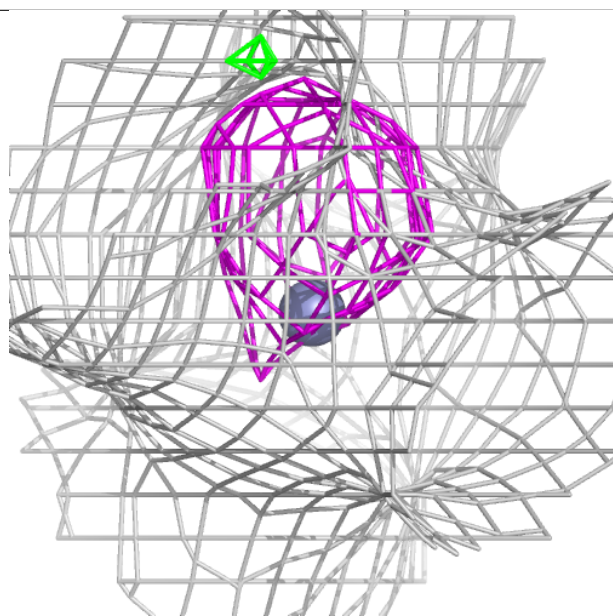
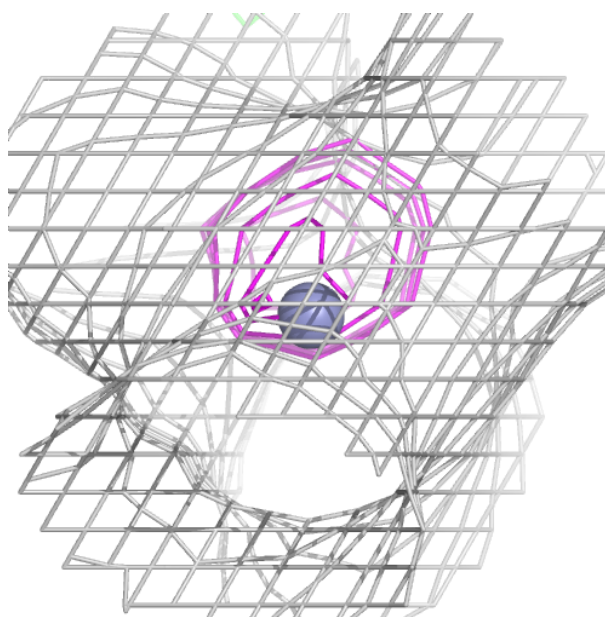
Electron density around ZN AAA 201:

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



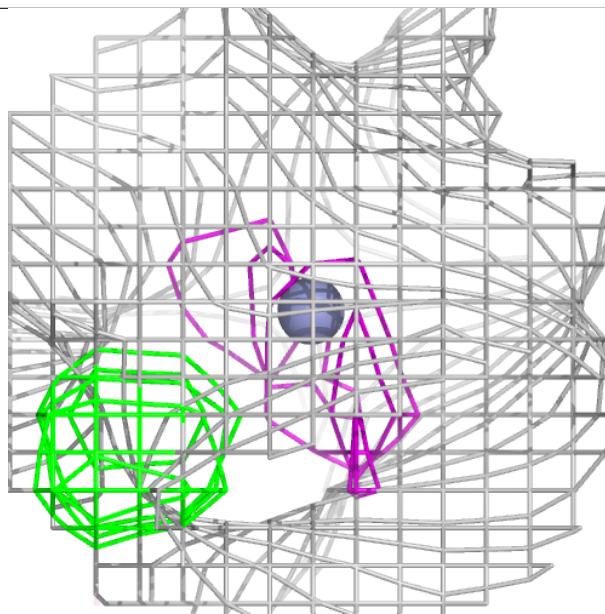
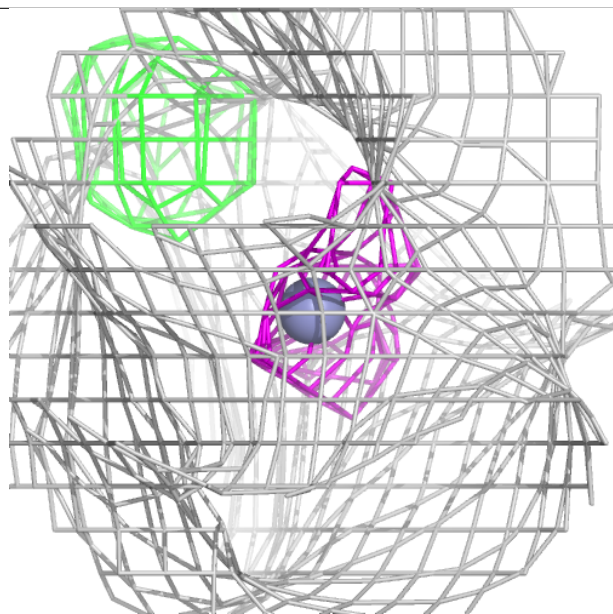
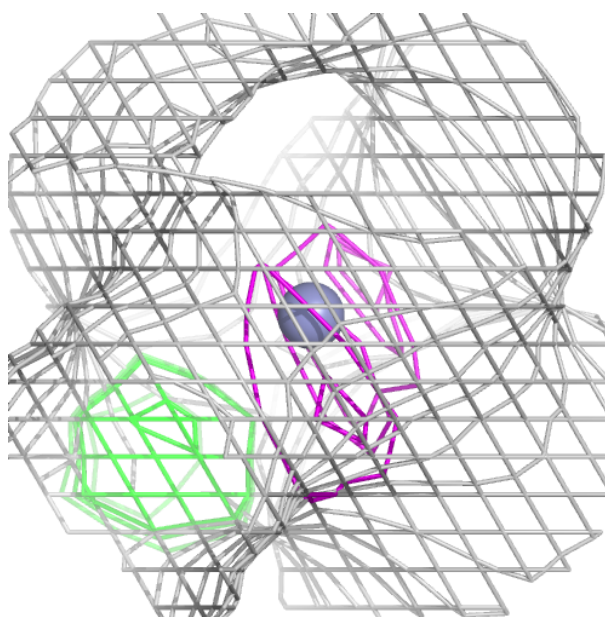
Electron density around ZN DDD 201:

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



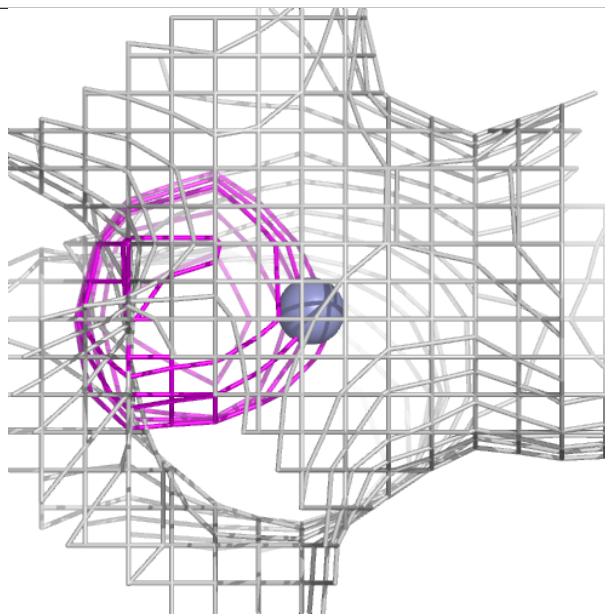
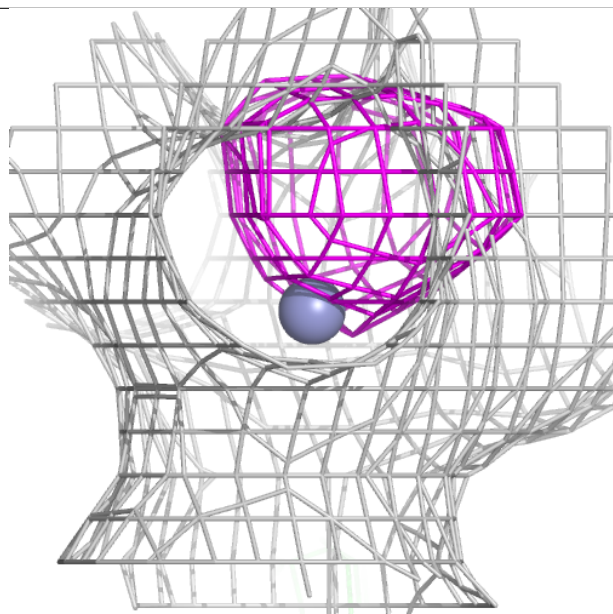
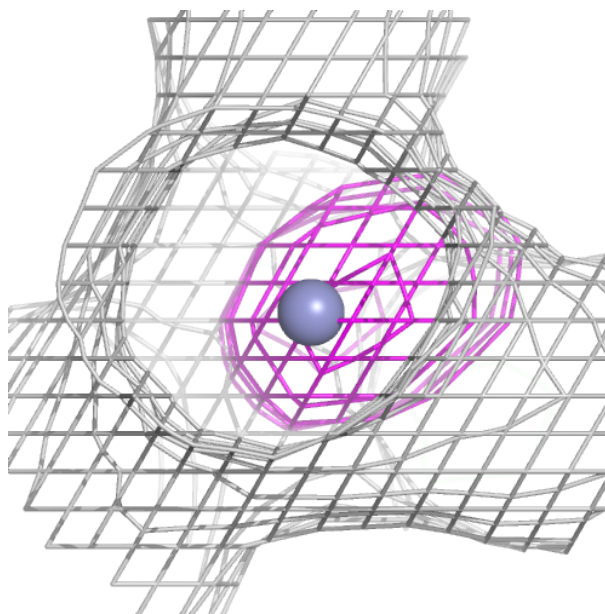
Electron density around ZN DDD 202:

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



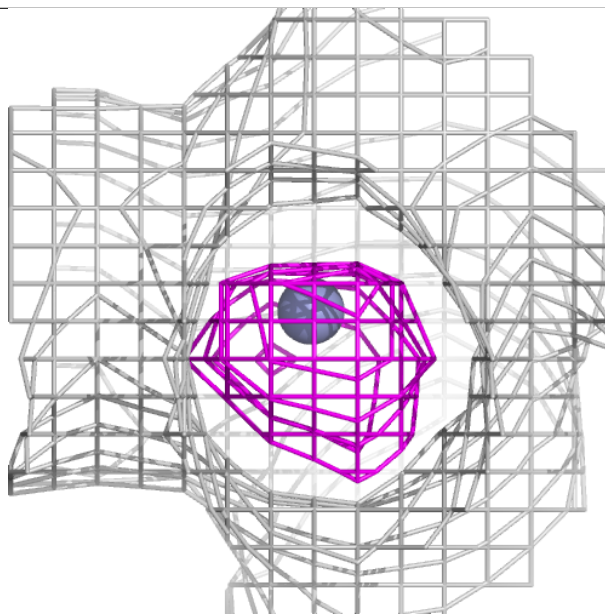
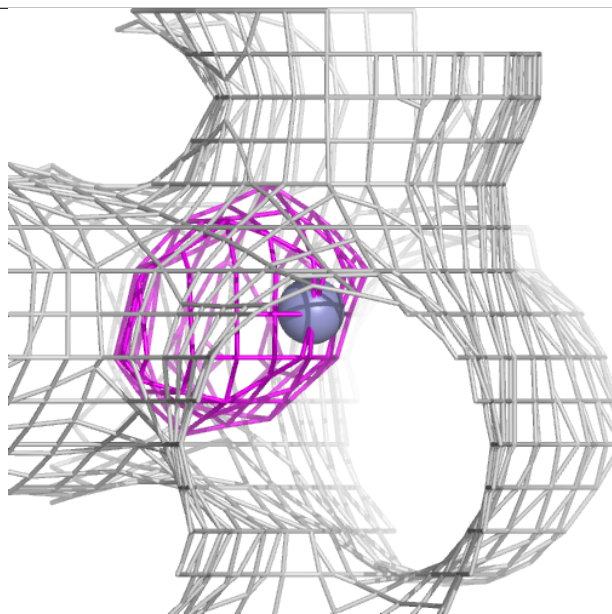
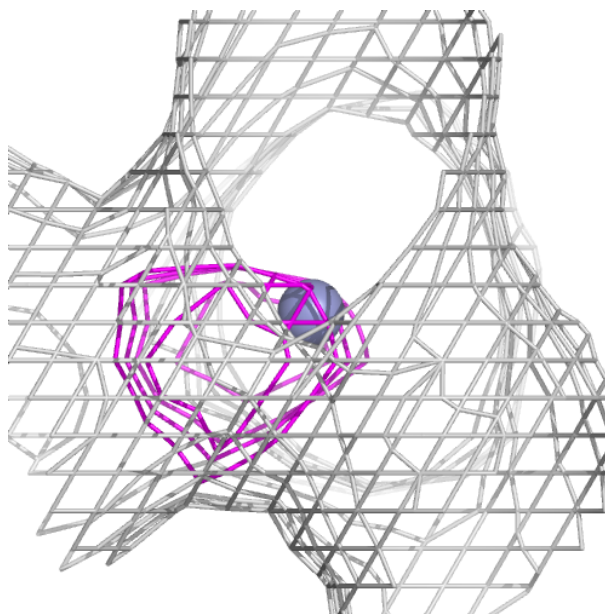
Electron density around ZN CCC 201:

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



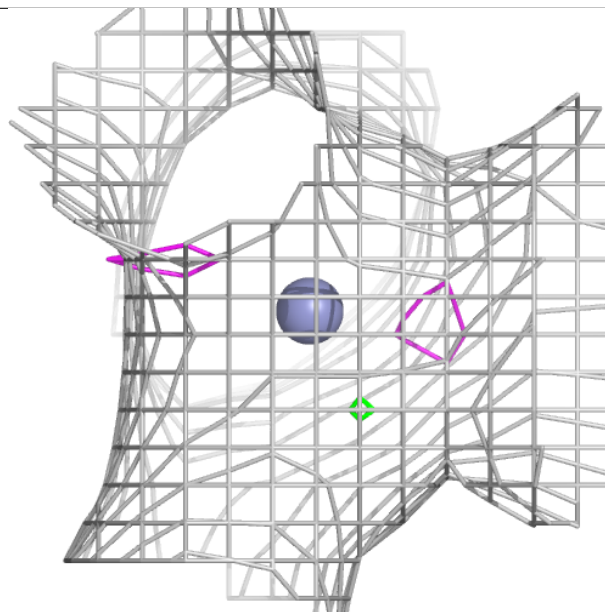
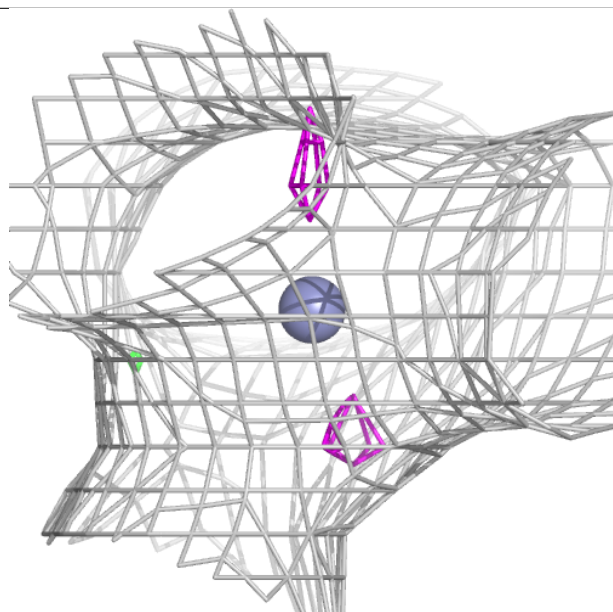
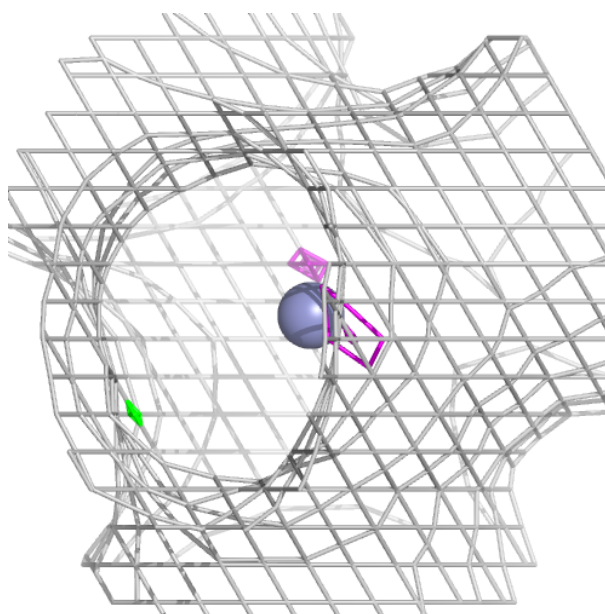
Electron density around ZN BBB 202:

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



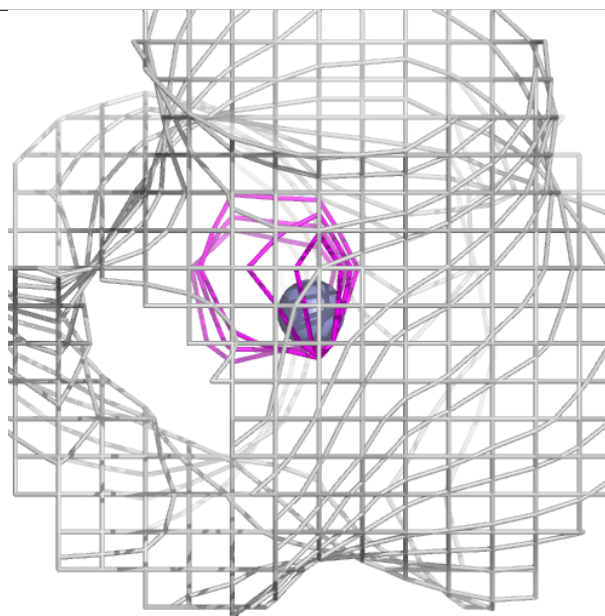
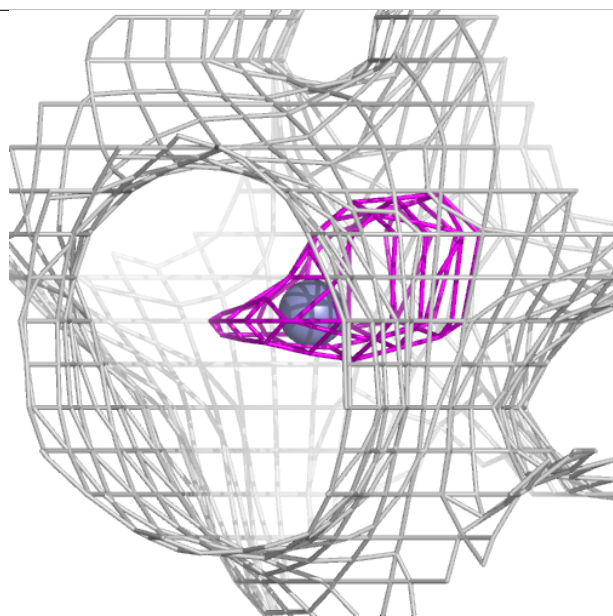
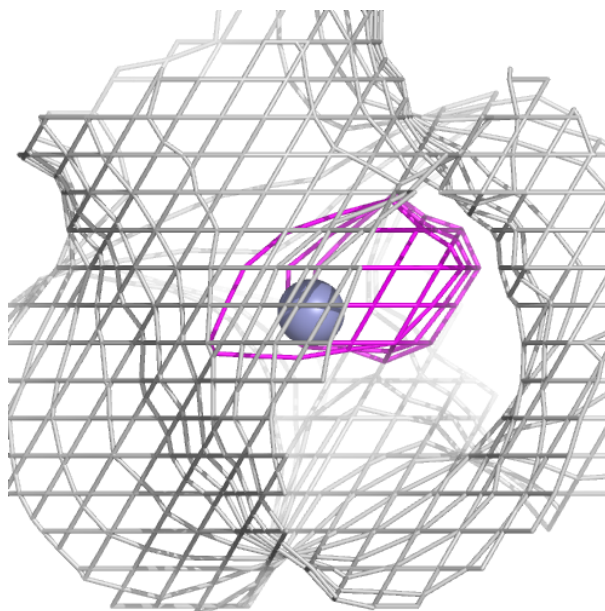
Electron density around ZN BBB 203:

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



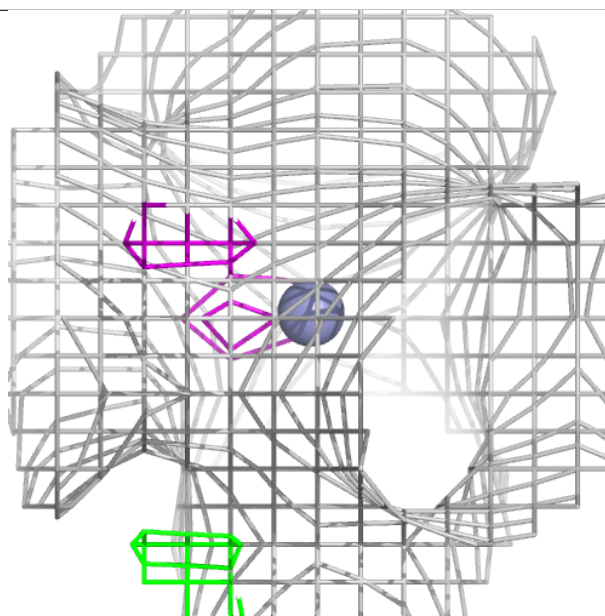
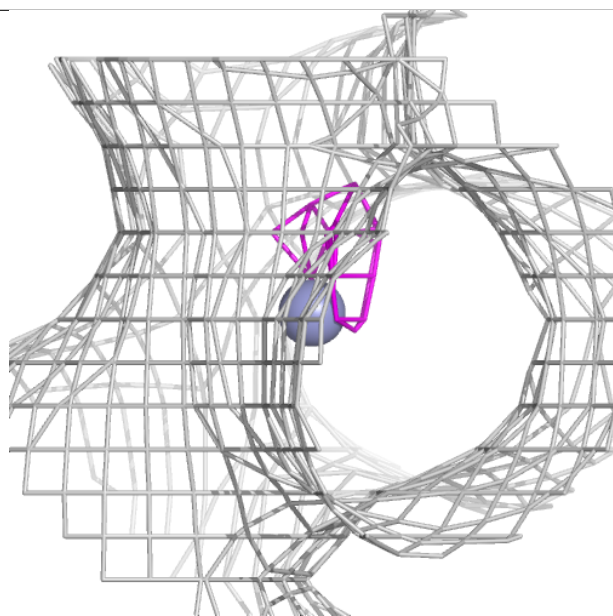
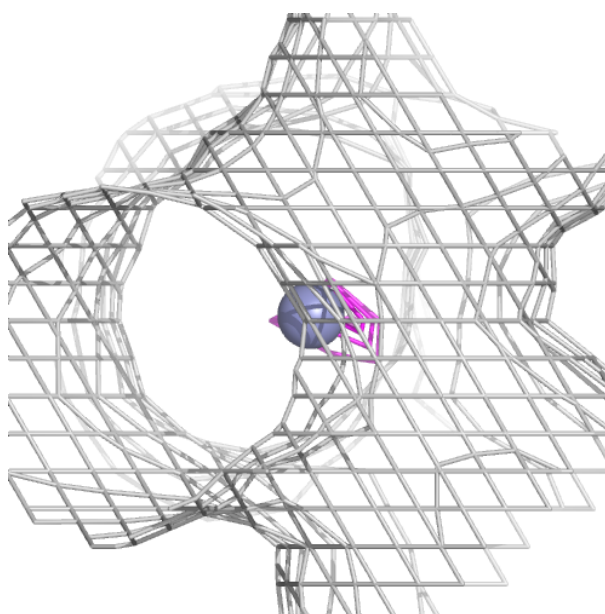
Electron density around ZN AAA 202:

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



Electron density around ZN CCC 202:

$2mF_o-DF_c$ (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.