



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 11:16 PM EDT

PDB ID : 7T3V
Title : Metal dependent activation of Plasmodium falciparum M17 aminopeptidase, spacegroup P22121 after crystals soaked with Zn²⁺
Authors : Webb, C.T.; McGowan, S.
Deposited on : 2021-12-08
Resolution : 2.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

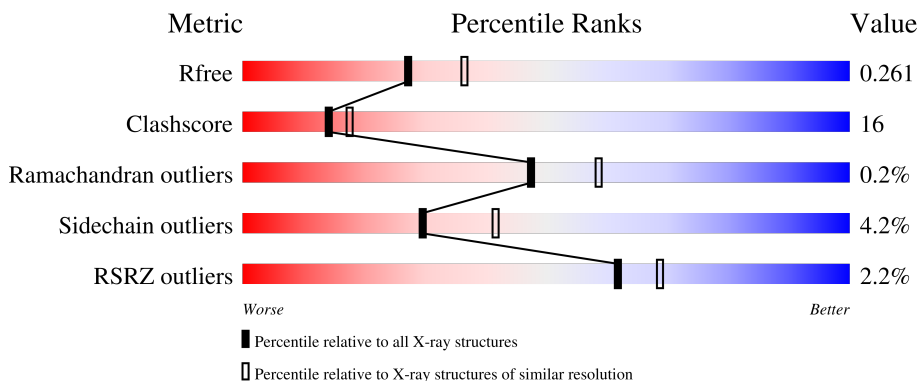
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	527	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">73% 24% ..</p>
1	B	527	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">65% 33% .</p>
1	C	527	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">68% 28% ..</p>
1	D	527	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">71% 25% ..</p>
1	E	527	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">67% 29% ..</p>

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Mol	Chain	Length	Quality of chain
1	F	527	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CO3	B	701	-	-	X	-
2	CO3	C	702	-	-	X	-
2	CO3	F	701	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23536 atoms, of which 28 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	3932	2527	635	750	20	0	0	0
1	B	518	3846	2472	621	733	20	0	0	0
1	C	518	3921	2524	628	749	20	0	0	0
1	D	517	3870	2490	623	738	19	0	0	0
1	E	511	3866	2489	623	735	19	0	0	0
1	F	509	3732	2399	605	709	19	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

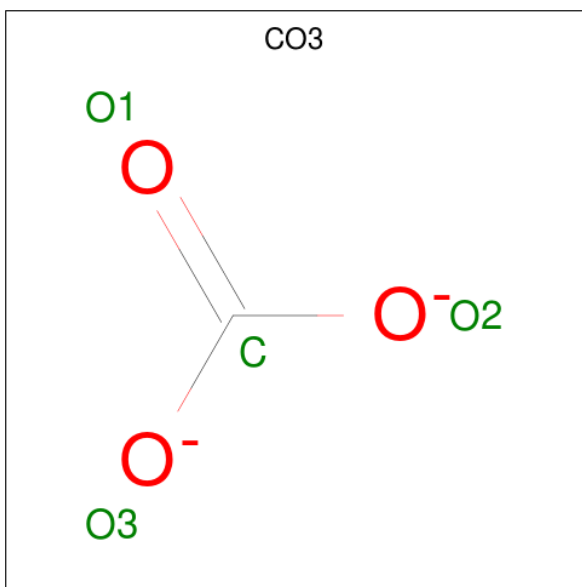
Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	conflict	UNP Q8IL11
A	515	GLN	ASN	conflict	UNP Q8IL11
A	546	GLN	ASN	conflict	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	conflict	UNP Q8IL11
B	515	GLN	ASN	conflict	UNP Q8IL11
B	546	GLN	ASN	conflict	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	conflict	UNP Q8IL11
C	515	GLN	ASN	conflict	UNP Q8IL11
C	546	GLN	ASN	conflict	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	conflict	UNP Q8IL11
D	515	GLN	ASN	conflict	UNP Q8IL11
D	546	GLN	ASN	conflict	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	conflict	UNP Q8IL11
E	515	GLN	ASN	conflict	UNP Q8IL11
E	546	GLN	ASN	conflict	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	conflict	UNP Q8IL11
F	515	GLN	ASN	conflict	UNP Q8IL11
F	546	GLN	ASN	conflict	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 1 3	0	0
2	B	1	Total C O 4 1 3	0	0
2	C	1	Total C O 4 1 3	0	0
2	D	1	Total C O 4 1 3	0	0
2	E	1	Total C O 4 1 3	0	0
2	F	1	Total C O 4 1 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

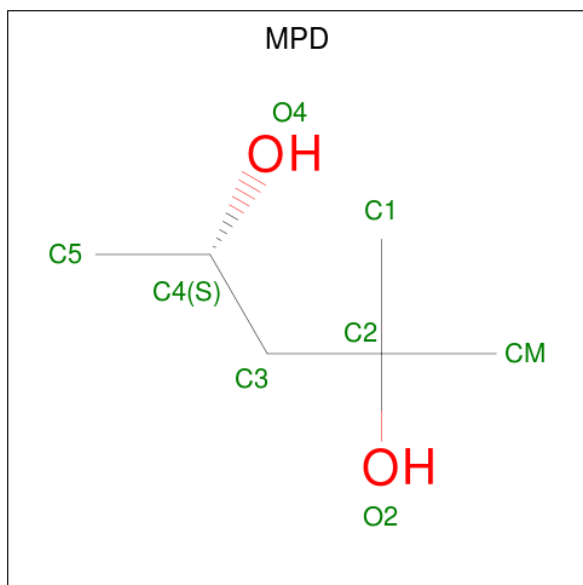
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0

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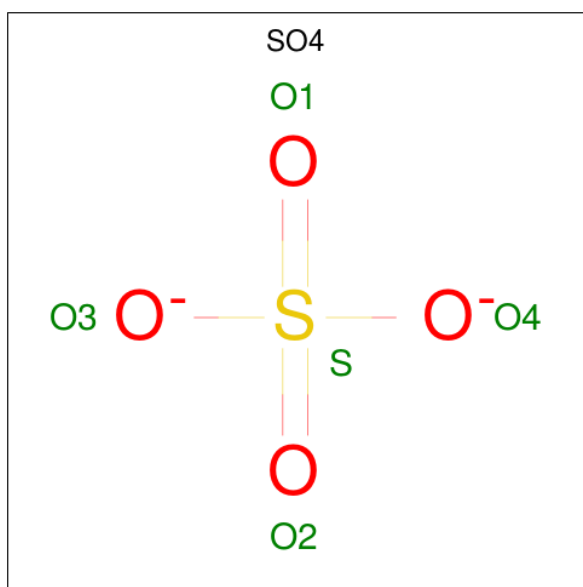
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Zn	0	0
			2	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			22	6	14	2		
4	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

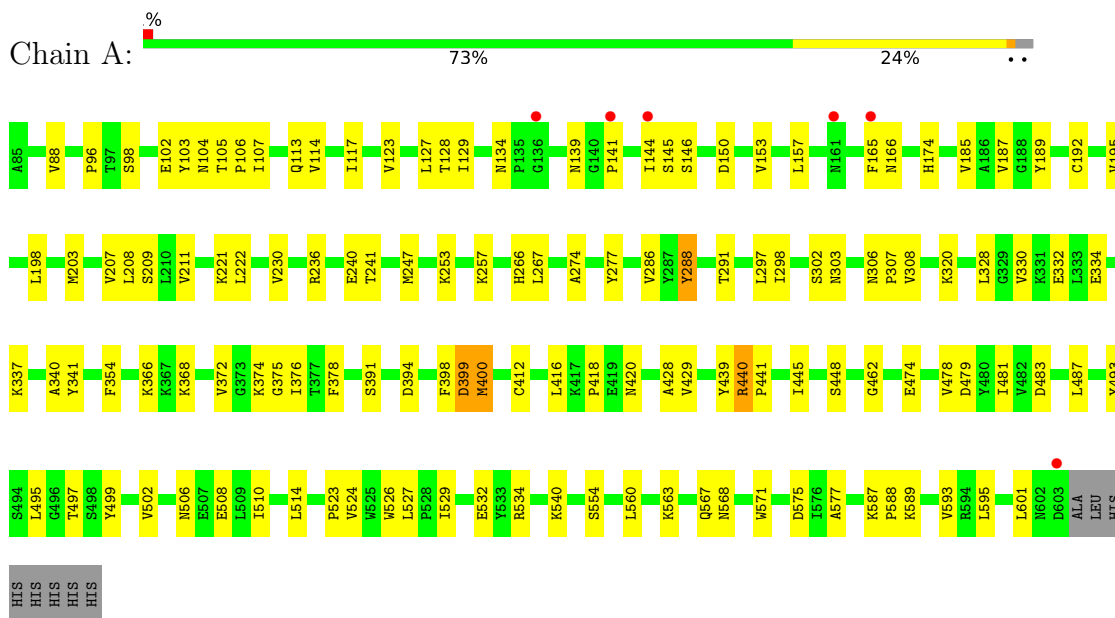
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	48	Total	O	0	0
			48	48		
6	B	46	Total	O	0	0
			46	46		
6	C	62	Total	O	0	0
			62	62		
6	D	42	Total	O	0	0
			42	42		
6	E	43	Total	O	0	0
			43	43		
6	F	38	Total	O	0	0
			38	38		

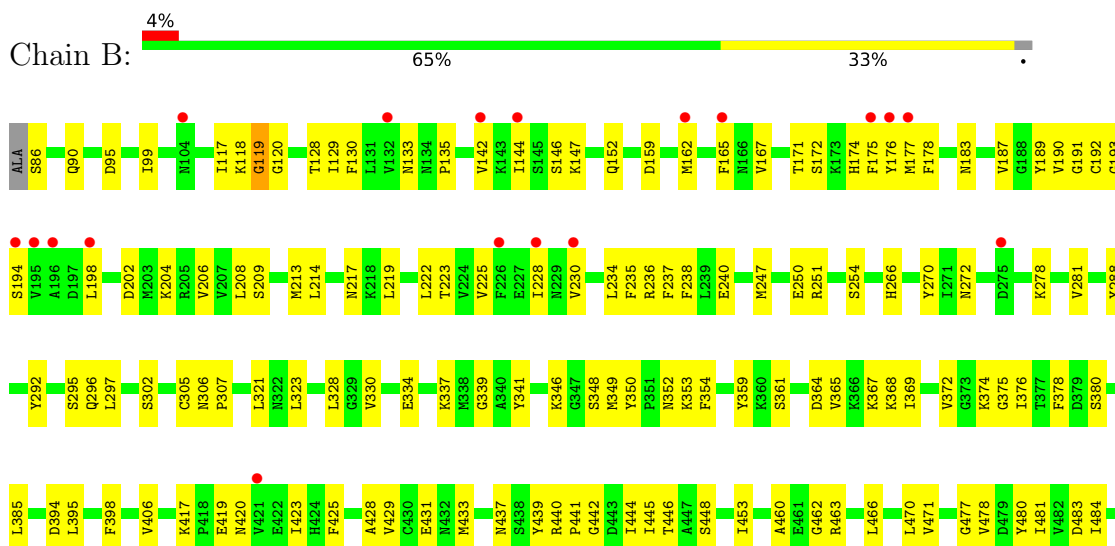
3 Residue-property plots i

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: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.76Å 172.76Å 176.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 2.30 47.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.24-2.30) 95.5 (47.24-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.264 0.219 , 0.261	Depositor DCC
R_{free} test set	1994 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtrriage
Anisotropy	0.704	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23536	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CO3, SO4, 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	0.28	0/4010	0.47	0/5450
1	B	0.28	0/3922	0.47	0/5342
1	C	0.31	0/3999	0.49	0/5433
1	D	0.29	0/3947	0.47	0/5368
1	E	0.29	0/3943	0.48	0/5357
1	F	0.28	0/3807	0.48	0/5189
All	All	0.29	0/23628	0.48	0/32139

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3932	0	3820	98	0
1	B	3846	0	3674	141	0
1	C	3921	0	3809	113	2
1	D	3870	0	3706	110	0
1	E	3866	0	3761	142	1
1	F	3732	0	3496	148	1
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	2	0
2	C	4	0	0	2	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	C	8	14	14	0	0
4	D	8	14	14	5	0
5	C	5	0	0	0	0
5	E	5	0	0	1	0
6	A	48	0	0	10	0
6	B	46	0	0	10	0
6	C	62	0	0	9	0
6	D	42	0	0	8	0
6	E	43	0	0	14	0
6	F	38	0	0	10	0
All	All	23508	28	22294	708	2

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 16.

The worst 5 of 708 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:B:230:VAL:HG23	1:B:234:LEU:HD23	1.35	1.07
1:B:133:ASN:HA	1:B:167:VAL:HG11	1.34	1.03
1:A:495:LEU:HD11	1:A:527:LEU:HD21	1.46	0.98
1:F:463:ARG:HD2	2:F:701:CO3:O3	1.63	0.97
1:C:456:GLY:O	6:C:801:HOH:O	1.84	0.96

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LYS:NZ	1:E:364:ASP:OD2[3_555]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASN:O	1:F:326:LYS:NZ[1_455]	2.18	0.02

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	517/527 (98%)	494 (96%)	23 (4%)	0	100	100
1	B	516/527 (98%)	484 (94%)	29 (6%)	3 (1%)	25	31
1	C	516/527 (98%)	498 (96%)	17 (3%)	1 (0%)	47	58
1	D	513/527 (97%)	492 (96%)	21 (4%)	0	100	100
1	E	507/527 (96%)	486 (96%)	20 (4%)	1 (0%)	47	58
1	F	503/527 (95%)	480 (95%)	21 (4%)	2 (0%)	34	42
All	All	3072/3162 (97%)	2934 (96%)	131 (4%)	7 (0%)	47	58

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	357	LEU
1	E	137	LYS
1	F	477	GLY
1	B	119	GLY
1	B	553	ALA

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	412/454 (91%)	401 (97%)	11 (3%)	44	61
1	B	392/454 (86%)	378 (96%)	14 (4%)	35	49
1	C	411/454 (90%)	388 (94%)	23 (6%)	21	29
1	D	395/454 (87%)	375 (95%)	20 (5%)	24	33
1	E	405/454 (89%)	389 (96%)	16 (4%)	31	44
1	F	369/454 (81%)	353 (96%)	16 (4%)	29	40
All	All	2384/2724 (88%)	2284 (96%)	100 (4%)	30	42

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	435	SER
1	E	219	LEU
1	F	483	ASP
1	D	439	TYR
1	D	518	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	215	HIS
1	E	166	ASN
1	E	538	ASN
1	E	420	ASN
1	B	217	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CO3	B	701	-	2,3,3	0.40	0	2,3,3	0.24	0
2	CO3	A	701	-	2,3,3	0.39	0	2,3,3	0.27	0
2	CO3	F	701	1	2,3,3	0.31	0	2,3,3	1.51	0
4	MPD	C	701	-	7,7,7	0.26	0	9,10,10	0.58	0
4	MPD	D	701	-	7,7,7	0.23	0	9,10,10	0.40	0
5	SO4	C	705	-	4,4,4	0.16	0	6,6,6	0.12	0
2	CO3	D	702	1	2,3,3	0.36	0	2,3,3	0.50	0
2	CO3	C	702	-	2,3,3	0.48	0	2,3,3	0.61	0
5	SO4	E	704	-	4,4,4	0.16	0	6,6,6	0.14	0
2	CO3	E	701	-	2,3,3	0.38	0	2,3,3	0.12	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	MPD	C	701	-	-	0/5/5/5	-
4	MPD	D	701	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	701	MPD	C2-C3-C4-O4
4	D	701	MPD	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	CO3	2	0
2	F	701	CO3	5	0
4	D	701	MPD	5	0
2	C	702	CO3	2	0
5	E	704	SO4	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 [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	519/527 (98%)	0.21	6 (1%) 79 83	41, 52, 74, 92	0
1	B	518/527 (98%)	0.24	19 (3%) 41 48	41, 56, 87, 97	0
1	C	518/527 (98%)	0.20	11 (2%) 63 70	40, 50, 78, 90	0
1	D	517/527 (98%)	0.13	10 (1%) 66 73	41, 53, 76, 89	0
1	E	511/527 (96%)	0.15	9 (1%) 68 74	40, 54, 73, 86	0
1	F	509/527 (96%)	0.27	13 (2%) 56 63	43, 57, 87, 98	0
All	All	3092/3162 (97%)	0.20	68 (2%) 62 69	40, 54, 81, 98	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	140	GLY	4.4
1	F	144	ILE	4.3
1	F	128	THR	4.2
1	C	141	PRO	4.1
1	B	230	VAL	3.9

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 monosaccharides in this entry.

6.4 Ligands [i](#)

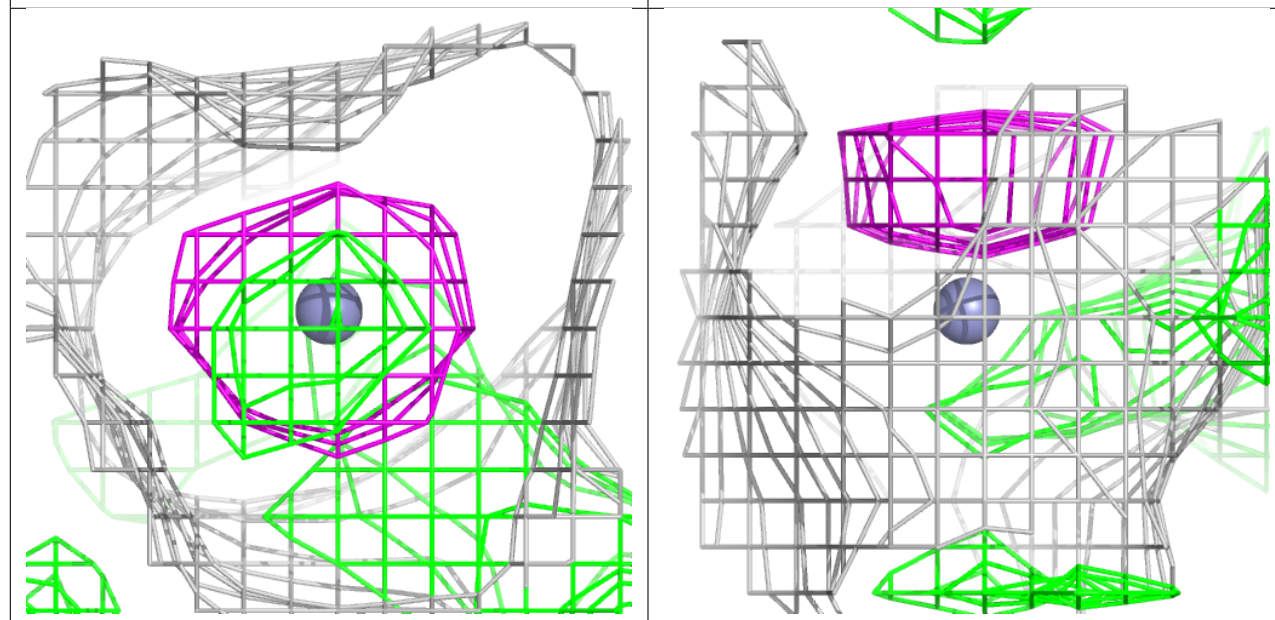
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CO3	F	701	4/4	0.61	0.25	49,53,55,62	0
2	CO3	D	702	4/4	0.69	0.19	52,54,62,62	0
3	ZN	B	702	1/1	0.70	0.13	51,51,51,51	0
3	ZN	B	703	1/1	0.73	0.13	52,52,52,52	0
3	ZN	D	704	1/1	0.80	0.12	52,52,52,52	0
2	CO3	C	702	4/4	0.91	0.21	49,50,52,57	0
4	MPD	D	701	8/8	0.91	0.27	51,70,86,90	0
2	CO3	A	701	4/4	0.92	0.19	44,46,48,55	0
3	ZN	F	703	1/1	0.92	0.15	54,54,54,54	0
3	ZN	C	704	1/1	0.92	0.12	50,50,50,50	0
3	ZN	A	702	1/1	0.93	0.13	48,48,48,48	1
3	ZN	E	703	1/1	0.93	0.12	47,47,47,47	0
3	ZN	F	702	1/1	0.93	0.13	55,55,55,55	0
2	CO3	B	701	4/4	0.93	0.15	52,52,53,62	0
3	ZN	D	703	1/1	0.93	0.15	49,49,49,49	0
4	MPD	C	701	8/8	0.94	0.13	51,63,69,69	0
3	ZN	C	703	1/1	0.95	0.13	49,49,49,49	0
3	ZN	E	702	1/1	0.96	0.14	50,50,50,50	0
3	ZN	A	703	1/1	0.96	0.12	50,50,50,50	0
2	CO3	E	701	4/4	0.97	0.13	49,52,56,63	0
5	SO4	C	705	5/5	0.97	0.13	42,46,50,57	0
5	SO4	E	704	5/5	0.98	0.12	46,47,51,53	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.

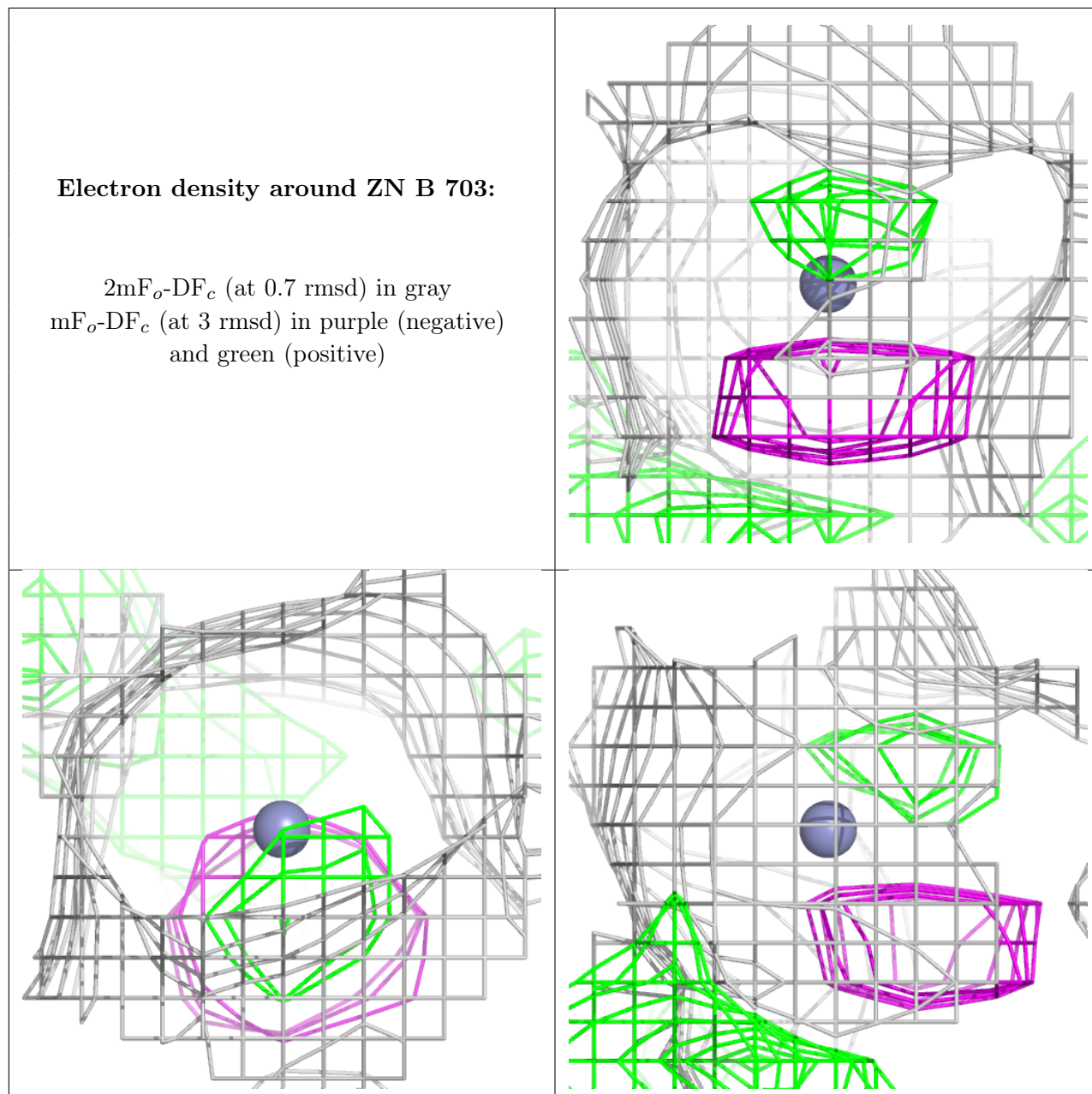
Electron density around ZN B 702:

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



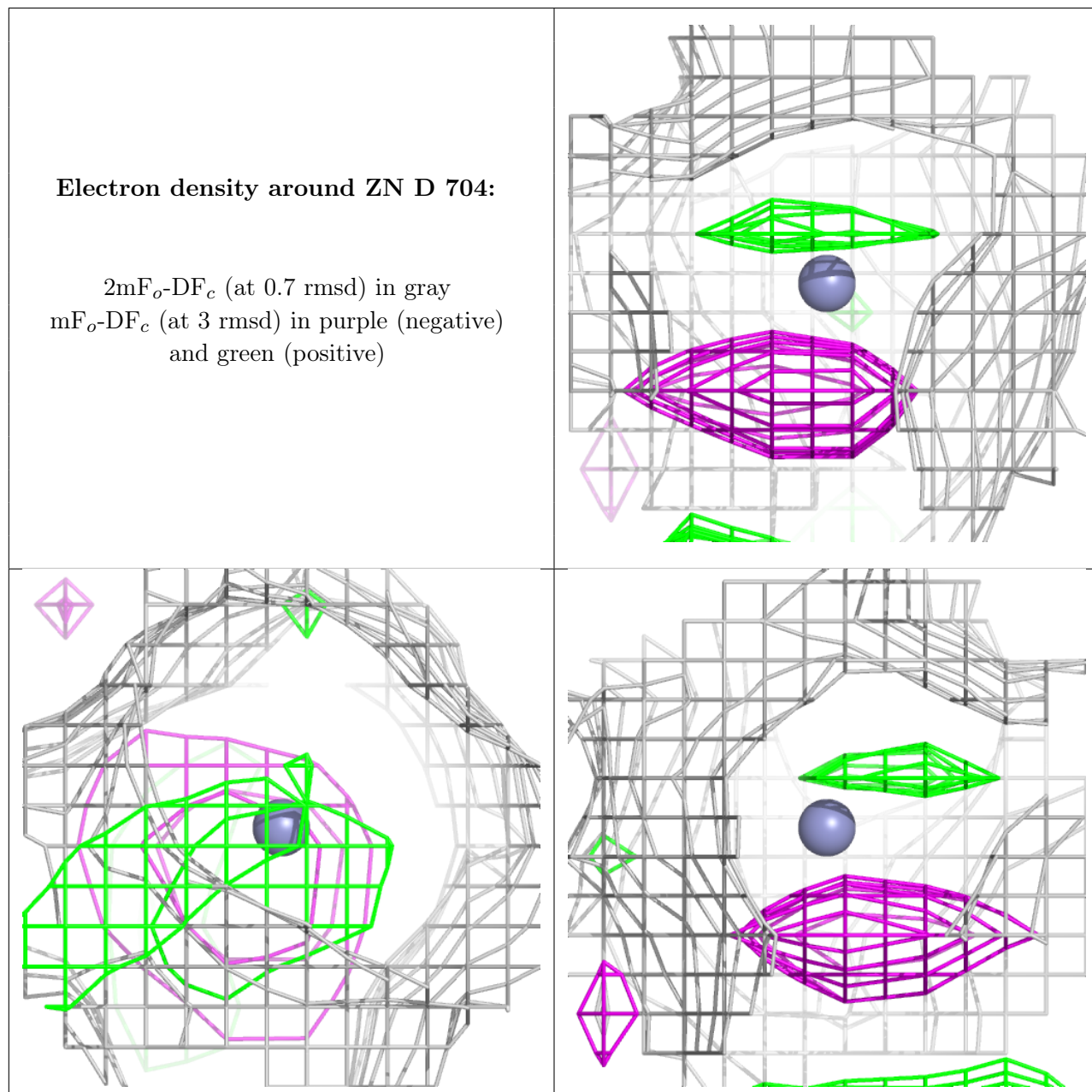
Electron density around ZN B 703:

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



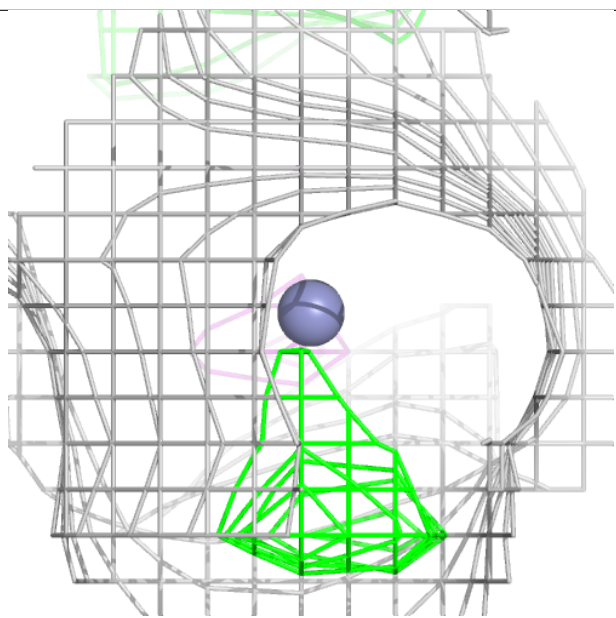
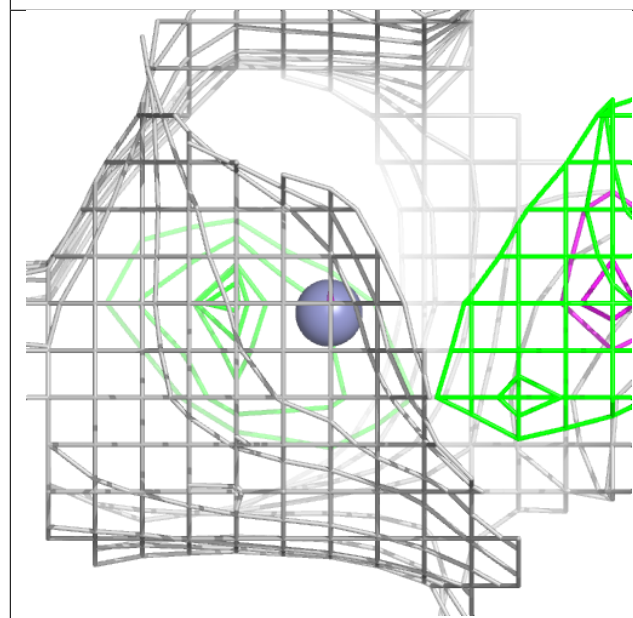
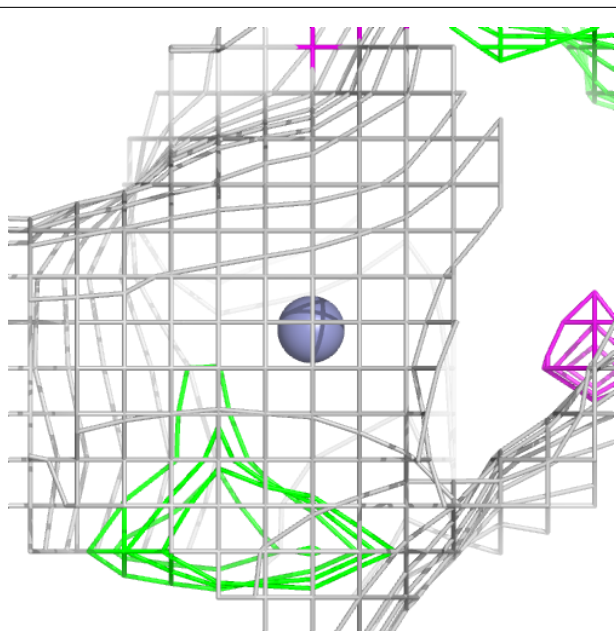
Electron density around ZN D 704:

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



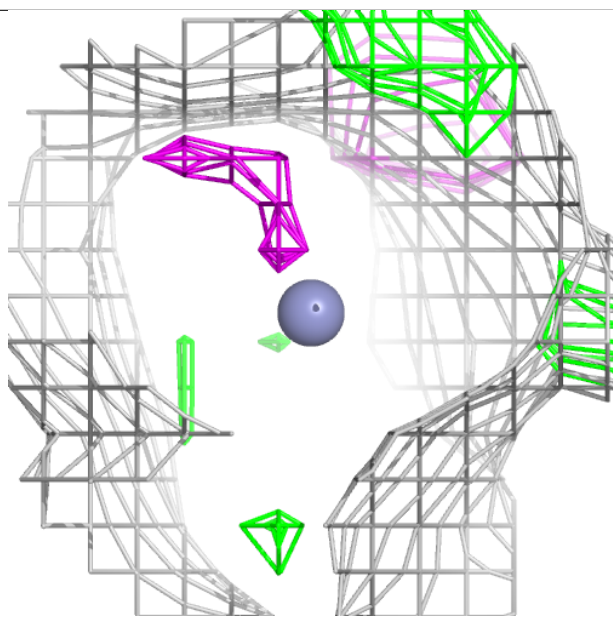
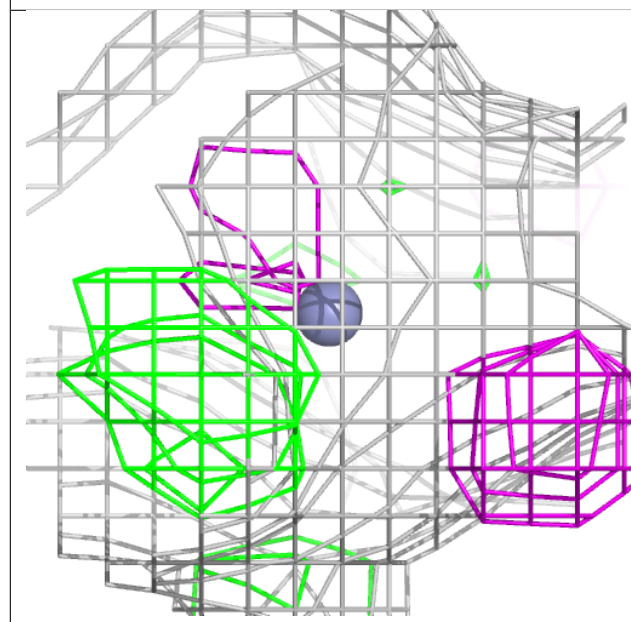
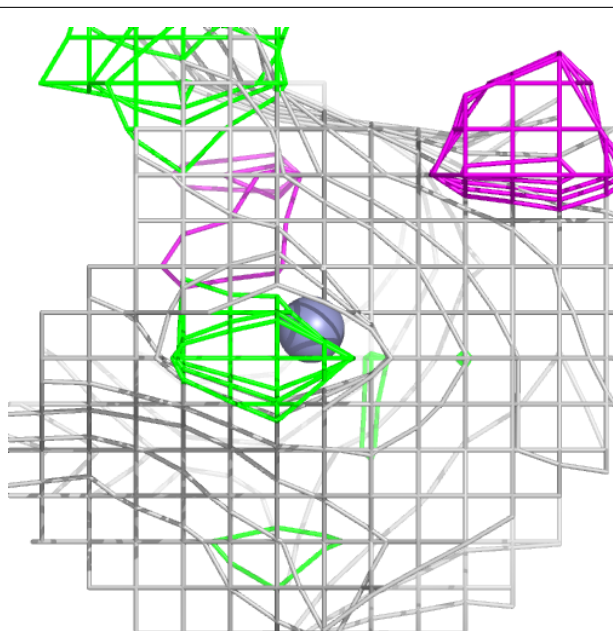
Electron density around ZN F 703:

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



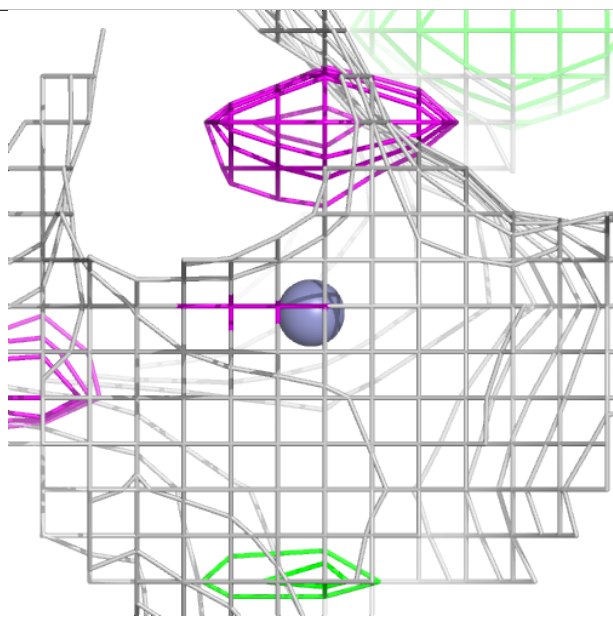
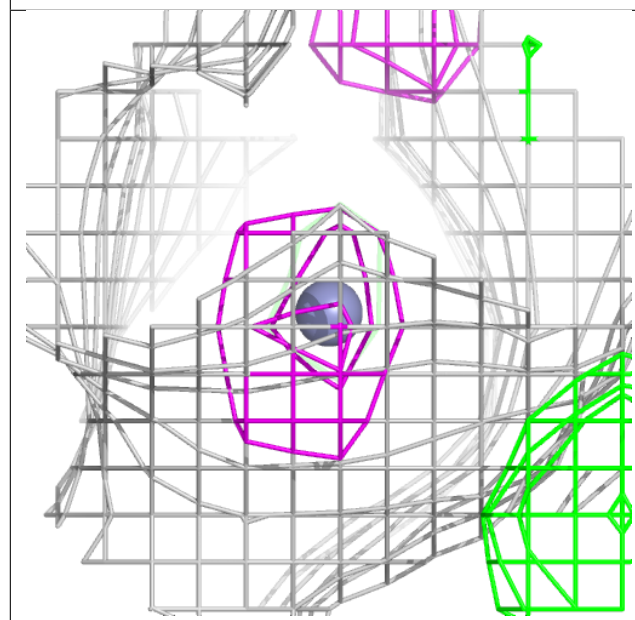
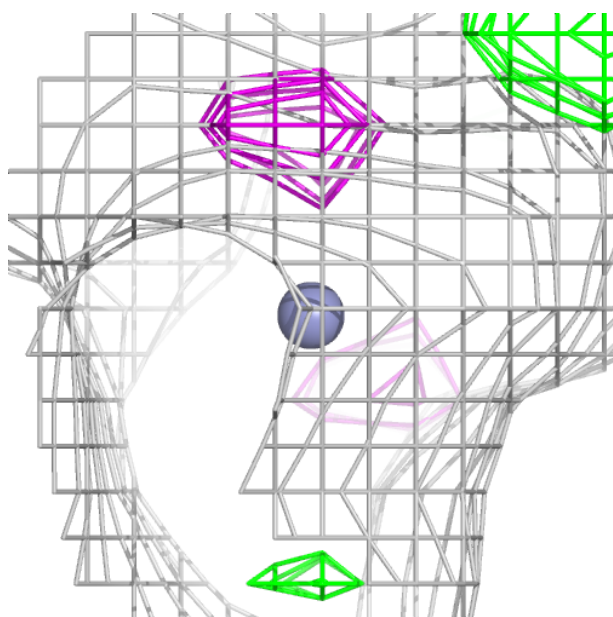
Electron density around ZN C 704:

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and green (positive)



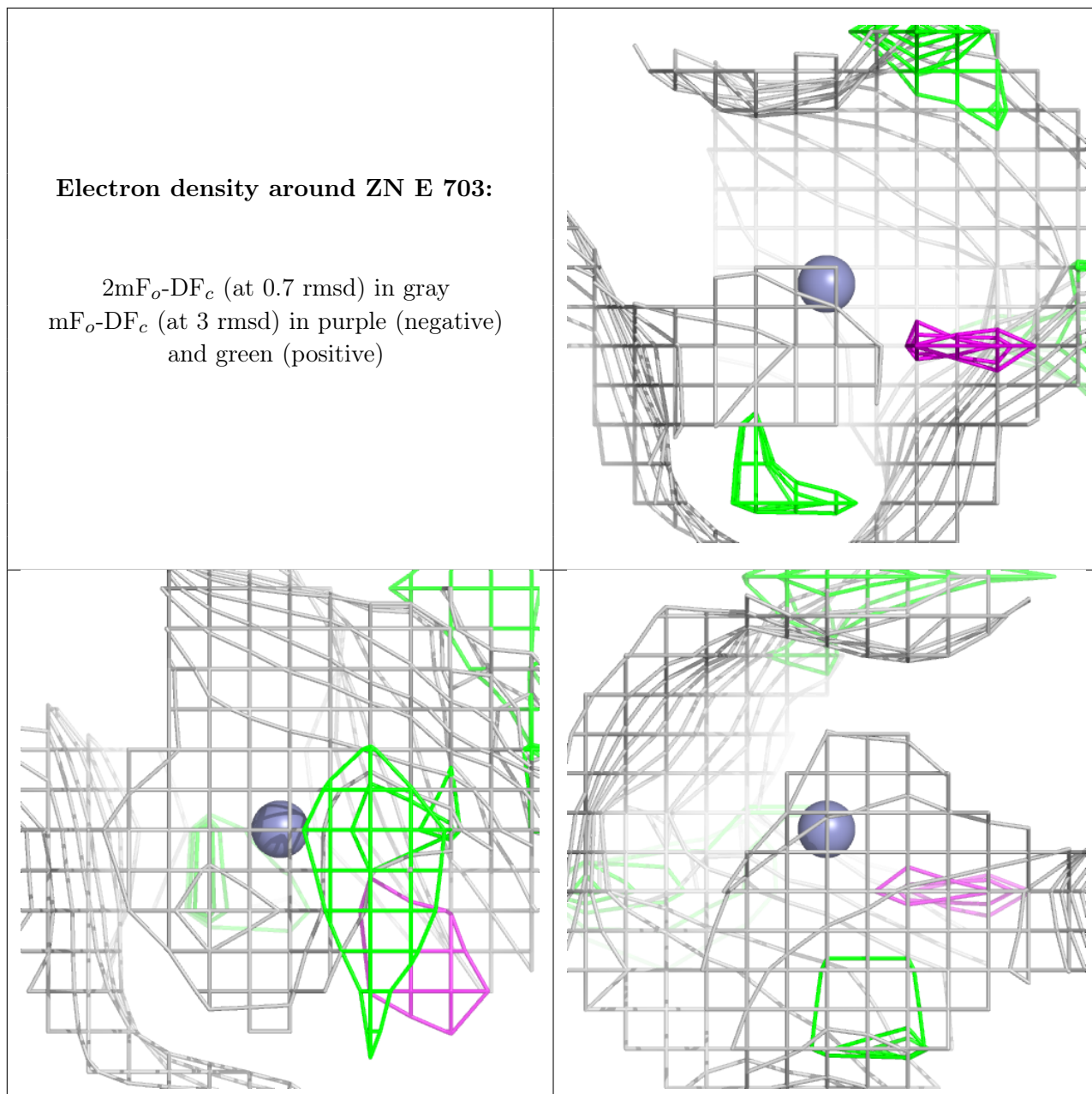
Electron density around ZN A 702:

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



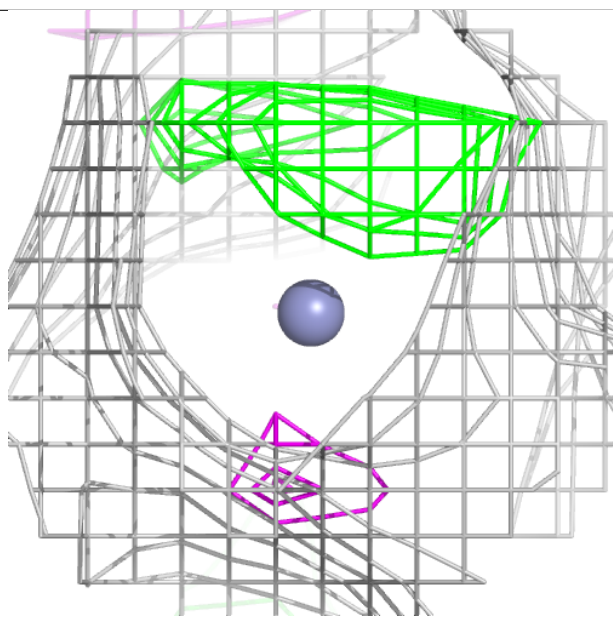
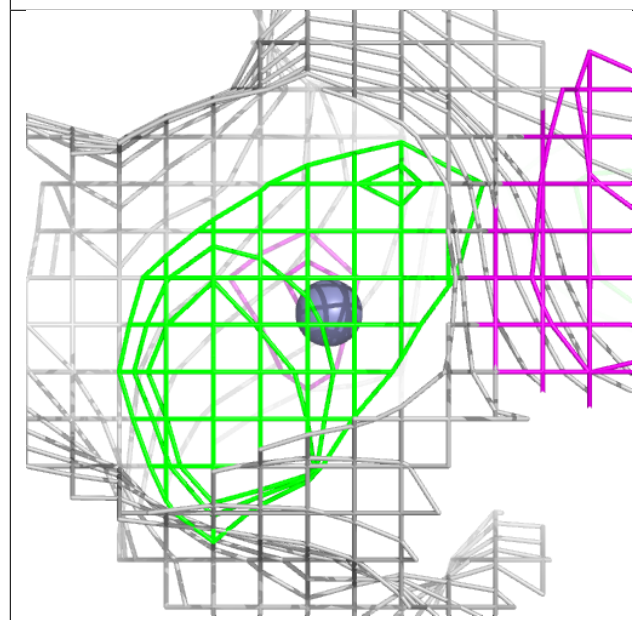
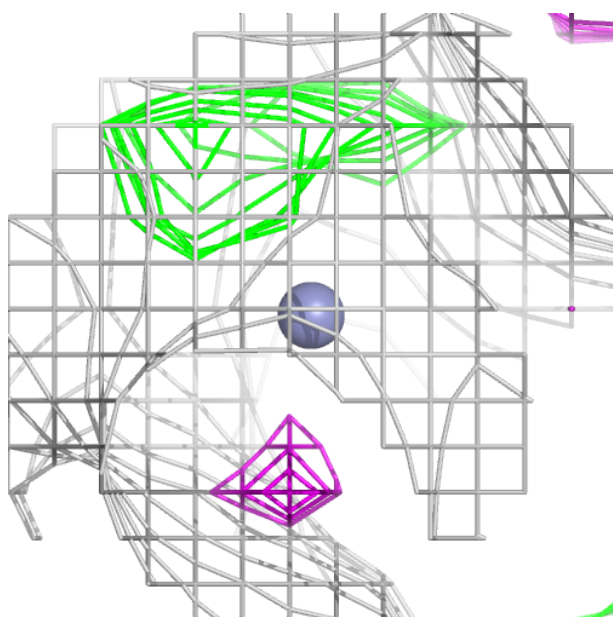
Electron density around ZN E 703:

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



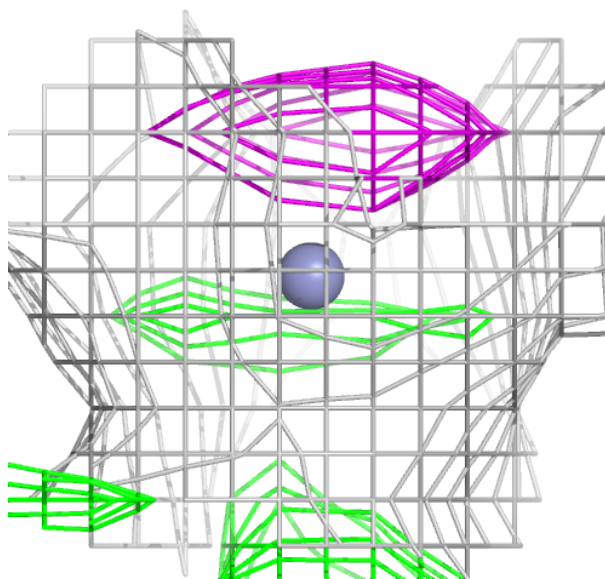
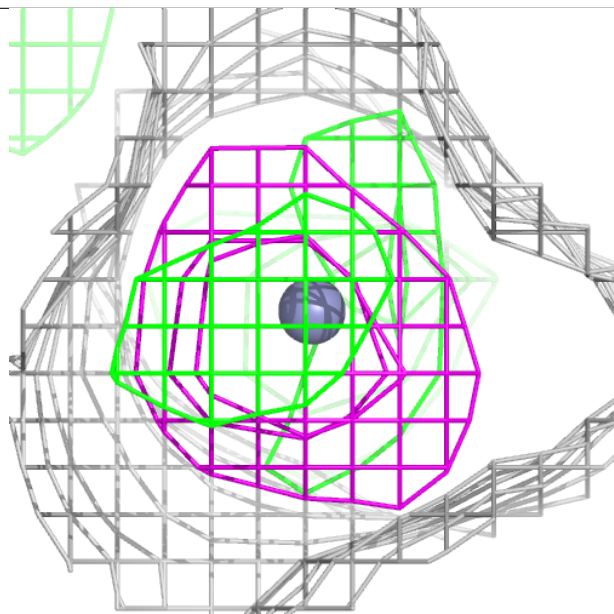
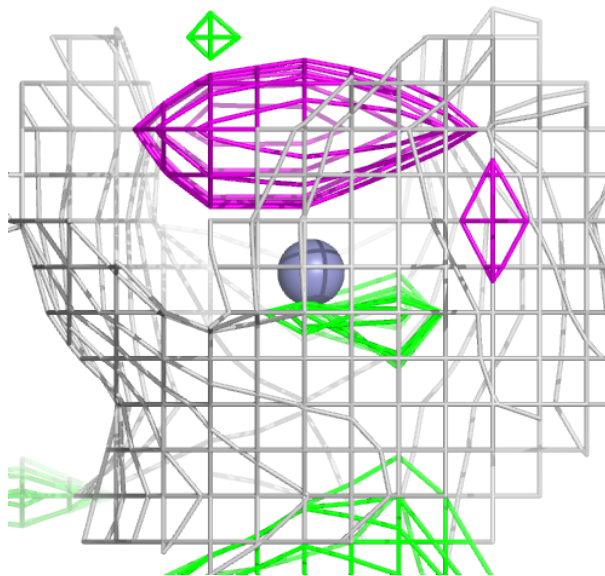
Electron density around ZN F 702:

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



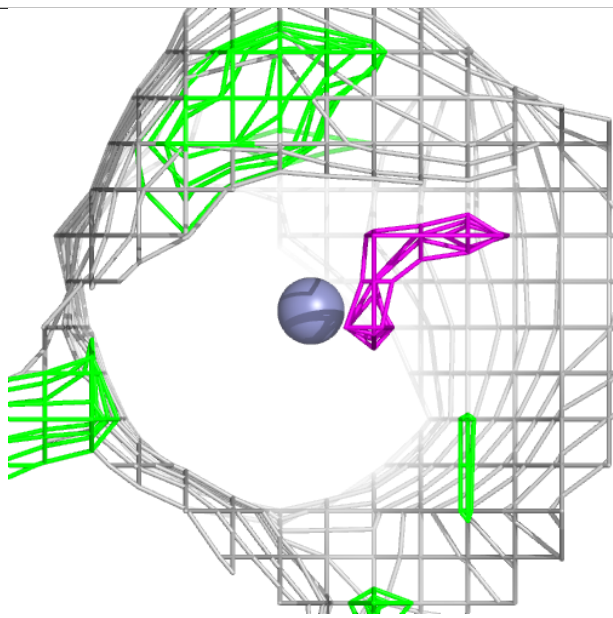
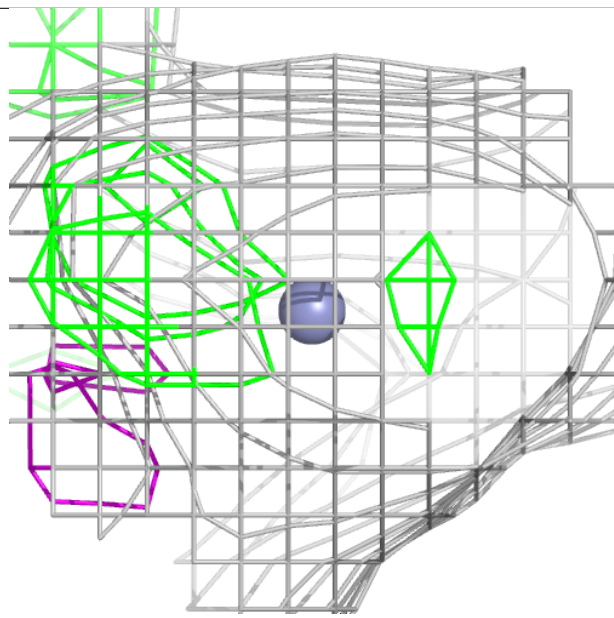
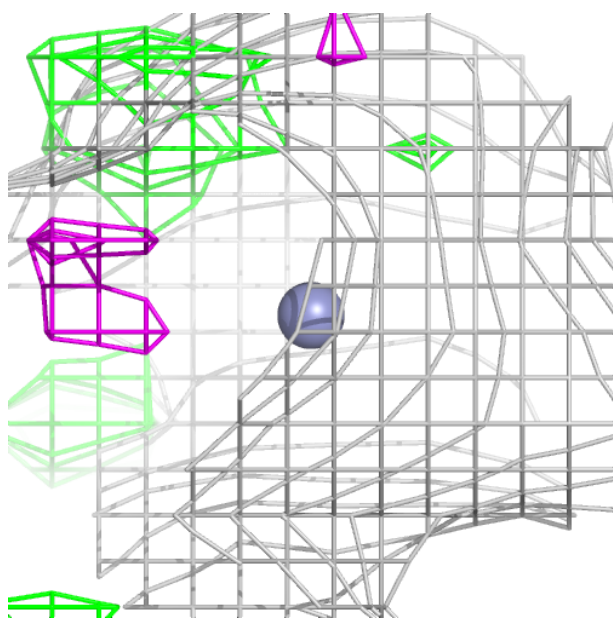
Electron density around ZN D 703:

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



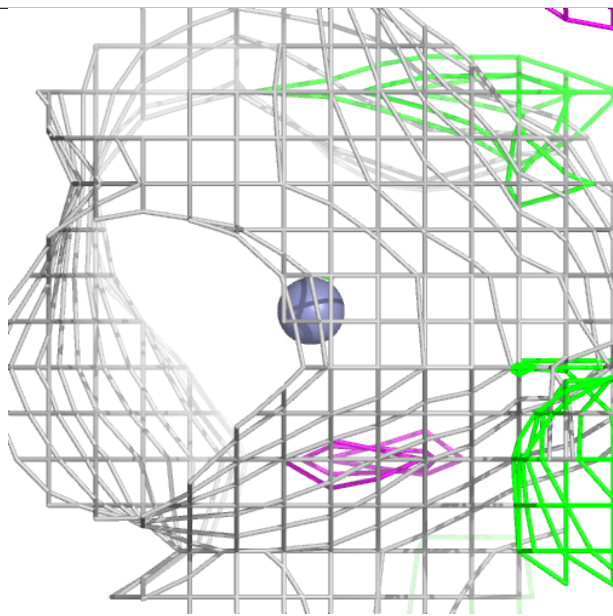
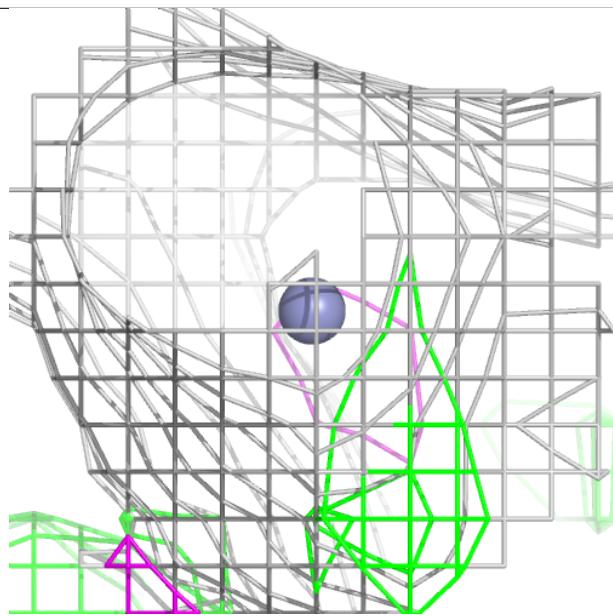
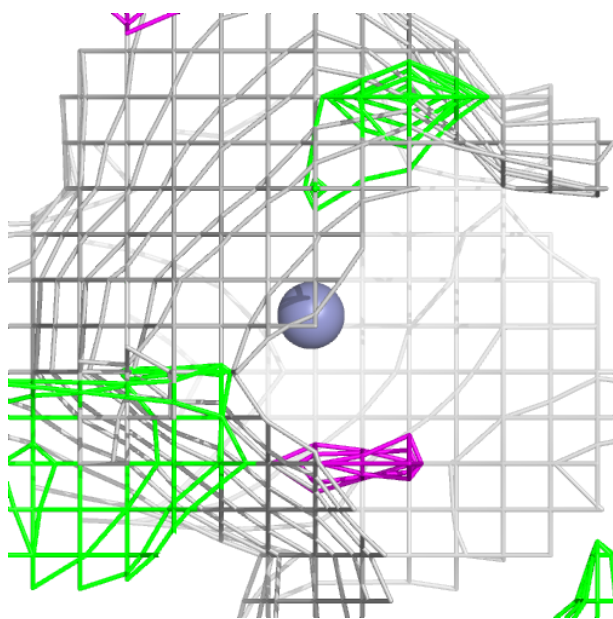
Electron density around ZN C 703:

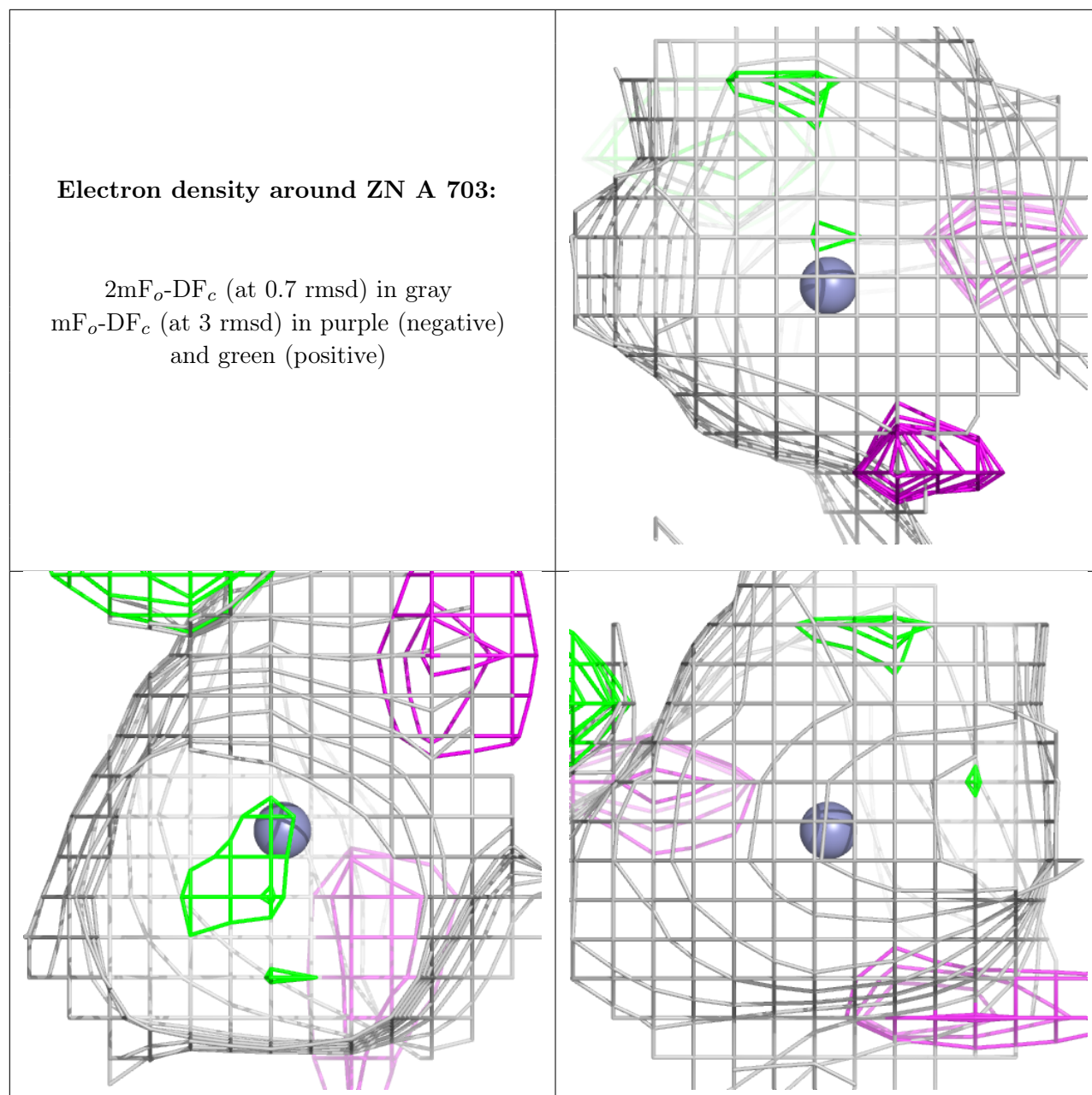
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN E 702:

$2mF_o-DF_c$ (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.