



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 23, 2022 – 04:23 PM EST

PDB ID : 7TM9
Title : Crystal structure of Bacterial alkaline phosphatase from *Klebsiella pneumoniae*
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2022-01-19
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

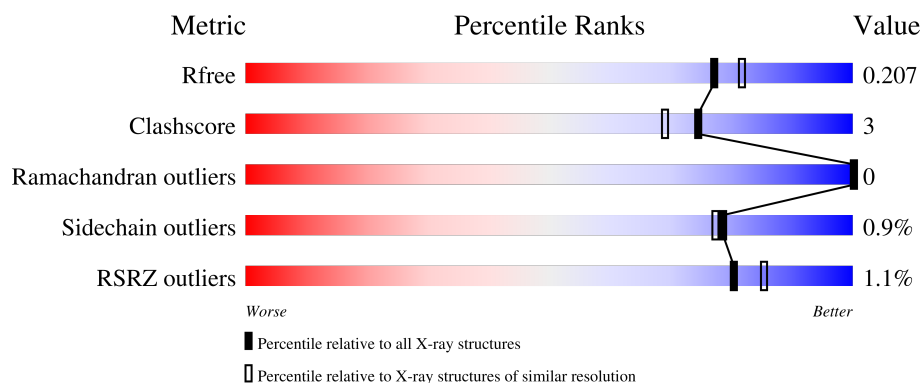
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	464	<div> <div>2%</div> <div>89% 6% 5%</div> </div>
1	B	464	<div> <div>%</div> <div>88% 7% 5%</div> </div>
1	C	464	<div> <div>%</div> <div>90% 5% 5%</div> </div>
1	D	464	<div> <div>%</div> <div>87% 8% 5%</div> </div>
1	E	464	<div> <div>%</div> <div>88% 7% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	464	<div><div>%</div><div><div></div><div>88%</div><div>7% 5%</div></div></div>
1	G	464	<div><div>%</div><div><div></div><div>87%</div><div>8% 5%</div></div></div>
1	H	464	<div><div>%</div><div><div></div><div>88%</div><div>7% 5%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29621 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 Bacterial alkaline phosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	P	S	0	0	0
			3228	1992	570	654	1	11			
1	B	441	Total	C	N	O	P	S	0	3	0
			3237	1999	569	657	1	11			
1	C	441	Total	C	N	O	P	S	0	2	0
			3238	2000	572	654	1	11			
1	D	441	Total	C	N	O	P	S	0	0	0
			3236	1996	570	658	1	11			
1	E	441	Total	C	N	O	P	S	0	1	0
			3229	1993	568	656	1	11			
1	F	441	Total	C	N	O	P	S	0	1	0
			3233	1995	572	654	1	11			
1	G	441	Total	C	N	O	P	S	0	2	0
			3241	1998	570	661	1	11			
1	H	441	Total	C	N	O	P	S	0	1	0
			3234	1996	570	656	1	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A0A0H3GK94
A	2	ALA	-	expression tag	UNP A0A0H3GK94
A	3	HIS	-	expression tag	UNP A0A0H3GK94
A	4	HIS	-	expression tag	UNP A0A0H3GK94
A	5	HIS	-	expression tag	UNP A0A0H3GK94
A	6	HIS	-	expression tag	UNP A0A0H3GK94
A	7	HIS	-	expression tag	UNP A0A0H3GK94
A	8	HIS	-	expression tag	UNP A0A0H3GK94
B	1	MET	-	expression tag	UNP A0A0H3GK94
B	2	ALA	-	expression tag	UNP A0A0H3GK94
B	3	HIS	-	expression tag	UNP A0A0H3GK94
B	4	HIS	-	expression tag	UNP A0A0H3GK94
B	5	HIS	-	expression tag	UNP A0A0H3GK94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP A0A0H3GK94
B	7	HIS	-	expression tag	UNP A0A0H3GK94
B	8	HIS	-	expression tag	UNP A0A0H3GK94
C	1	MET	-	expression tag	UNP A0A0H3GK94
C	2	ALA	-	expression tag	UNP A0A0H3GK94
C	3	HIS	-	expression tag	UNP A0A0H3GK94
C	4	HIS	-	expression tag	UNP A0A0H3GK94
C	5	HIS	-	expression tag	UNP A0A0H3GK94
C	6	HIS	-	expression tag	UNP A0A0H3GK94
C	7	HIS	-	expression tag	UNP A0A0H3GK94
C	8	HIS	-	expression tag	UNP A0A0H3GK94
D	1	MET	-	expression tag	UNP A0A0H3GK94
D	2	ALA	-	expression tag	UNP A0A0H3GK94
D	3	HIS	-	expression tag	UNP A0A0H3GK94
D	4	HIS	-	expression tag	UNP A0A0H3GK94
D	5	HIS	-	expression tag	UNP A0A0H3GK94
D	6	HIS	-	expression tag	UNP A0A0H3GK94
D	7	HIS	-	expression tag	UNP A0A0H3GK94
D	8	HIS	-	expression tag	UNP A0A0H3GK94
E	1	MET	-	expression tag	UNP A0A0H3GK94
E	2	ALA	-	expression tag	UNP A0A0H3GK94
E	3	HIS	-	expression tag	UNP A0A0H3GK94
E	4	HIS	-	expression tag	UNP A0A0H3GK94
E	5	HIS	-	expression tag	UNP A0A0H3GK94
E	6	HIS	-	expression tag	UNP A0A0H3GK94
E	7	HIS	-	expression tag	UNP A0A0H3GK94
E	8	HIS	-	expression tag	UNP A0A0H3GK94
F	1	MET	-	expression tag	UNP A0A0H3GK94
F	2	ALA	-	expression tag	UNP A0A0H3GK94
F	3	HIS	-	expression tag	UNP A0A0H3GK94
F	4	HIS	-	expression tag	UNP A0A0H3GK94
F	5	HIS	-	expression tag	UNP A0A0H3GK94
F	6	HIS	-	expression tag	UNP A0A0H3GK94
F	7	HIS	-	expression tag	UNP A0A0H3GK94
F	8	HIS	-	expression tag	UNP A0A0H3GK94
G	1	MET	-	expression tag	UNP A0A0H3GK94
G	2	ALA	-	expression tag	UNP A0A0H3GK94
G	3	HIS	-	expression tag	UNP A0A0H3GK94
G	4	HIS	-	expression tag	UNP A0A0H3GK94
G	5	HIS	-	expression tag	UNP A0A0H3GK94
G	6	HIS	-	expression tag	UNP A0A0H3GK94
G	7	HIS	-	expression tag	UNP A0A0H3GK94

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Chain	Residue	Modelled	Actual	Comment	Reference
G	8	HIS	-	expression tag	UNP A0A0H3GK94
H	1	MET	-	expression tag	UNP A0A0H3GK94
H	2	ALA	-	expression tag	UNP A0A0H3GK94
H	3	HIS	-	expression tag	UNP A0A0H3GK94
H	4	HIS	-	expression tag	UNP A0A0H3GK94
H	5	HIS	-	expression tag	UNP A0A0H3GK94
H	6	HIS	-	expression tag	UNP A0A0H3GK94
H	7	HIS	-	expression tag	UNP A0A0H3GK94
H	8	HIS	-	expression tag	UNP A0A0H3GK94

- Molecule 2 is ZINC ION (three-letter code: 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
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

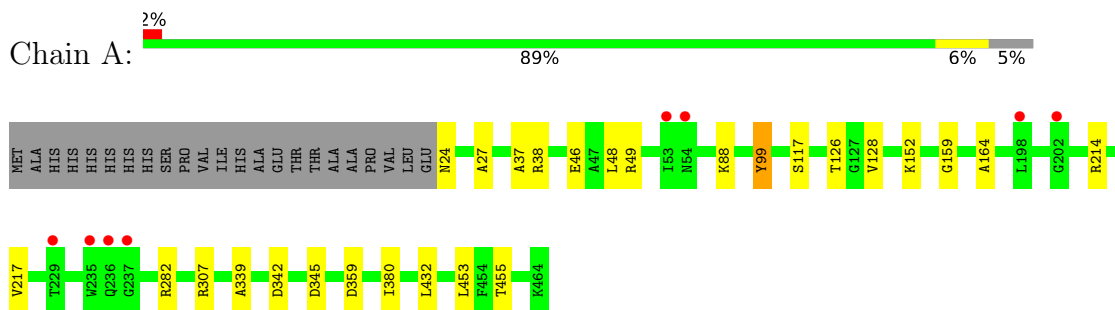
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	424	Total 424	O 424	0	0
4	B	471	Total 471	O 471	0	0
4	C	454	Total 454	O 454	0	0
4	D	505	Total 505	O 505	0	0
4	E	469	Total 469	O 469	0	0
4	F	425	Total 425	O 425	0	0
4	G	524	Total 524	O 524	0	0
4	H	449	Total 449	O 449	0	0

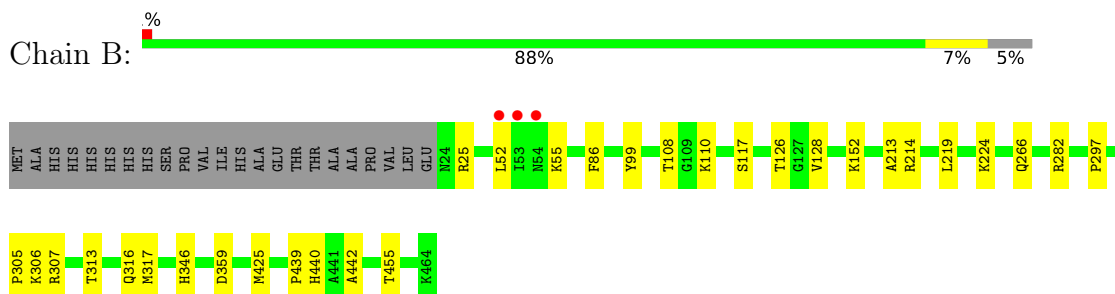
3 Residue-property plots [i](#)

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.

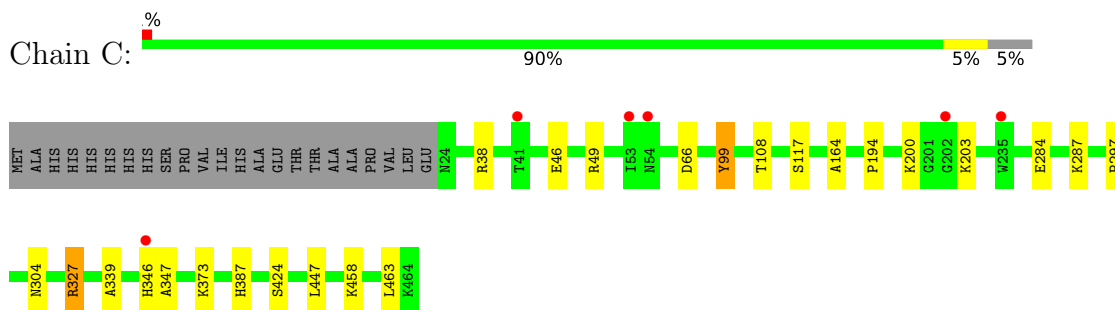
- Molecule 1: Bacterial alkaline phosphatase



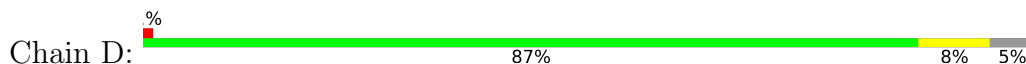
- Molecule 1: Bacterial alkaline phosphatase

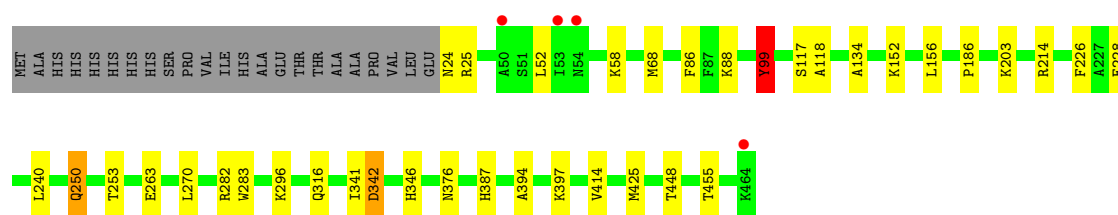


- Molecule 1: Bacterial alkaline phosphatase

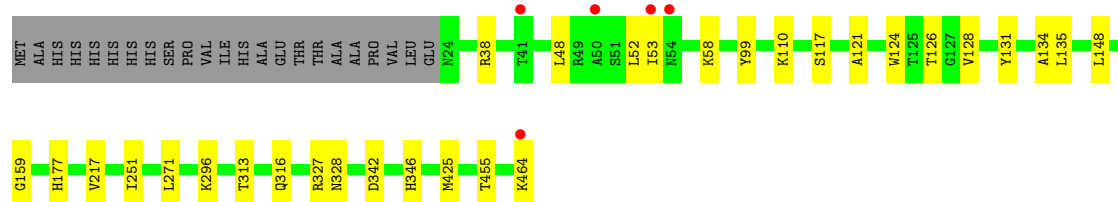
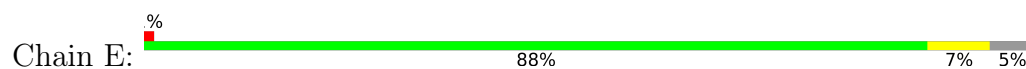


- Molecule 1: Bacterial alkaline phosphatase

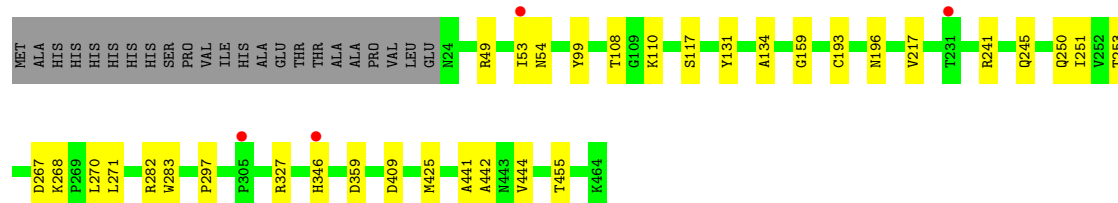
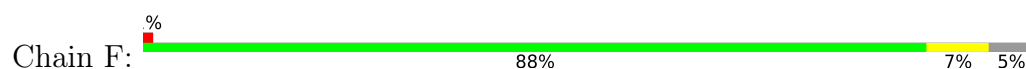




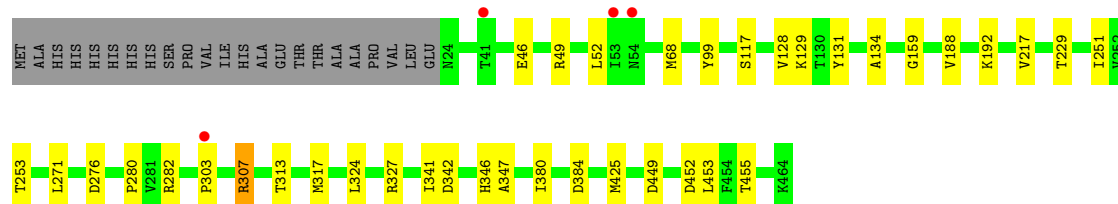
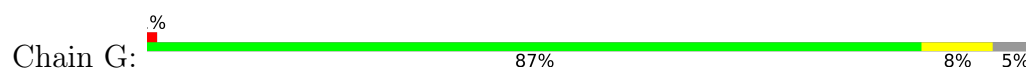
• Molecule 1: Bacterial alkaline phosphatase



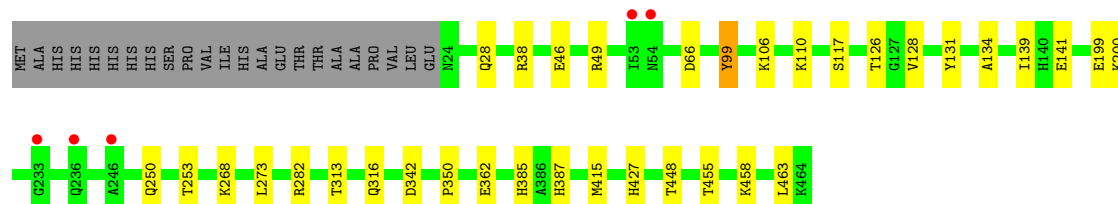
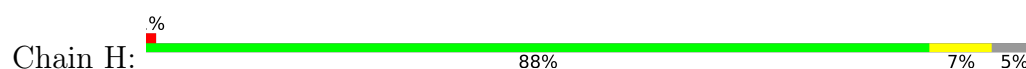
• Molecule 1: Bacterial alkaline phosphatase



• Molecule 1: Bacterial alkaline phosphatase



• Molecule 1: Bacterial alkaline phosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.95Å 240.60Å 101.48Å 90.00° 105.13° 90.00°	Depositor
Resolution (Å)	46.09 – 1.95 49.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.09-1.95) 97.7 (49.66-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.172 , 0.211 0.165 , 0.207	Depositor DCC
R_{free} test set	11767 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29621	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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 56.01 % 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 2.9133e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, SEP, 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	A	0.50	0/3271	0.70	1/4446 (0.0%)
1	B	0.52	0/3286	0.69	0/4469
1	C	0.53	0/3284	0.71	3/4464 (0.1%)
1	D	0.52	0/3279	0.72	2/4456 (0.0%)
1	E	0.52	0/3275	0.71	0/4454
1	F	0.51	0/3276	0.70	0/4453
1	G	0.54	0/3287	0.74	1/4470 (0.0%)
1	H	0.52	0/3280	0.70	0/4458
All	All	0.52	0/26238	0.71	7/35670 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	342	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	C	66	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	99	TYR	CA-CB-CG	5.36	123.59	113.40
1	D	99	TYR	CA-CB-CG	5.33	123.53	113.40
1	G	384	ASP	CB-CG-OD1	5.25	123.02	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3228	0	3154	18	0
1	B	3237	0	3156	26	0
1	C	3238	0	3168	16	0
1	D	3236	0	3162	29	0
1	E	3229	0	3147	20	0
1	F	3233	0	3157	20	0
1	G	3241	0	3154	24	0
1	H	3234	0	3160	24	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
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	424	0	0	3	0
4	B	471	0	0	9	0
4	C	454	0	0	5	0
4	D	505	0	0	5	0
4	E	469	0	0	5	0
4	F	425	0	0	2	0
4	G	524	0	0	7	0
4	H	449	0	0	4	0
All	All	29621	0	25258	163	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 3.

The worst 5 of 163 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:F:282:ARG:HG3	1:F:283:TRP:CD1	2.15	0.80
1:H:250:GLN:HG3	1:H:268:LYS:HE3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LEU:O	1:F:49:ARG:NH2	2.30	0.65
1:H:110:LYS:HE2	4:H:673:HOH:O	1.96	0.65
1:B:108:THR:HB	4:B:1238:HOH:O	1.95	0.65

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	438/464 (94%)	431 (98%)	7 (2%)	0	100	100
1	B	441/464 (95%)	434 (98%)	7 (2%)	0	100	100
1	C	440/464 (95%)	434 (99%)	6 (1%)	0	100	100
1	D	438/464 (94%)	433 (99%)	5 (1%)	0	100	100
1	E	439/464 (95%)	434 (99%)	5 (1%)	0	100	100
1	F	439/464 (95%)	433 (99%)	6 (1%)	0	100	100
1	G	440/464 (95%)	436 (99%)	4 (1%)	0	100	100
1	H	439/464 (95%)	435 (99%)	4 (1%)	0	100	100
All	All	3514/3712 (95%)	3470 (99%)	44 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/352 (93%)	325 (99%)	3 (1%)	78	77
1	B	329/352 (94%)	327 (99%)	2 (1%)	86	85
1	C	329/352 (94%)	326 (99%)	3 (1%)	78	77
1	D	330/352 (94%)	327 (99%)	3 (1%)	78	77
1	E	328/352 (93%)	324 (99%)	4 (1%)	71	68
1	F	328/352 (93%)	325 (99%)	3 (1%)	78	77
1	G	330/352 (94%)	326 (99%)	4 (1%)	71	68
1	H	329/352 (94%)	327 (99%)	2 (1%)	86	85
All	All	2631/2816 (93%)	2607 (99%)	24 (1%)	78	77

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	464	LYS
1	F	267	ASP
1	F	99	TYR
1	G	99	TYR
1	C	327	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	376	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	SEP	B	117	2,1	8,9,10	1.64	2 (25%)	8,12,14	1.57	1 (12%)
1	SEP	F	117	2,1	8,9,10	1.75	1 (12%)	8,12,14	1.13	0
1	SEP	D	117	2,1	8,9,10	1.78	1 (12%)	8,12,14	1.09	1 (12%)
1	SEP	G	117	2,1	8,9,10	1.73	1 (12%)	8,12,14	1.67	2 (25%)
1	SEP	H	117	2,1	8,9,10	1.60	1 (12%)	8,12,14	1.61	2 (25%)
1	SEP	C	117	2,1	8,9,10	1.56	1 (12%)	8,12,14	1.47	3 (37%)
1	SEP	A	117	2,1	8,9,10	1.63	2 (25%)	8,12,14	1.58	2 (25%)
1	SEP	E	117	2,1	8,9,10	1.59	1 (12%)	8,12,14	1.63	2 (25%)

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	SEP	B	117	2,1	-	1/5/8/10	-
1	SEP	F	117	2,1	-	0/5/8/10	-
1	SEP	D	117	2,1	-	1/5/8/10	-
1	SEP	G	117	2,1	-	1/5/8/10	-
1	SEP	H	117	2,1	-	1/5/8/10	-
1	SEP	C	117	2,1	-	0/5/8/10	-
1	SEP	A	117	2,1	-	1/5/8/10	-
1	SEP	E	117	2,1	-	1/5/8/10	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	SEP	P-O1P	3.94	1.63	1.50
1	F	117	SEP	P-O1P	3.73	1.62	1.50
1	E	117	SEP	P-O1P	3.51	1.61	1.50
1	G	117	SEP	P-O1P	3.39	1.61	1.50
1	B	117	SEP	P-O1P	3.07	1.60	1.50

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	SEP	OG-CB-CA	3.70	111.74	108.14
1	E	117	SEP	OG-CB-CA	3.64	111.69	108.14
1	A	117	SEP	OG-CB-CA	3.39	111.45	108.14
1	H	117	SEP	O2P-P-OG	-3.20	98.23	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	117	SEP	O2P-P-OG	-2.99	98.76	106.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	117	SEP	CA-CB-OG-P
1	B	117	SEP	CA-CB-OG-P
1	D	117	SEP	CA-CB-OG-P
1	E	117	SEP	CA-CB-OG-P
1	G	117	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/464 (94%)	0.11	8 (1%) 68 76	6, 13, 27, 40	0
1	B	440/464 (94%)	-0.02	3 (0%) 87 92	5, 11, 25, 47	0
1	C	440/464 (94%)	0.03	6 (1%) 75 82	5, 12, 24, 37	0
1	D	440/464 (94%)	-0.04	4 (0%) 84 89	5, 11, 25, 41	0
1	E	440/464 (94%)	-0.02	5 (1%) 80 85	5, 13, 26, 46	0
1	F	440/464 (94%)	0.04	4 (0%) 84 89	6, 13, 27, 41	0
1	G	440/464 (94%)	-0.08	4 (0%) 84 89	4, 11, 24, 39	0
1	H	440/464 (94%)	0.03	5 (1%) 80 85	5, 13, 28, 37	0
All	All	3520/3712 (94%)	0.01	39 (1%) 80 85	4, 12, 27, 47	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	ILE	4.7
1	B	53	ILE	4.5
1	G	54	ASN	3.8
1	F	305	PRO	3.7
1	A	53	ILE	3.4

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, 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
1	SEP	F	117	10/11	0.83	0.19	4,13,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	H	117	10/11	0.85	0.19	9,15,25,27	0
1	SEP	D	117	10/11	0.86	0.15	6,10,28,31	0
1	SEP	A	117	10/11	0.87	0.17	6,14,25,27	0
1	SEP	B	117	10/11	0.87	0.16	5,11,26,27	0
1	SEP	C	117	10/11	0.87	0.17	5,14,29,30	0
1	SEP	G	117	10/11	0.88	0.15	5,12,22,30	0
1	SEP	E	117	10/11	0.88	0.15	5,10,25,25	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
3	MG	F	503	1/1	0.93	0.08	13,13,13,13	0
3	MG	A	503	1/1	0.94	0.05	14,14,14,14	0
3	MG	H	503	1/1	0.95	0.06	12,12,12,12	0
3	MG	D	503	1/1	0.96	0.09	8,8,8,8	0
2	ZN	B	501	1/1	0.97	0.11	37,37,37,37	0
2	ZN	C	502	1/1	0.97	0.11	39,39,39,39	0
2	ZN	F	501	1/1	0.97	0.17	41,41,41,41	0
2	ZN	F	502	1/1	0.97	0.12	37,37,37,37	0
2	ZN	B	502	1/1	0.98	0.08	32,32,32,32	0
2	ZN	H	501	1/1	0.98	0.14	38,38,38,38	0
2	ZN	C	501	1/1	0.98	0.18	42,42,42,42	0
3	MG	C	503	1/1	0.98	0.04	8,8,8,8	0
2	ZN	A	502	1/1	0.98	0.10	34,34,34,34	0
3	MG	E	503	1/1	0.98	0.04	7,7,7,7	0
2	ZN	D	502	1/1	0.98	0.10	33,33,33,33	0
2	ZN	A	501	1/1	0.98	0.17	39,39,39,39	0
2	ZN	D	501	1/1	0.99	0.12	42,42,42,42	0
3	MG	B	503	1/1	0.99	0.07	10,10,10,10	0
2	ZN	E	501	1/1	0.99	0.13	36,36,36,36	0
2	ZN	G	501	1/1	0.99	0.13	34,34,34,34	0
2	ZN	G	502	1/1	0.99	0.10	30,30,30,30	0

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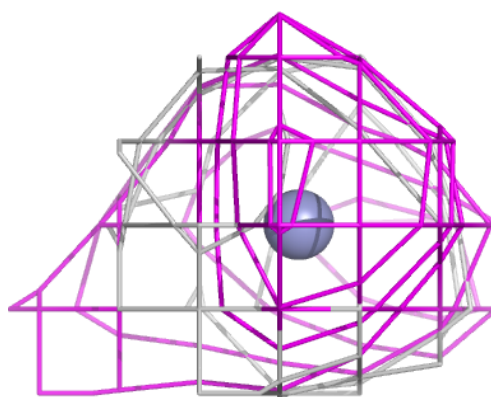
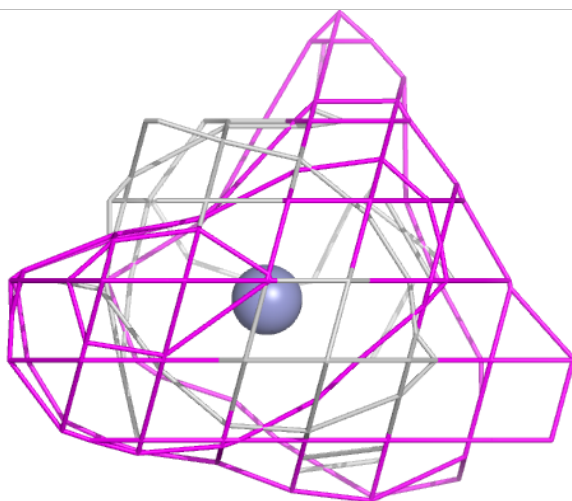
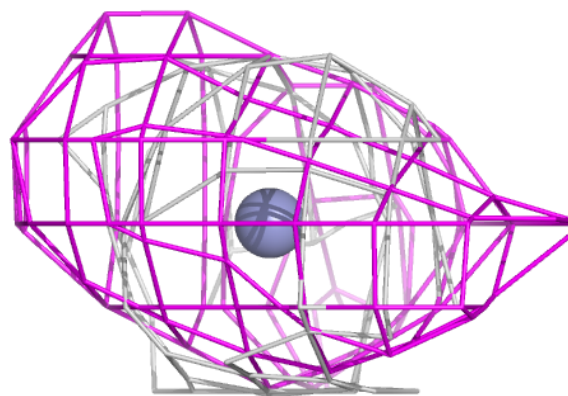
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	E	502	1/1	0.99	0.08	31,31,31,31	0
3	MG	G	503	1/1	0.99	0.04	8,8,8,8	0
2	ZN	H	502	1/1	0.99	0.13	37,37,37,37	0

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.

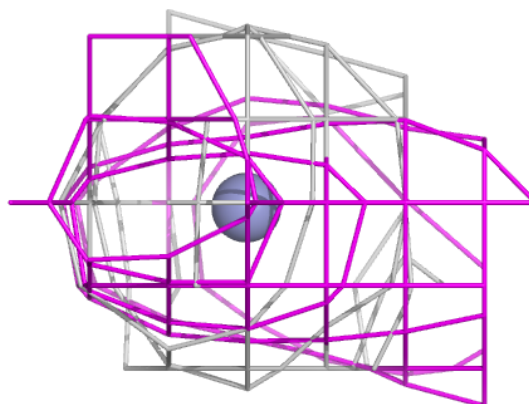
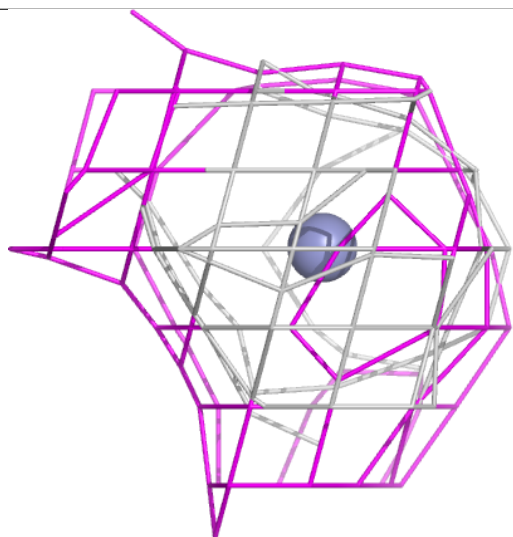
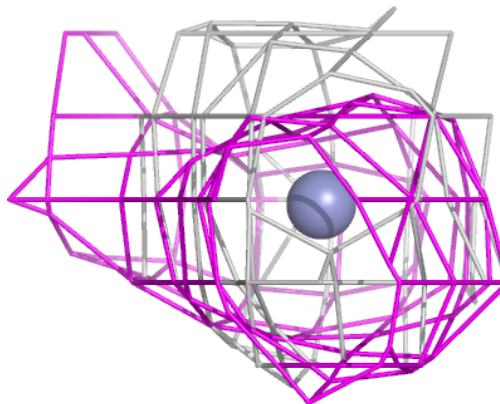
Electron density around ZN B 501:

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



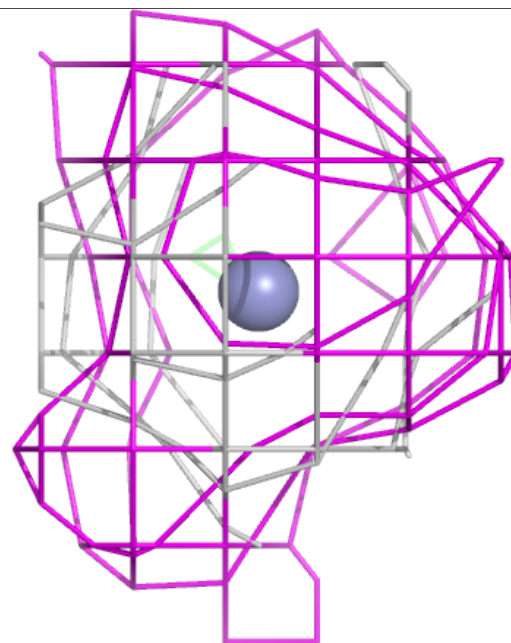
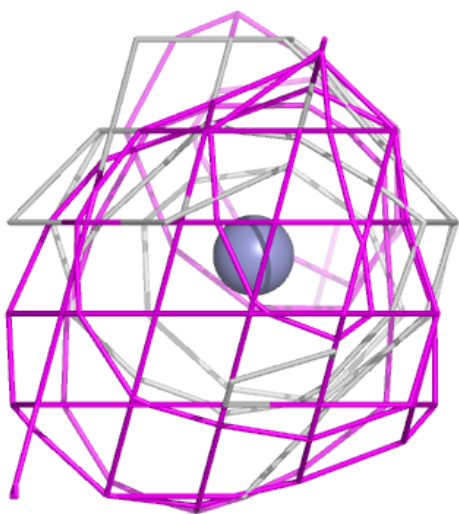
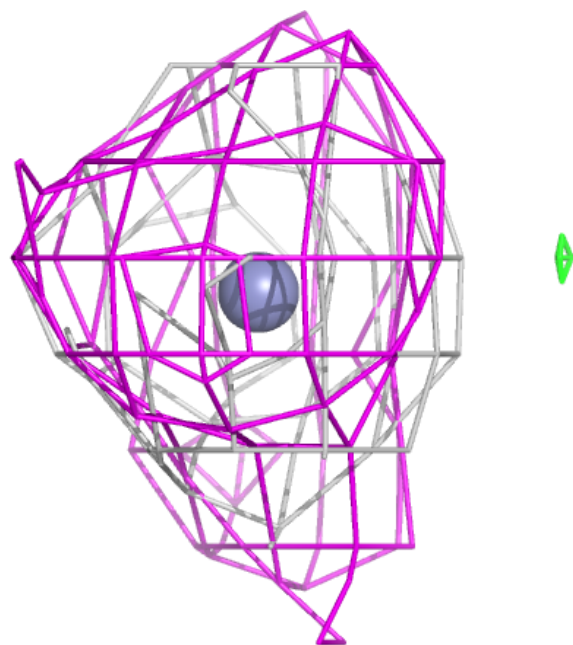
Electron density around ZN C 502:

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and green (positive)



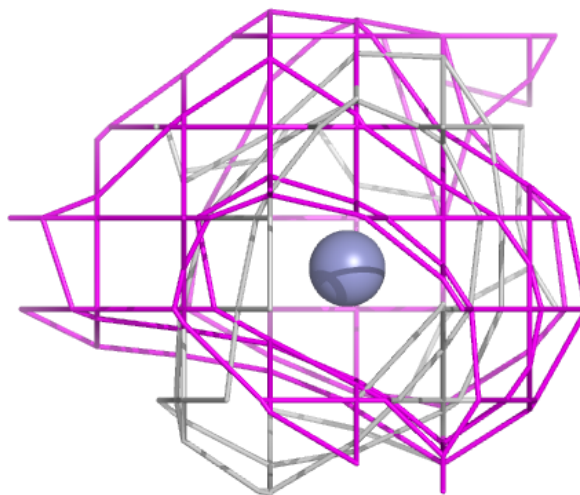
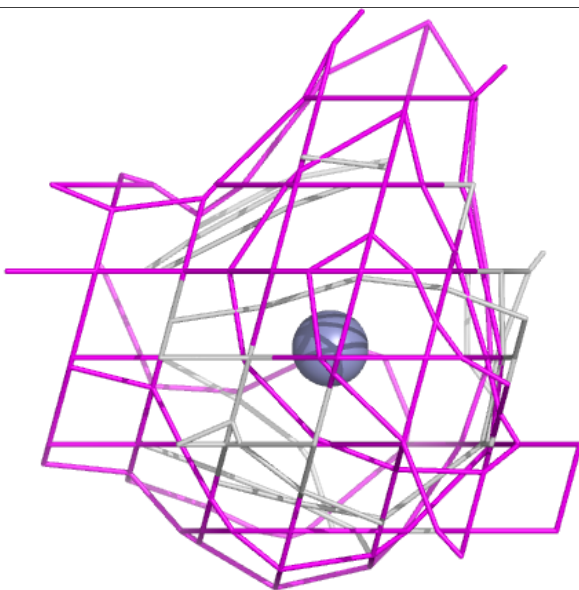
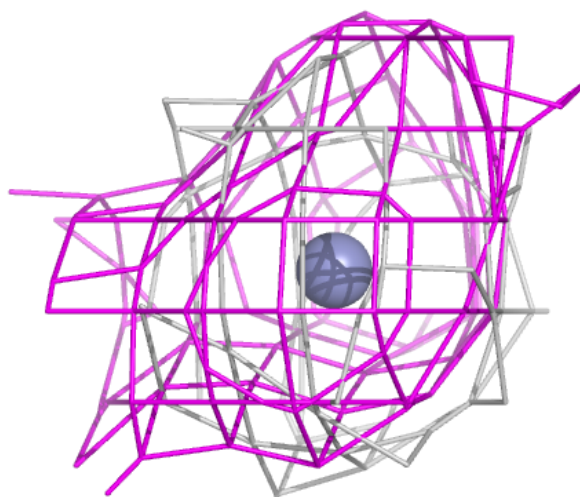
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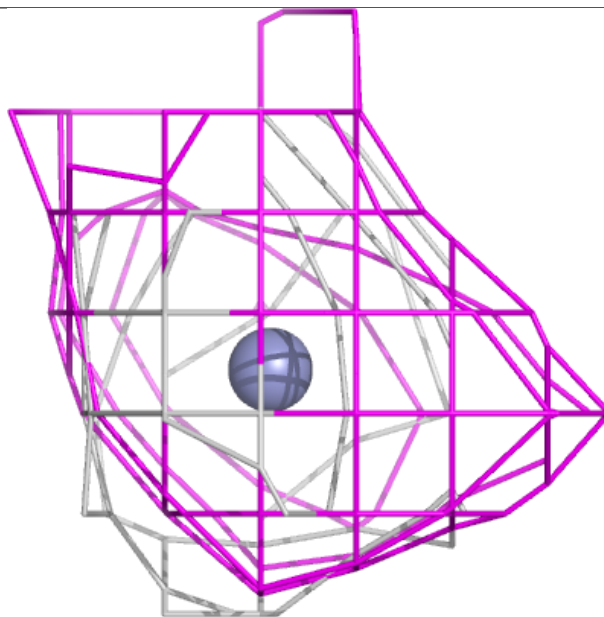
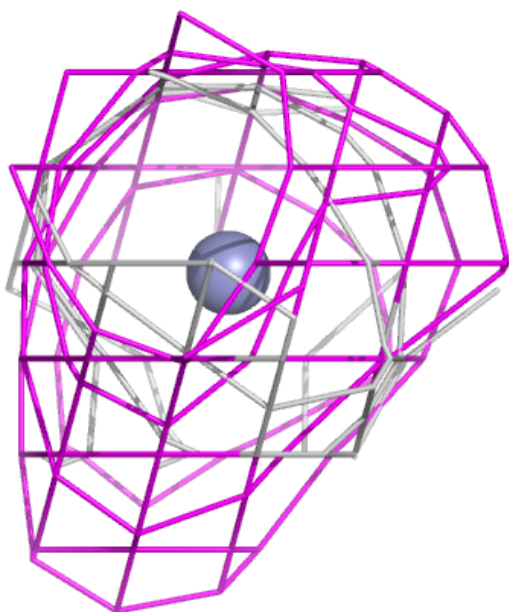
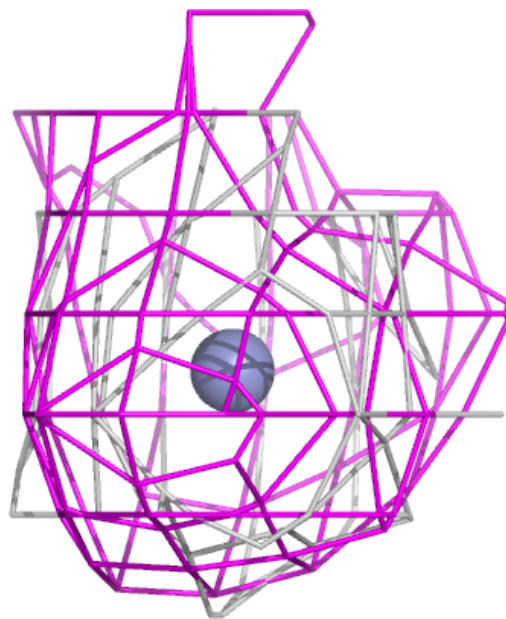
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and green (positive)



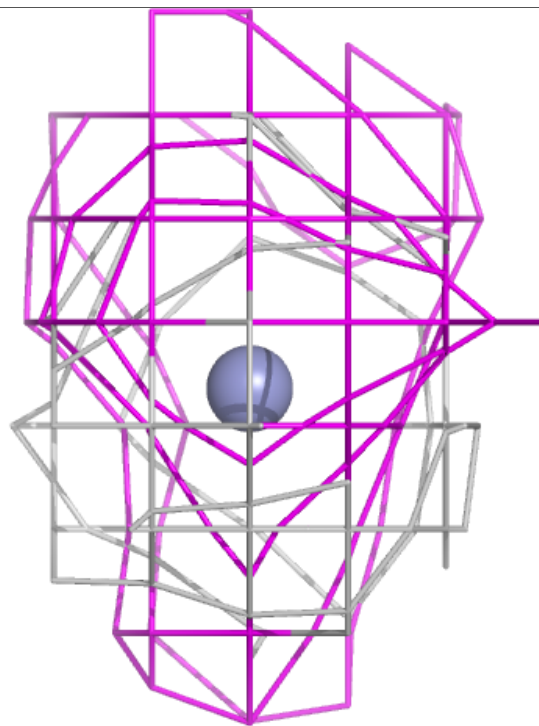
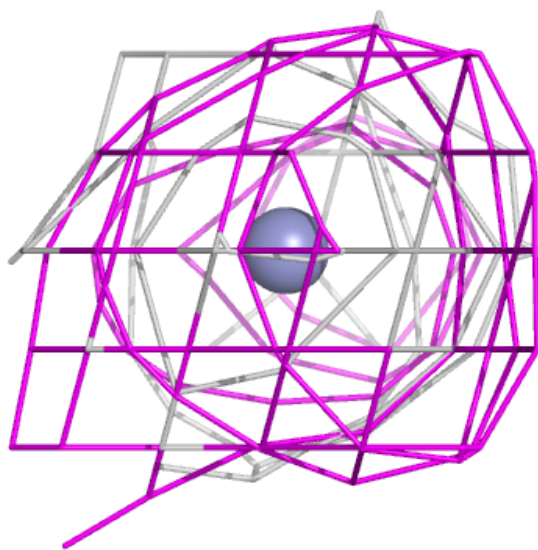
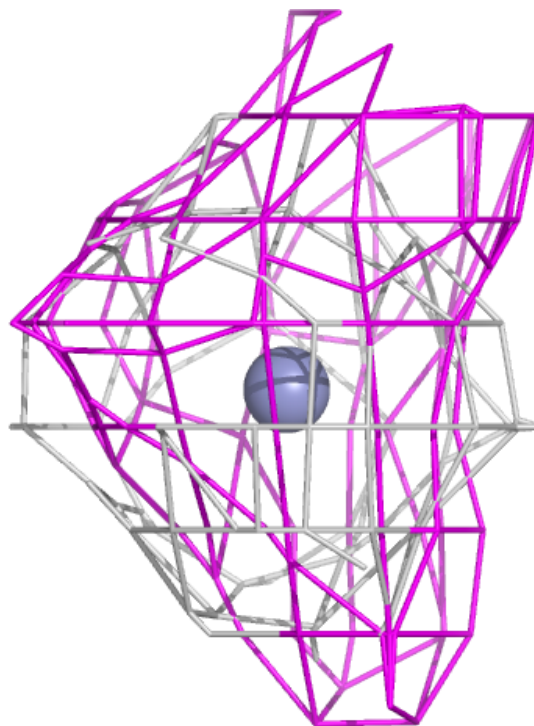
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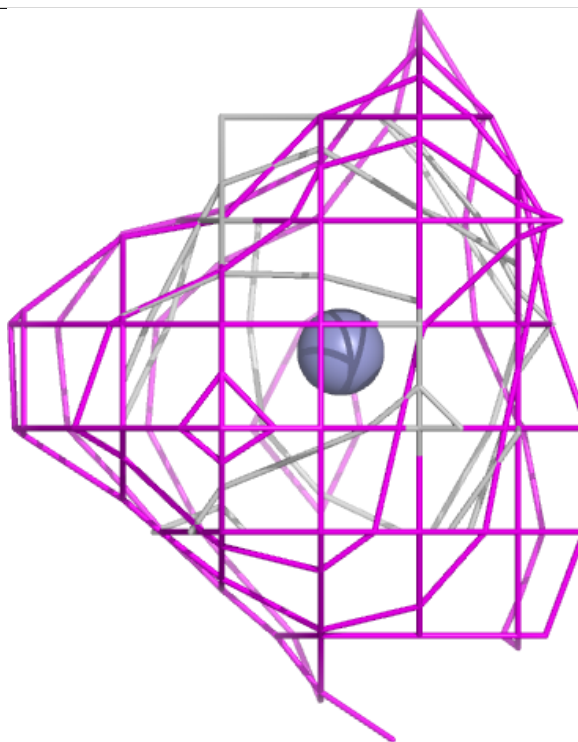
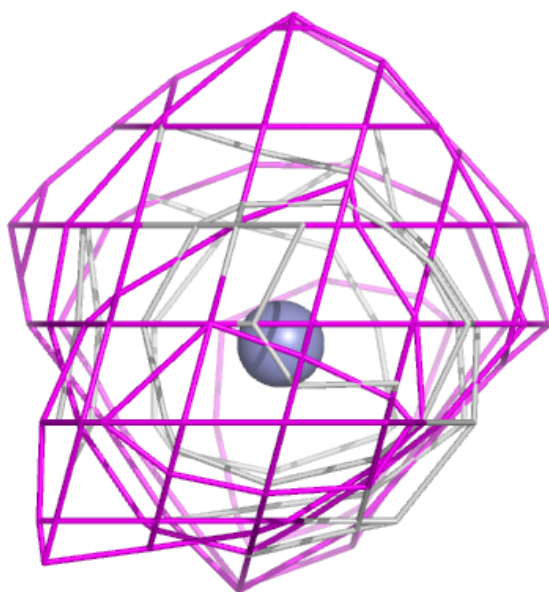
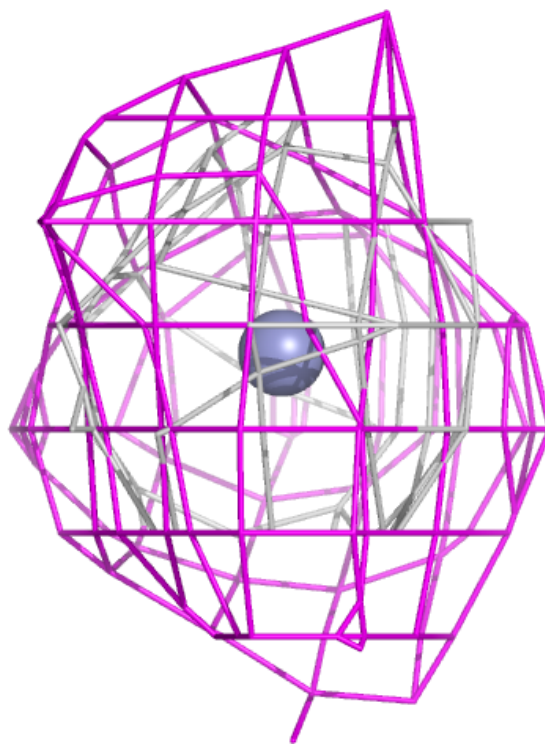
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and green (positive)



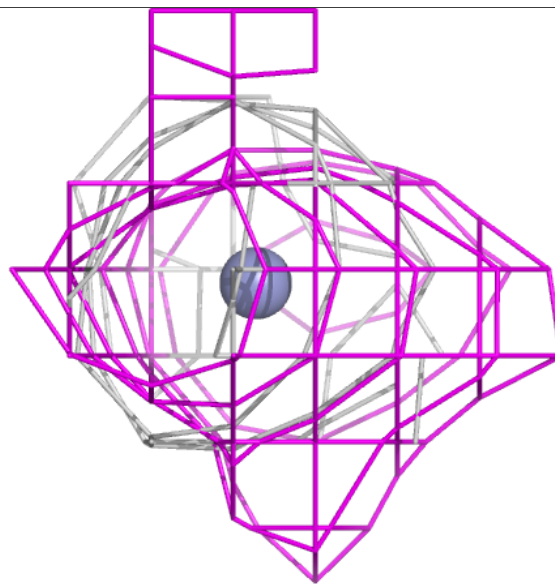
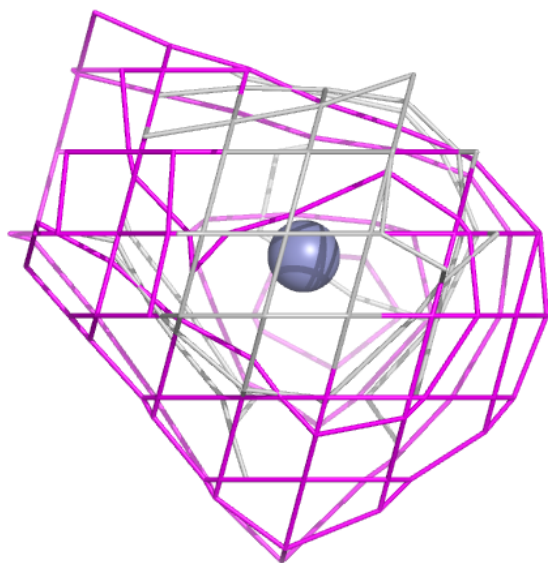
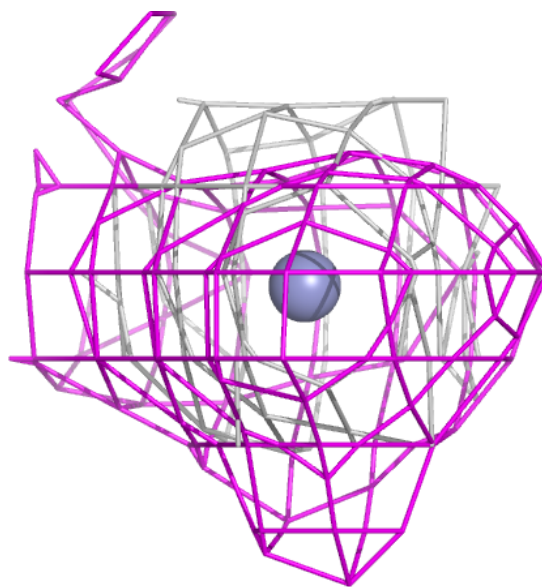
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and green (positive)



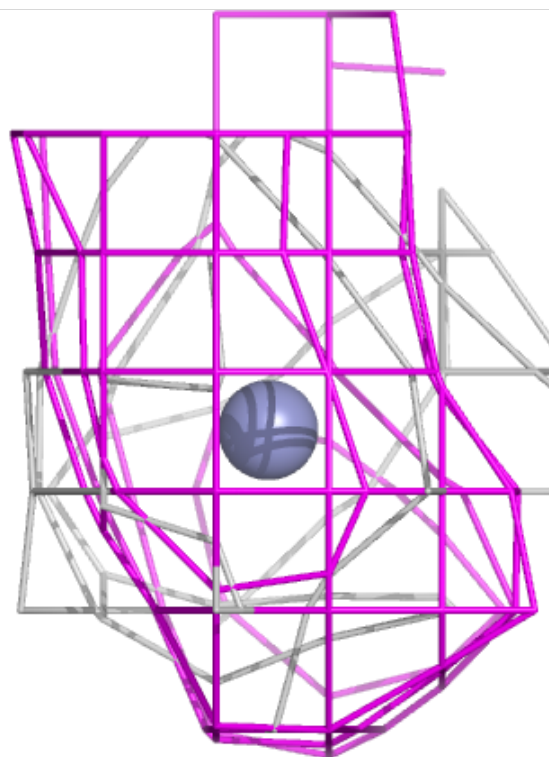
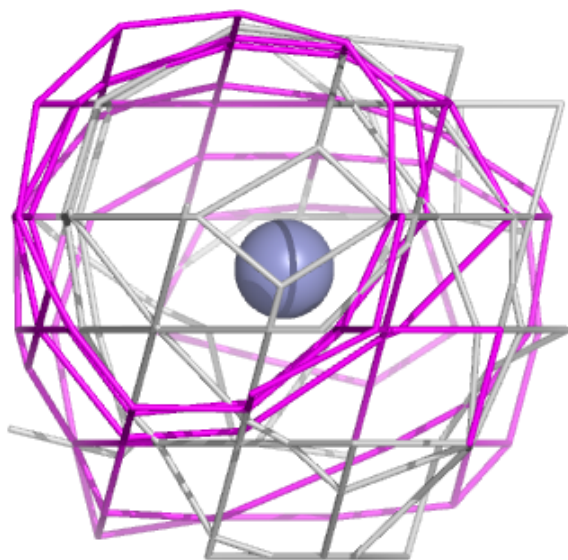
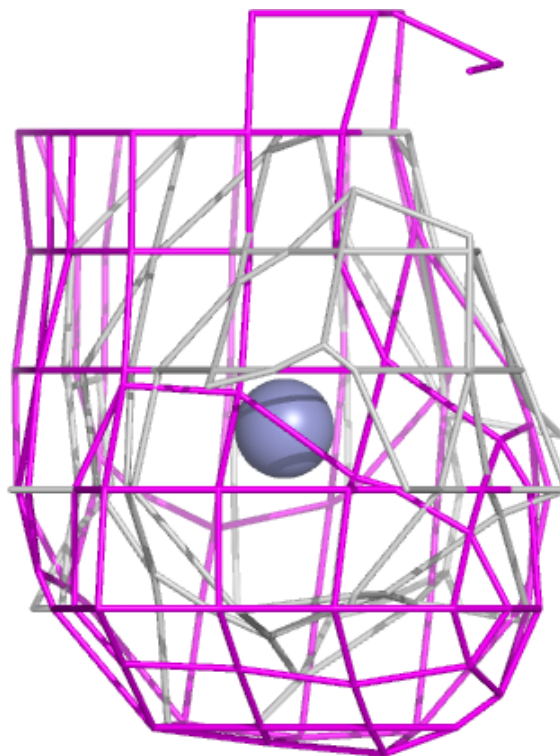
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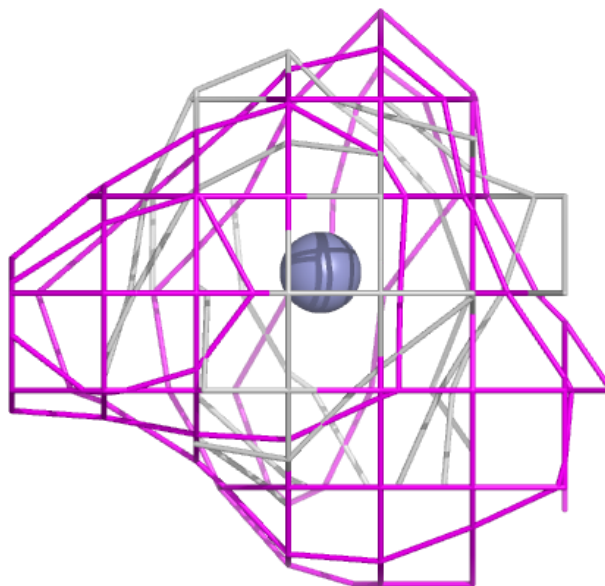
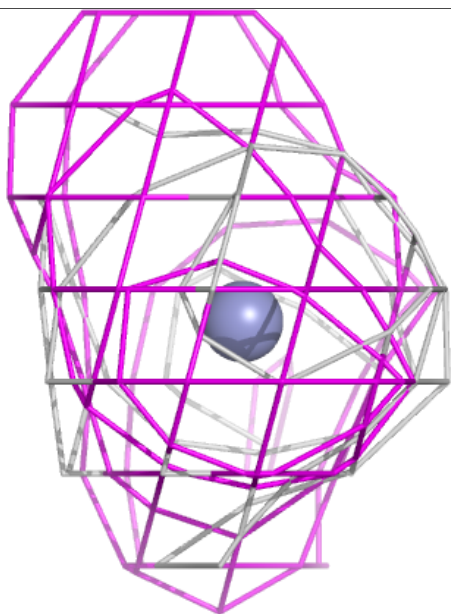
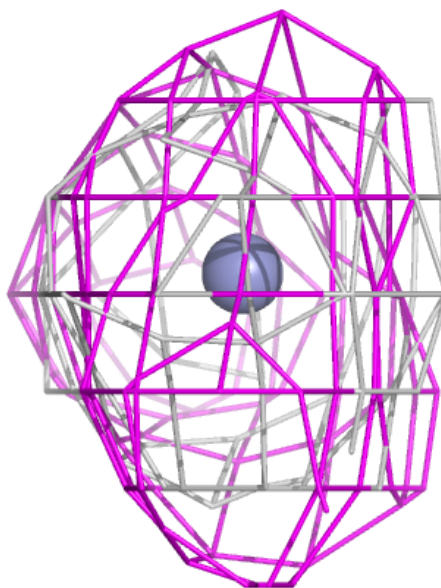
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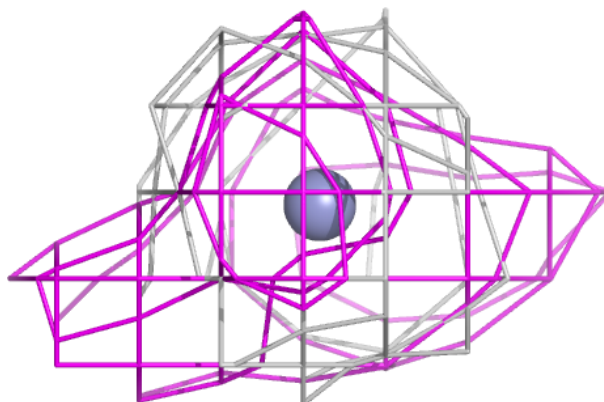
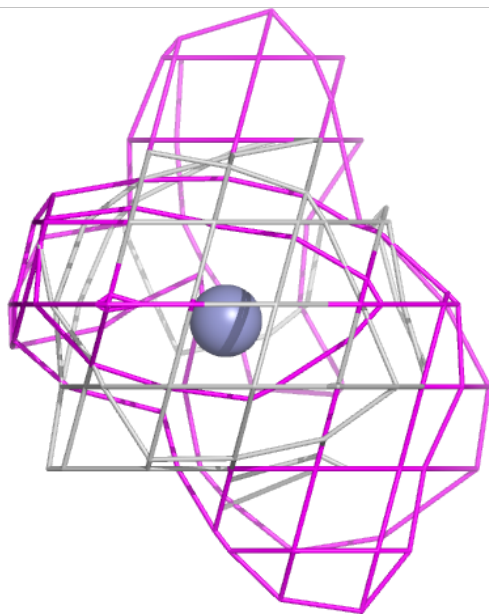
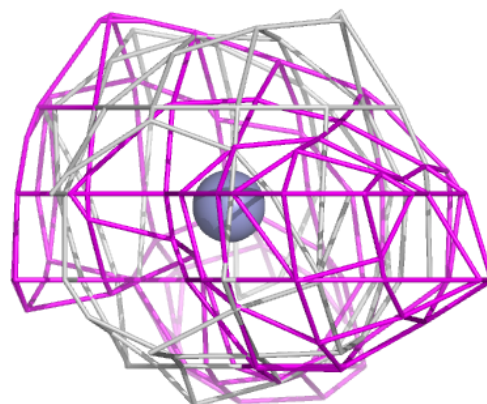
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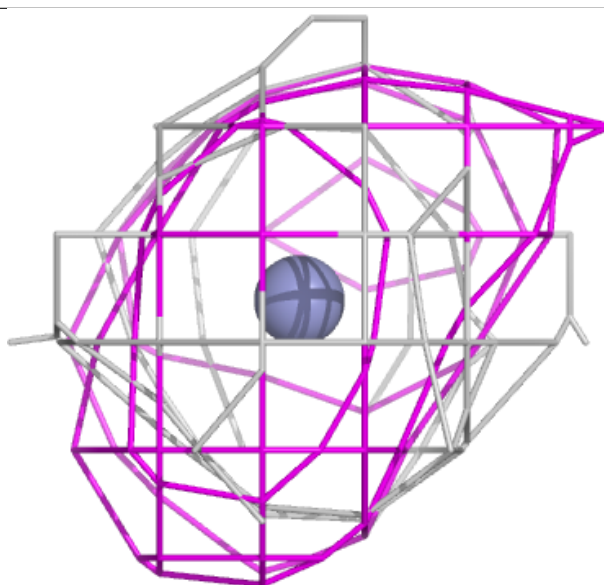
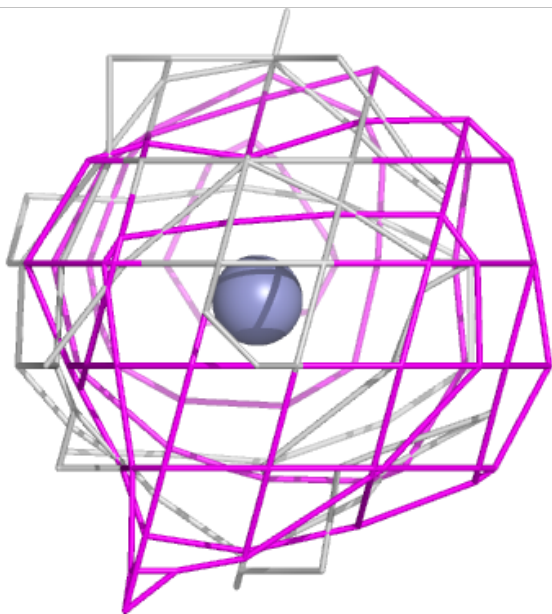
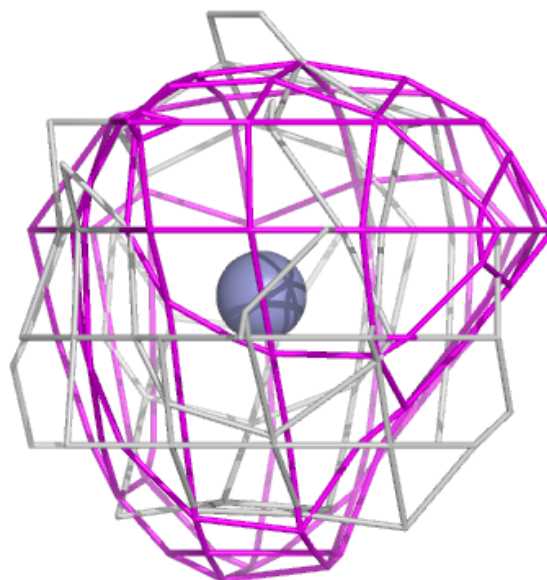
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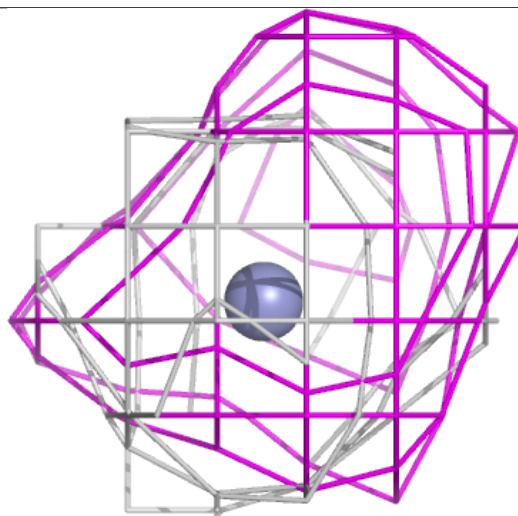
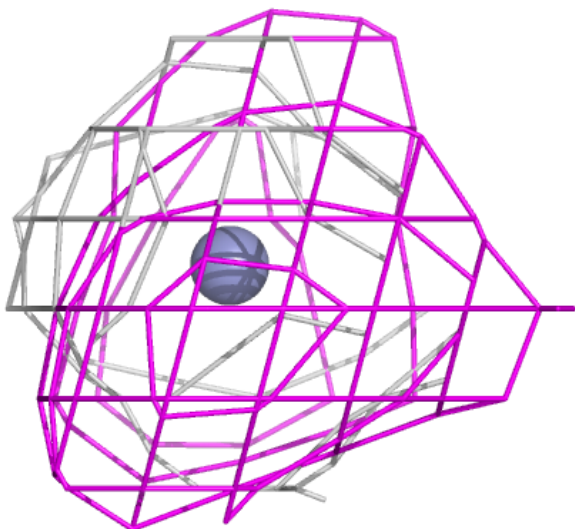
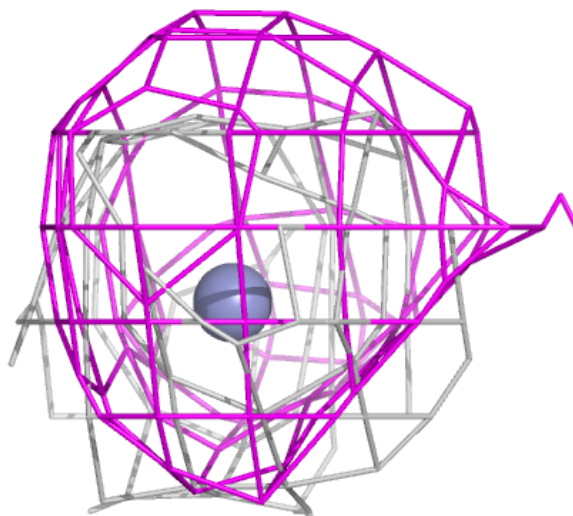
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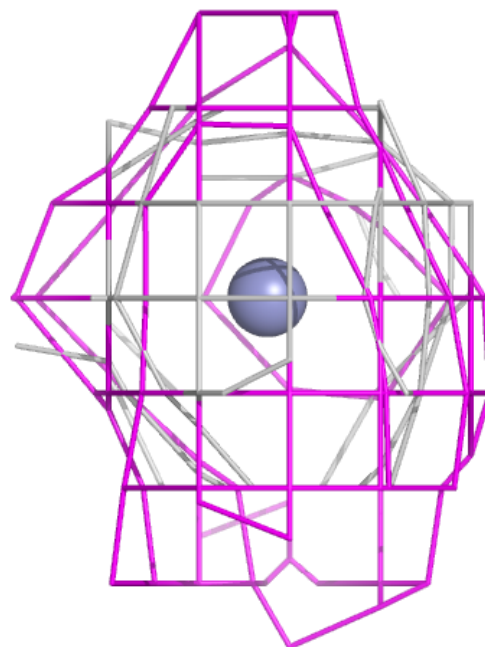
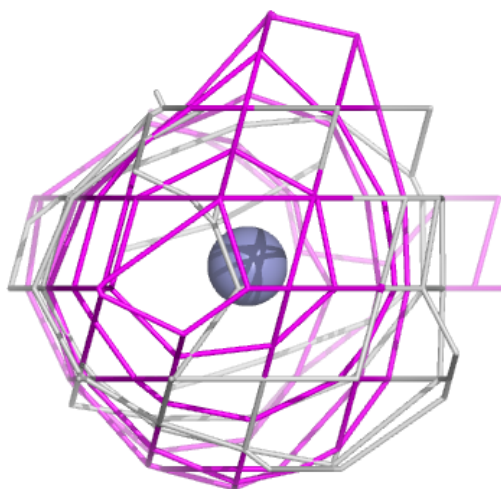
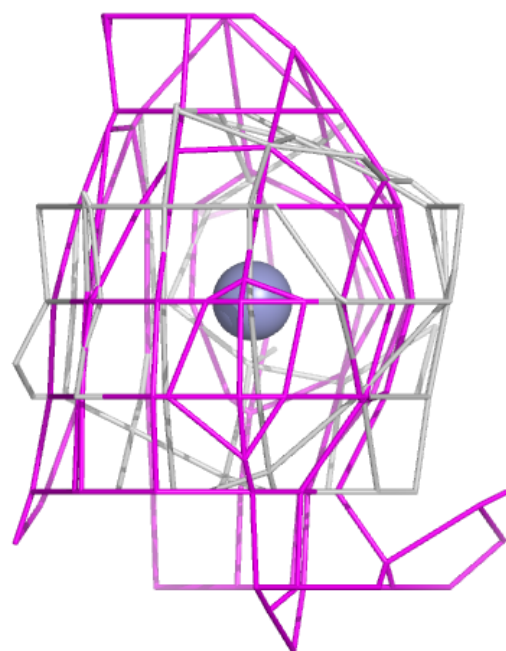
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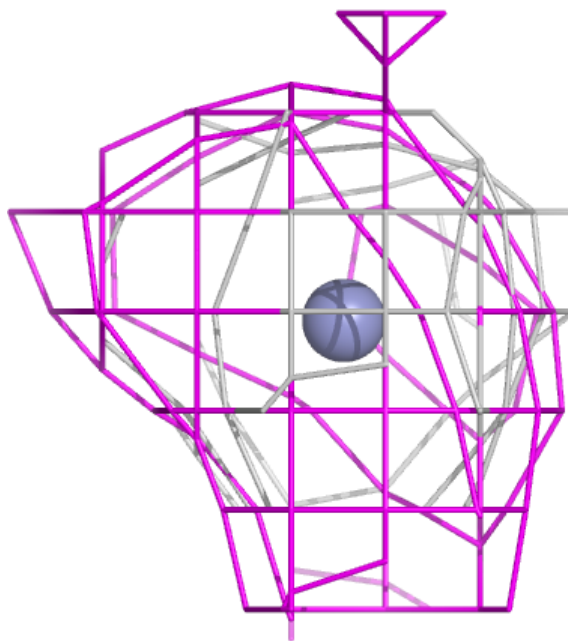
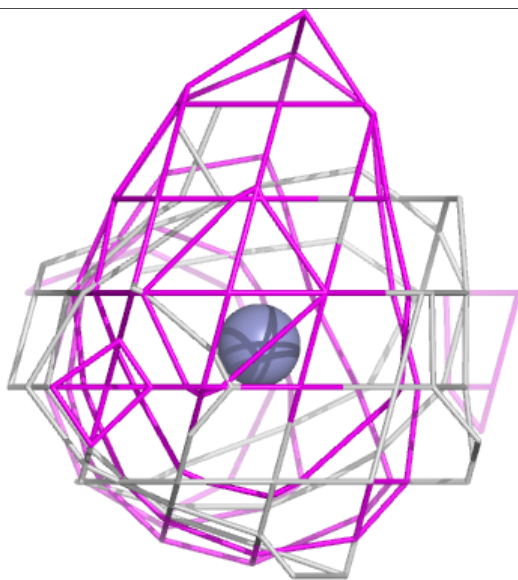
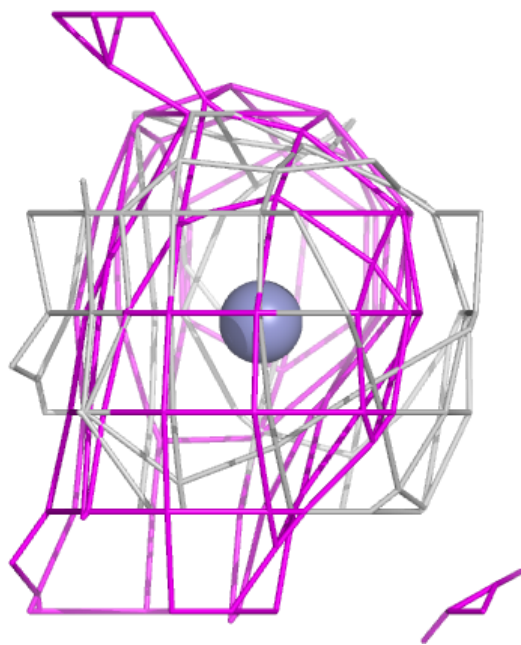
Electron density around ZN G 502:

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



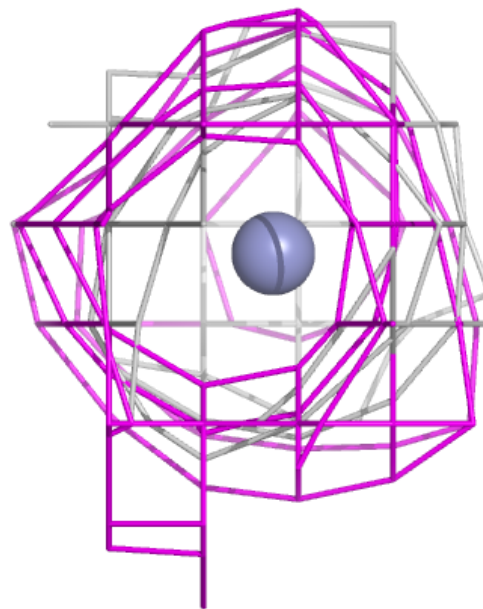
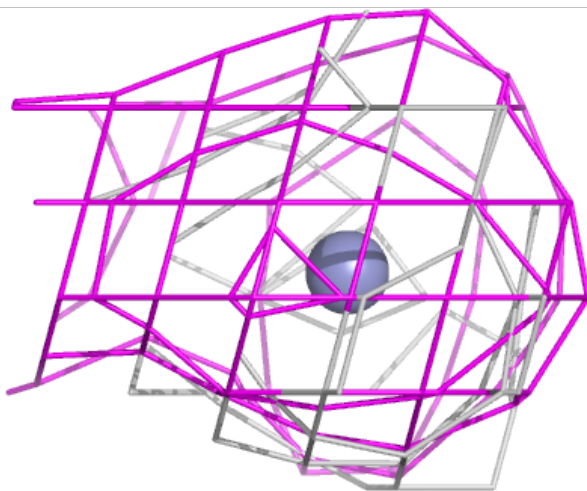
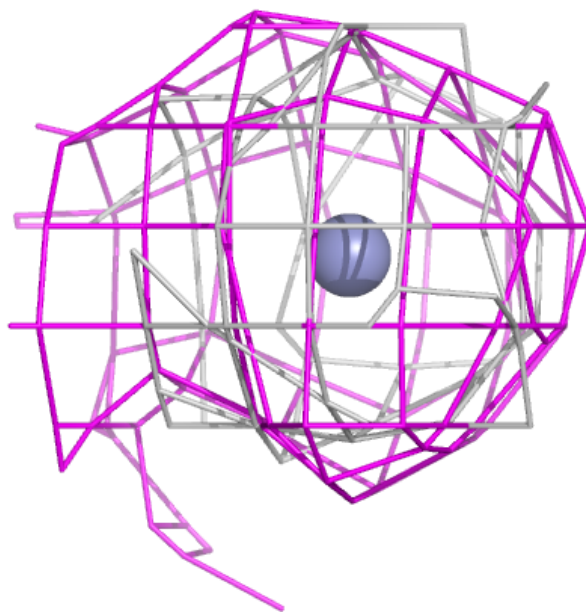
Electron density around ZN E 502:

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



Electron density around ZN H 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.