



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 1, 2025 – 06:19 pm GMT

PDB ID : 9QEZ / pdb_00009qez
Title : Carbonic anhydrase mutant
Authors : Mohsin, I.; Papageorgiou, A.C.
Deposited on : 2025-03-11
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

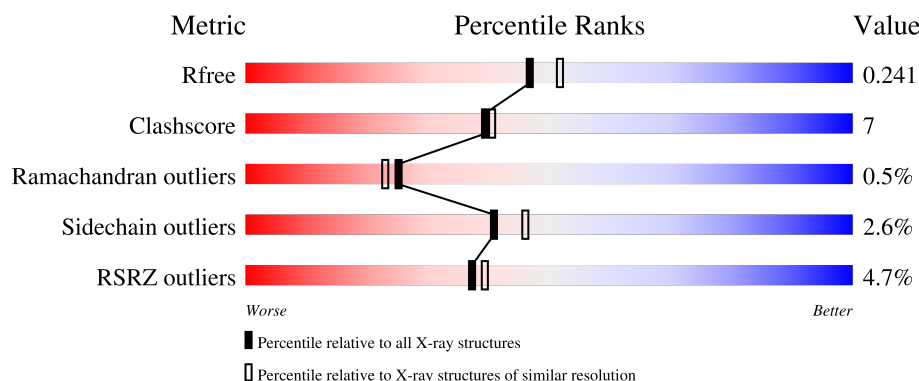
1 Overall quality at a glance

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}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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	A	180	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	180	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	C	180	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div> </div>
1	D	180	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>•</div> </div> </div>
1	E	180	<div> <div>•</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	180	
1	G	180	
1	H	180	
1	I	180	
2	L	8	

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
4	NA	D	204	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12598 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 Carbonic anhydrase mutant.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	174	Total	C	N	O	S	0	2	0
			1376	863	243	264	6			
1	B	172	Total	C	N	O	S	0	0	0
			1345	844	236	259	6			
1	F	169	Total	C	N	O	S	0	0	0
			1315	826	227	256	6			
1	E	167	Total	C	N	O	S	0	0	0
			1294	812	225	251	6			
1	H	171	Total	C	N	O	S	0	0	0
			1331	837	228	260	6			
1	C	169	Total	C	N	O	S	0	0	0
			1314	826	226	256	6			
1	A	168	Total	C	N	O	S	0	0	0
			1304	818	228	252	6			
1	I	173	Total	C	N	O	S	0	0	0
			1349	847	230	266	6			
1	G	168	Total	C	N	O	S	0	0	0
			1304	818	228	252	6			

- Molecule 2 is a protein called Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	8	Total	C	N	O	0	0	0
			70	47	13	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Zn 1	0	0
3	E	1	Total 1	Zn 1	0	0
3	H	2	Total 2	Zn 2	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	2	Total 2	Zn 2	0	0
3	I	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total 4	Na 4	0	0
4	B	1	Total 1	Na 1	0	0
4	F	1	Total 1	Na 1	0	0
4	E	2	Total 2	Na 2	0	0
4	C	1	Total 1	Na 1	0	0
4	A	1	Total 1	Na 1	0	0
4	I	1	Total 1	Na 1	0	0
4	G	2	Total 2	Na 2	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	3	Total	Mg	0	0
			3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	62	Total	O	0	0
			62	62		
7	B	66	Total	O	0	0
			66	66		
7	F	53	Total	O	0	0
			53	53		
7	E	55	Total	O	0	0
			55	55		

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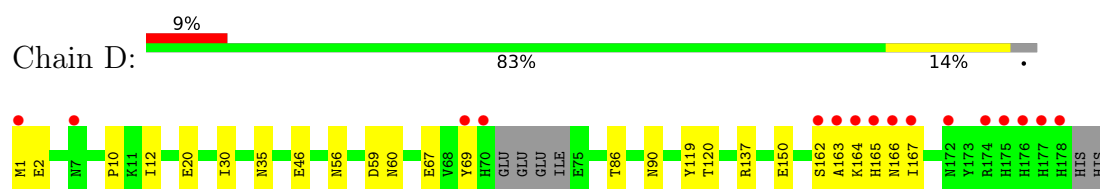
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	46	Total 46	O 46	0	0
7	C	86	Total 86	O 86	0	0
7	A	44	Total 44	O 44	0	0
7	I	62	Total 62	O 62	0	0
7	G	28	Total 28	O 28	0	0
7	L	6	Total 6	O 6	0	0

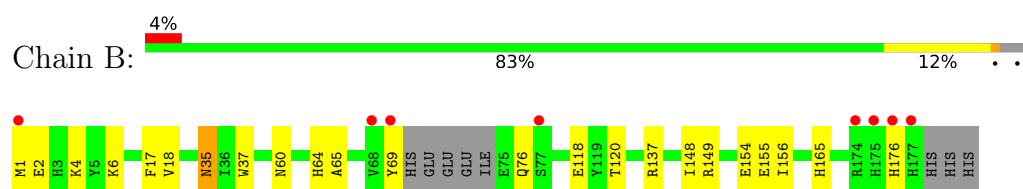
3 Residue-property plots [i](#)

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.

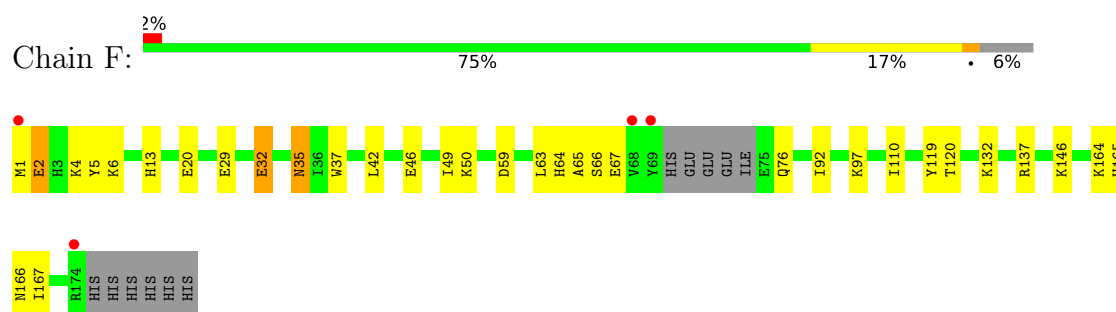
- Molecule 1: Carbonic anhydrase mutant



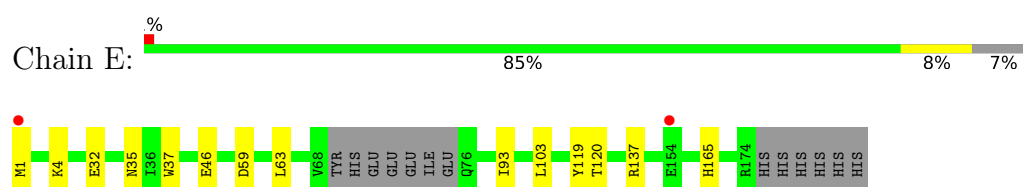
- Molecule 1: Carbonic anhydrase mutant



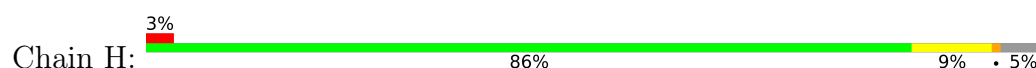
- Molecule 1: Carbonic anhydrase mutant



- Molecule 1: Carbonic anhydrase mutant

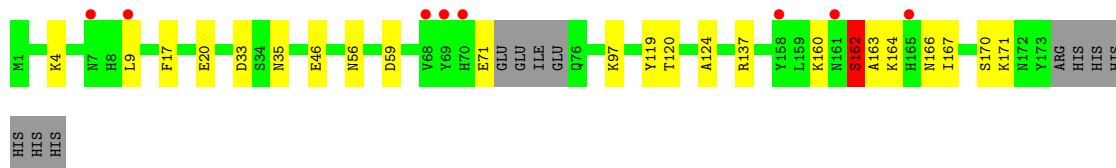
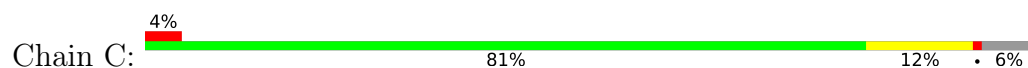


- Molecule 1: Carbonic anhydrase mutant

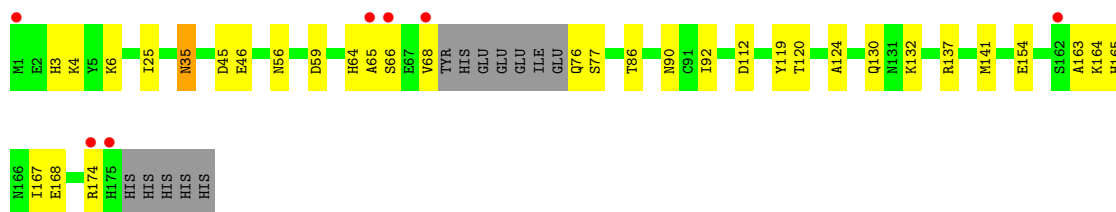
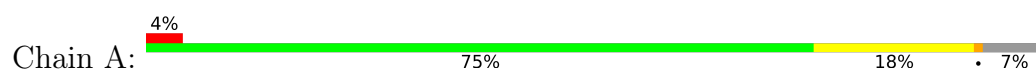




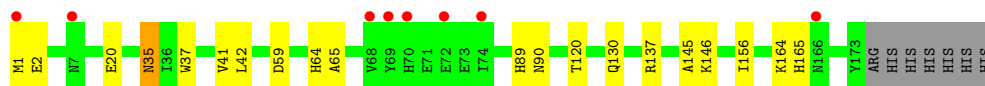
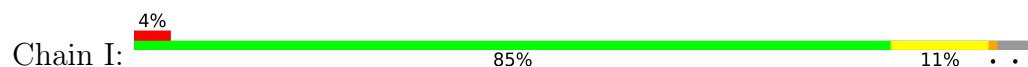
- Molecule 1: Carbonic anhydrase mutant



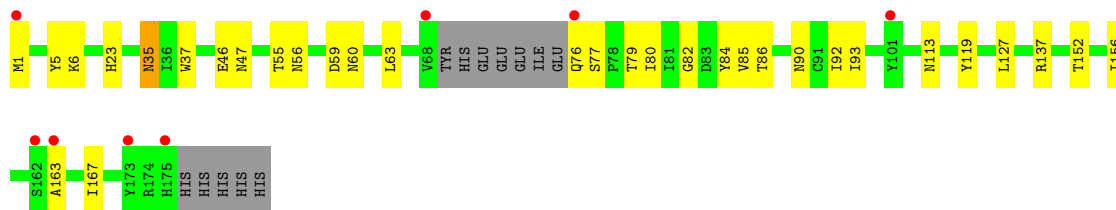
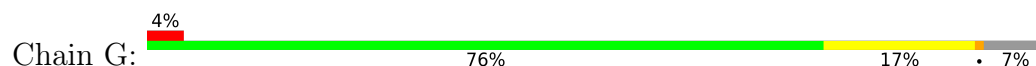
- Molecule 1: Carbonic anhydrase mutant



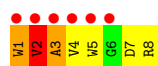
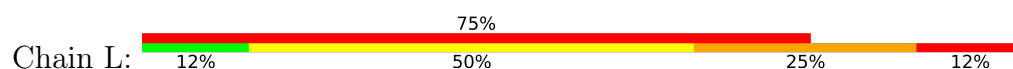
- Molecule 1: Carbonic anhydrase mutant



- Molecule 1: Carbonic anhydrase mutant



- Molecule 2: Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.69Å 164.96Å 165.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.78 – 2.10 45.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.78-2.10) 89.5 (45.78-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.240 0.200 , 0.241	Depositor DCC
R_{free} test set	2009 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12598	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 31.77 % 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 1.0485e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, EPE, ZN, MG

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	0.30	0/1326	0.55	0/1791
1	B	0.33	0/1370	0.53	0/1851
1	C	0.34	0/1337	0.53	0/1807
1	D	0.35	0/1409	0.55	0/1904
1	E	0.34	0/1315	0.53	0/1776
1	F	0.34	0/1337	0.52	0/1806
1	G	0.27	0/1326	0.45	0/1791
1	H	0.30	0/1354	0.47	0/1830
1	I	0.32	0/1373	0.53	0/1857
2	L	0.62	0/73	0.91	0/100
All	All	0.32	0/12220	0.52	0/16513

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	1304	0	1299	23	0
1	B	1345	0	1325	17	0
1	C	1314	0	1301	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1376	0	1352	18	0
1	E	1294	0	1292	9	0
1	F	1315	0	1307	28	0
1	G	1304	0	1299	21	0
1	H	1331	0	1318	10	0
1	I	1349	0	1331	15	0
2	L	70	0	65	11	0
3	A	2	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	2	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	I	1	0	0	0	0
5	A	30	0	34	6	0
5	B	15	0	17	1	0
5	C	15	0	18	5	0
6	I	3	0	0	0	0
7	A	44	0	0	3	0
7	B	66	0	0	4	0
7	C	86	0	0	6	1
7	D	62	0	0	3	1
7	E	55	0	0	1	0
7	F	53	0	0	2	1
7	G	28	0	0	2	0
7	H	46	0	0	2	1
7	I	62	0	0	3	0
7	L	6	0	0	4	0
All	All	12598	0	11958	159	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 7.

The worst 5 of 159 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:G:1:MET:N	7:G:301:HOH:O	2.05	0.88
1:A:56:ASN:HD21	1:A:86:THR:HG23	1.40	0.86
1:D:60:ASN:OD1	7:D:301:HOH:O	1.94	0.83
1:B:35:ASN:HD22	1:B:37:TRP:HE1	1.29	0.80
1:F:35:ASN:HD22	1:F:37:TRP:HE1	1.29	0.80

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)
7:F:325:HOH:O	7:H:342:HOH:O[4_655]	2.08	0.12
7:D:353:HOH:O	7:C:343:HOH:O[1_455]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	164/180 (91%)	162 (99%)	2 (1%)	0	100	100
1	B	168/180 (93%)	165 (98%)	3 (2%)	0	100	100
1	C	165/180 (92%)	160 (97%)	4 (2%)	1 (1%)	22	19
1	D	172/180 (96%)	164 (95%)	6 (4%)	2 (1%)	11	7
1	E	163/180 (91%)	159 (98%)	4 (2%)	0	100	100
1	F	165/180 (92%)	158 (96%)	6 (4%)	1 (1%)	22	19
1	G	164/180 (91%)	158 (96%)	6 (4%)	0	100	100
1	H	167/180 (93%)	162 (97%)	5 (3%)	0	100	100
1	I	171/180 (95%)	167 (98%)	4 (2%)	0	100	100
2	L	6/8 (75%)	3 (50%)	0	3 (50%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1505/1628 (92%)	1458 (97%)	40 (3%)	7 (0%)	25	23

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	2	VAL
2	L	3	ALA
1	D	162	SER
2	L	7	ASP
1	D	163	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/156 (92%)	138 (96%)	6 (4%)	25	26
1	B	148/156 (95%)	146 (99%)	2 (1%)	62	70
1	C	145/156 (93%)	141 (97%)	4 (3%)	38	43
1	D	152/156 (97%)	150 (99%)	2 (1%)	65	72
1	E	143/156 (92%)	139 (97%)	4 (3%)	38	43
1	F	145/156 (93%)	140 (97%)	5 (3%)	32	35
1	G	144/156 (92%)	141 (98%)	3 (2%)	48	55
1	H	147/156 (94%)	144 (98%)	3 (2%)	50	57
1	I	149/156 (96%)	145 (97%)	4 (3%)	40	44
2	L	6/6 (100%)	4 (67%)	2 (33%)	0	0
All	All	1323/1410 (94%)	1288 (97%)	35 (3%)	41	46

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	120	THR
1	I	164	LYS

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Mol	Chain	Res	Type
1	G	127	LEU
1	E	120	THR
1	E	59	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	8	HIS
1	G	35	ASN
1	G	131	ASN
1	H	113	ASN
1	H	58	GLN

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 32 ligands modelled in this entry, 28 are monoatomic - leaving 4 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	$\# Z > 2$
5	EPE	A	204	3	15,15,15	0.59	0	18,20,20	1.63	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EPE	C	203	-	15,15,15	0.98	1 (6%)	18,20,20	1.98	5 (27%)
5	EPE	A	205	-	15,15,15	0.88	1 (6%)	18,20,20	1.65	5 (27%)
5	EPE	B	201	-	15,15,15	1.27	1 (6%)	18,20,20	2.06	5 (27%)

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
5	EPE	A	204	3	-	6/9/19/19	0/1/1/1
5	EPE	C	203	-	-	4/9/19/19	0/1/1/1
5	EPE	A	205	-	-	6/9/19/19	0/1/1/1
5	EPE	B	201	-	-	3/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	EPE	C10-S	4.34	1.83	1.77
5	C	203	EPE	C10-S	3.22	1.82	1.77
5	A	205	EPE	C10-S	2.91	1.81	1.77

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	203	EPE	C7-N4-C3	4.01	121.49	111.23
5	B	201	EPE	C7-N4-C3	3.97	121.40	111.23
5	C	203	EPE	C7-N4-C5	3.97	121.40	111.23
5	B	201	EPE	C7-N4-C5	3.87	121.14	111.23
5	B	201	EPE	C5-N4-C3	3.71	117.19	108.83

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	203	EPE	C10-C9-N1-C2
5	C	203	EPE	C10-C9-N1-C6
5	A	204	EPE	C8-C7-N4-C5
5	A	204	EPE	C9-C10-S-O1S
5	A	205	EPE	C10-C9-N1-C6

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	204	EPE	3	0
5	C	203	EPE	5	0
5	A	205	EPE	3	0
5	B	201	EPE	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	168/180 (93%)	0.14	7 (4%) 41 43	34, 46, 67, 82	0
1	B	172/180 (95%)	0.00	8 (4%) 37 39	31, 43, 67, 104	0
1	C	169/180 (93%)	-0.04	8 (4%) 37 39	30, 39, 72, 120	0
1	D	174/180 (96%)	0.22	16 (9%) 16 17	26, 42, 81, 145	2 (1%)
1	E	167/180 (92%)	-0.05	2 (1%) 76 77	31, 42, 62, 91	0
1	F	169/180 (93%)	0.02	4 (2%) 59 61	33, 44, 64, 97	0
1	G	168/180 (93%)	0.46	8 (4%) 36 38	38, 55, 79, 98	0
1	H	171/180 (95%)	0.22	6 (3%) 47 49	35, 46, 75, 119	0
1	I	173/180 (96%)	0.13	8 (4%) 38 40	34, 44, 70, 91	0
2	L	8/8 (100%)	3.17	6 (75%) 0 0	53, 55, 65, 72	0
All	All	1539/1628 (94%)	0.14	73 (4%) 37 39	26, 45, 74, 145	2 (0%)

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	68	VAL	6.5
2	L	3	ALA	5.3
1	F	68	VAL	4.7
1	B	176	HIS	4.3
1	H	74	ILE	4.2

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

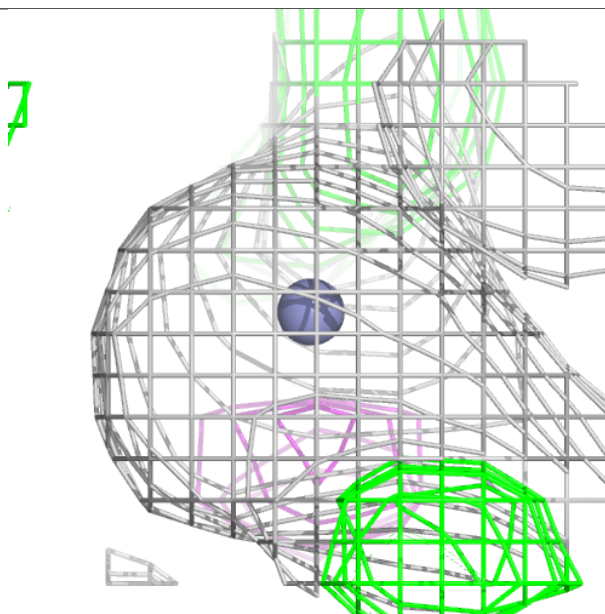
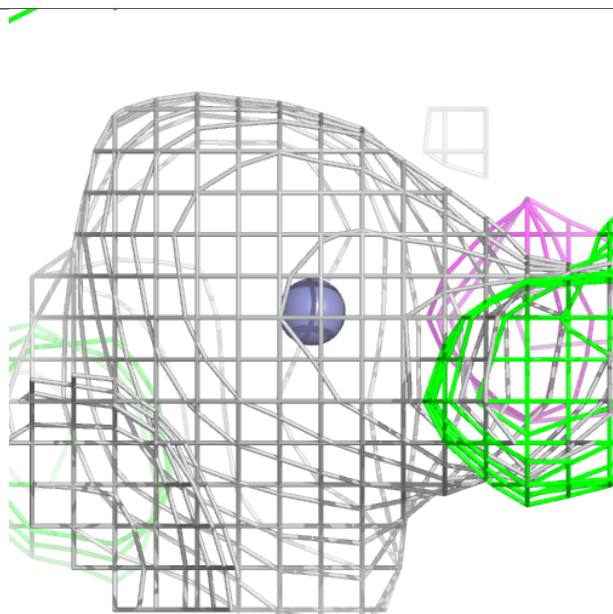
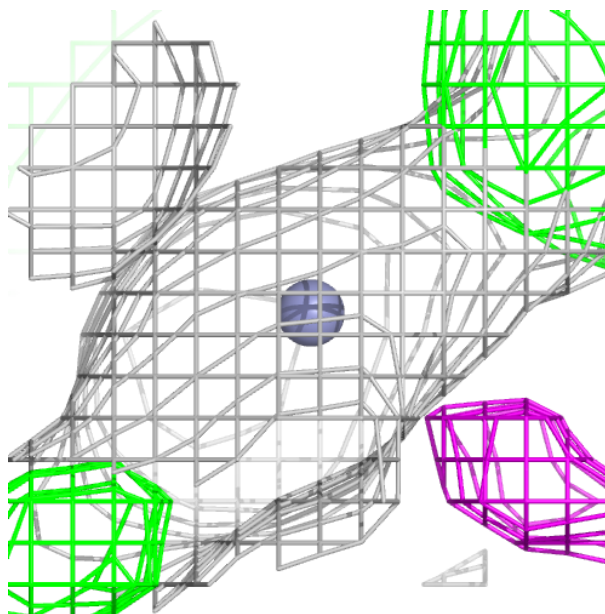
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EPE	B	201	15/15	0.65	0.24	59,73,87,87	0
5	EPE	A	205	15/15	0.71	0.18	56,74,84,85	0
4	NA	D	204	1/1	0.78	0.41	58,58,58,58	0
3	ZN	A	202	1/1	0.80	0.13	110,110,110,110	0
4	NA	E	202	1/1	0.80	0.23	63,63,63,63	1
5	EPE	C	203	15/15	0.81	0.17	39,61,84,90	0
4	NA	I	202	1/1	0.84	0.17	75,75,75,75	1
5	EPE	A	204	15/15	0.87	0.14	39,55,65,66	0
4	NA	G	203	1/1	0.87	0.12	54,54,54,54	0
4	NA	G	202	1/1	0.88	0.18	60,60,60,60	0
3	ZN	H	202	1/1	0.88	0.12	105,105,105,105	0
4	NA	D	205	1/1	0.93	0.12	61,61,61,61	0
4	NA	C	202	1/1	0.94	0.12	56,56,56,56	0
4	NA	D	203	1/1	0.94	0.10	62,62,62,62	0
4	NA	F	202	1/1	0.94	0.18	62,62,62,62	0
4	NA	D	202	1/1	0.94	0.19	55,55,55,55	0
4	NA	B	203	1/1	0.95	0.14	62,62,62,62	0
4	NA	E	203	1/1	0.95	0.09	55,55,55,55	0
4	NA	A	203	1/1	0.96	0.13	47,47,47,47	0
3	ZN	L	101	1/1	0.98	0.07	84,84,84,84	0
6	MG	I	204	1/1	0.98	0.14	52,52,52,52	0
6	MG	I	205	1/1	0.98	0.04	52,52,52,52	0
3	ZN	B	202	1/1	0.99	0.04	40,40,40,40	0
3	ZN	A	201	1/1	0.99	0.06	45,45,45,45	0
6	MG	I	203	1/1	0.99	0.05	52,52,52,52	0
3	ZN	E	201	1/1	0.99	0.06	41,41,41,41	0
3	ZN	G	201	1/1	0.99	0.03	49,49,49,49	0
3	ZN	D	201	1/1	1.00	0.01	41,41,41,41	0
3	ZN	H	201	1/1	1.00	0.03	49,49,49,49	0
3	ZN	I	201	1/1	1.00	0.05	41,41,41,41	0
3	ZN	F	201	1/1	1.00	0.03	40,40,40,40	0
3	ZN	C	201	1/1	1.00	0.03	42,42,42,42	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.

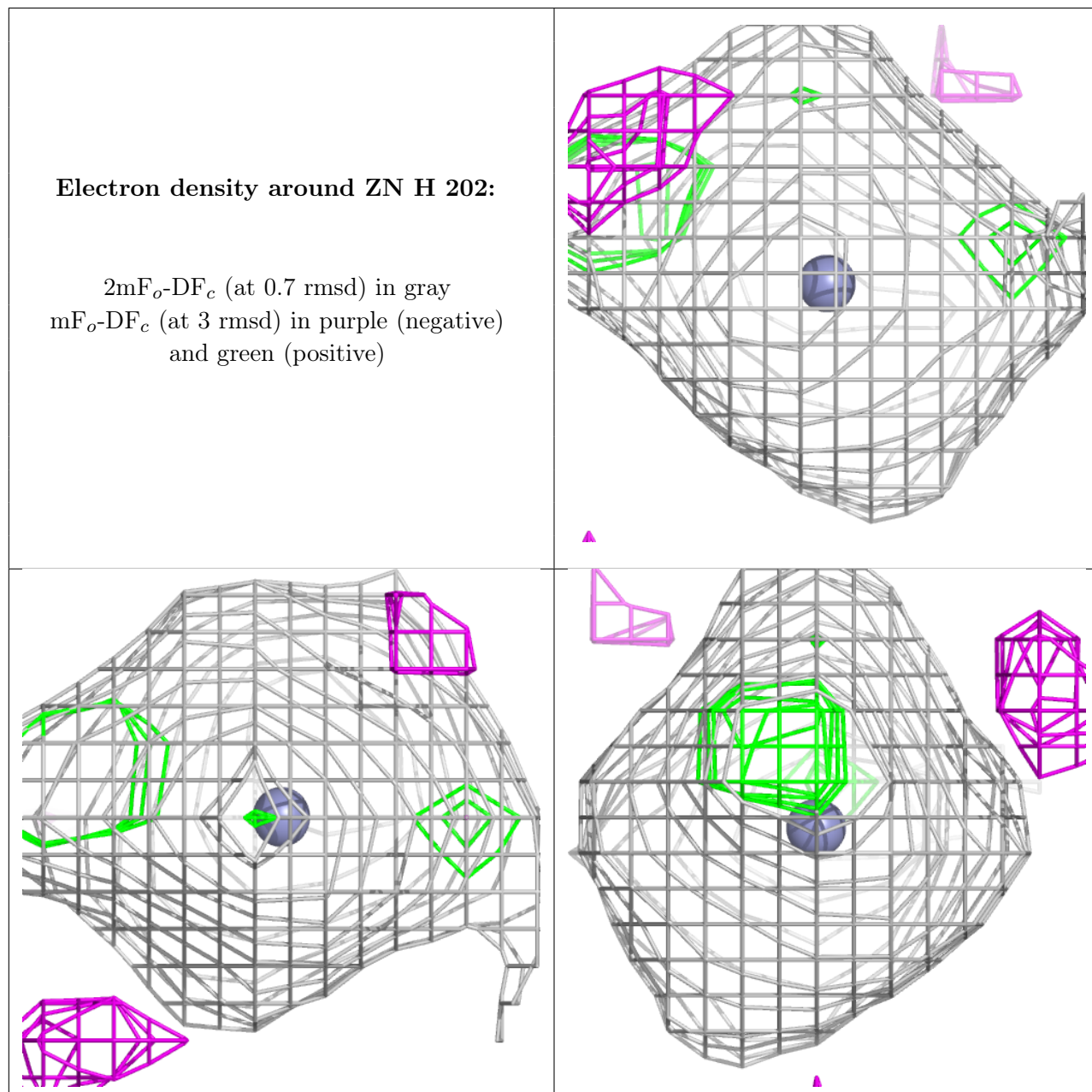
Electron density around ZN A 202:

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



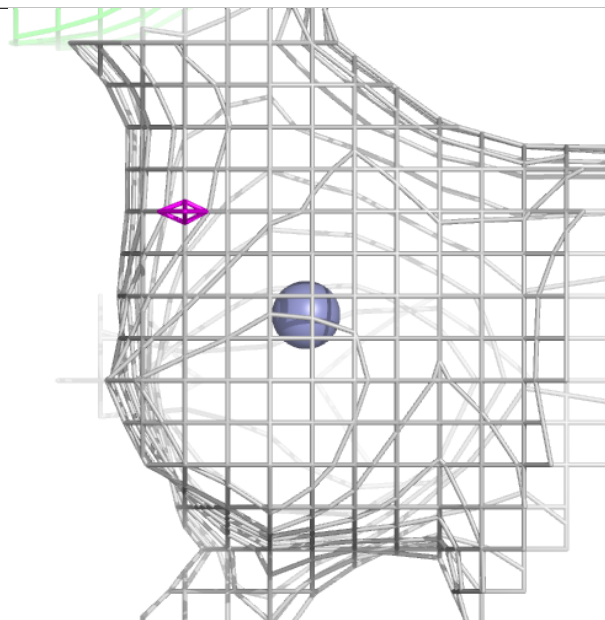
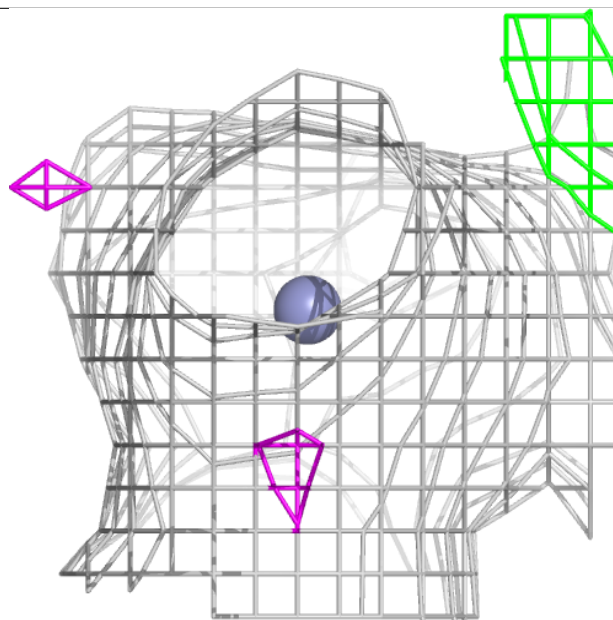
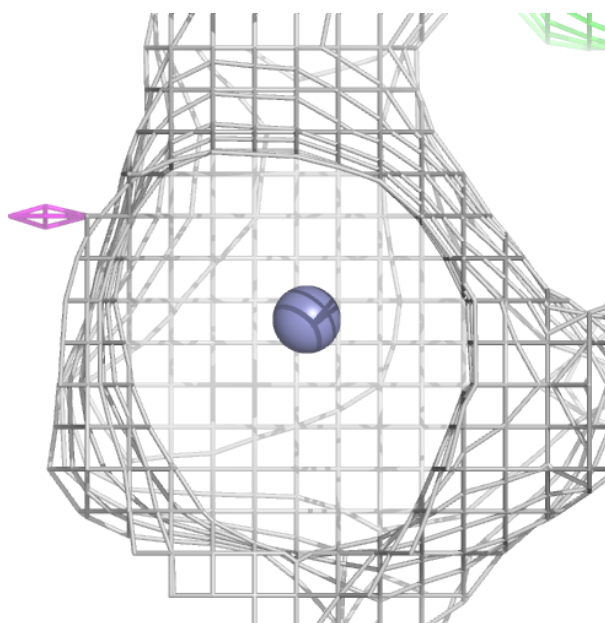
Electron density around ZN H 202:

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



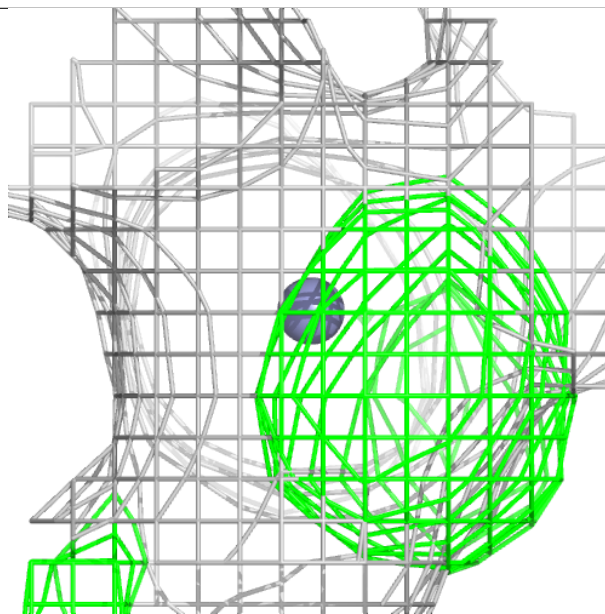
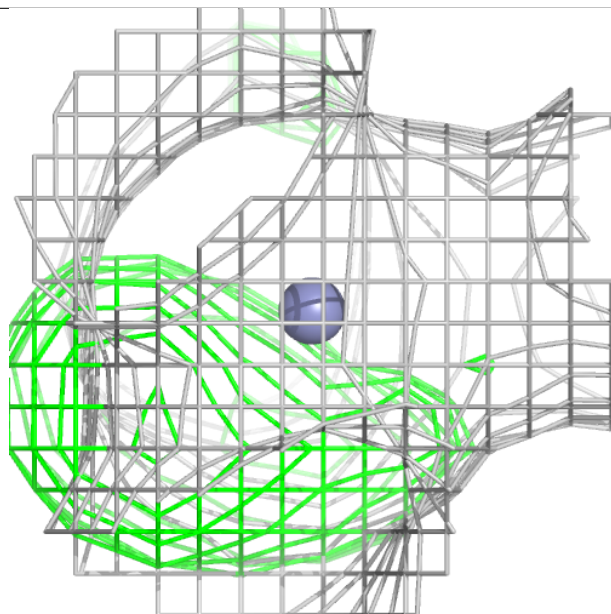
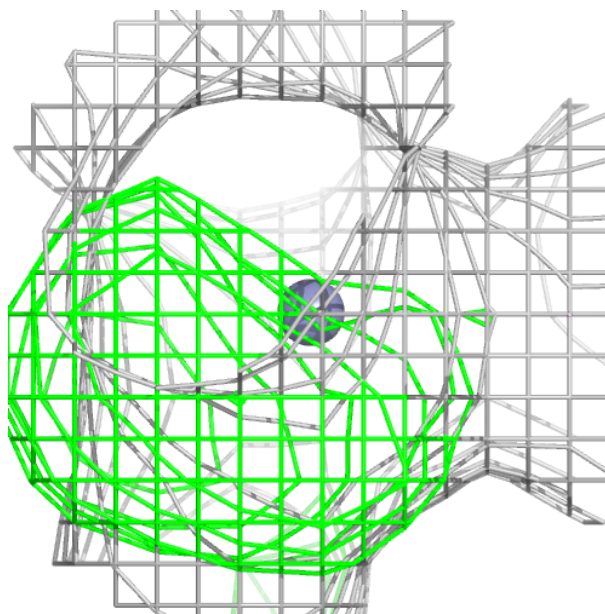
Electron density around ZN L 101:

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



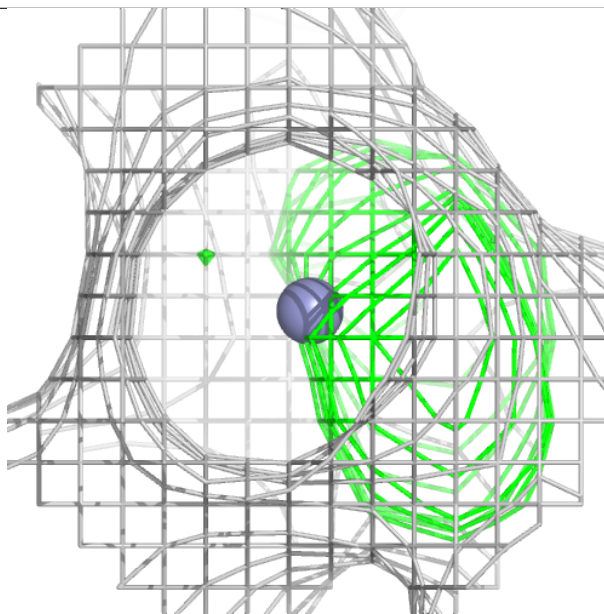
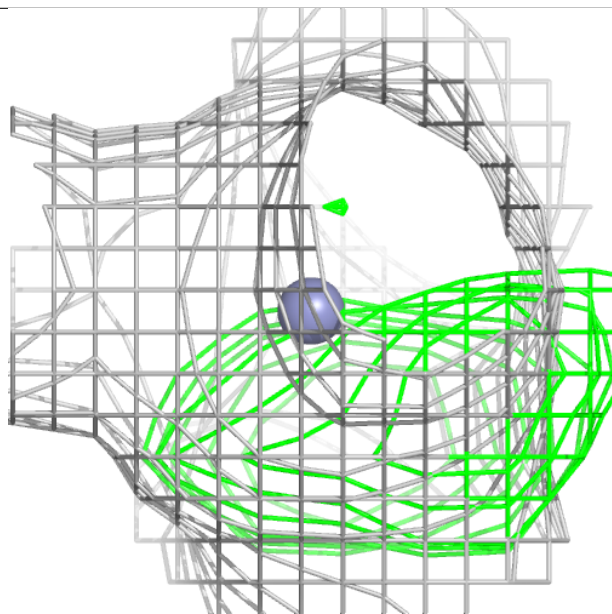
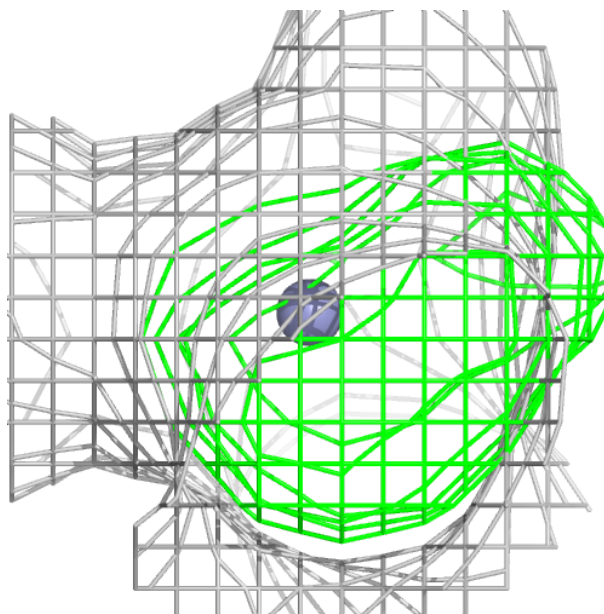
Electron density around ZN B 202:

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



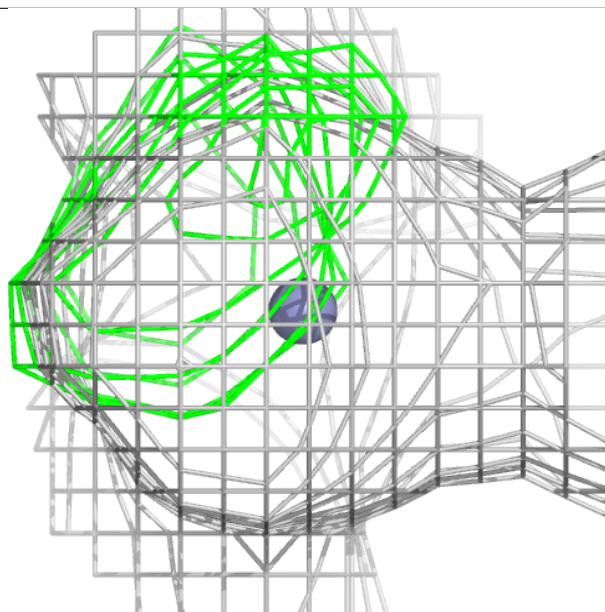
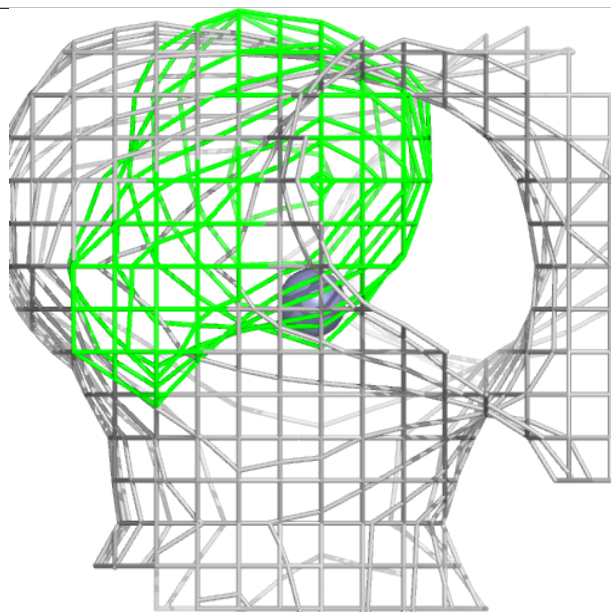
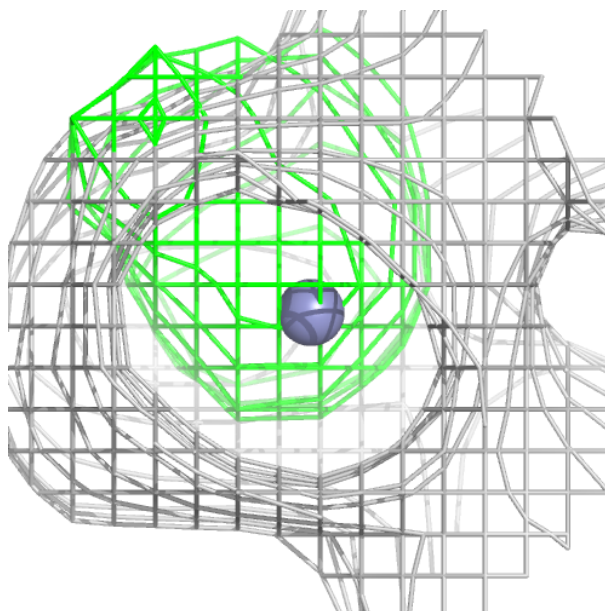
Electron density around ZN A 201:

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



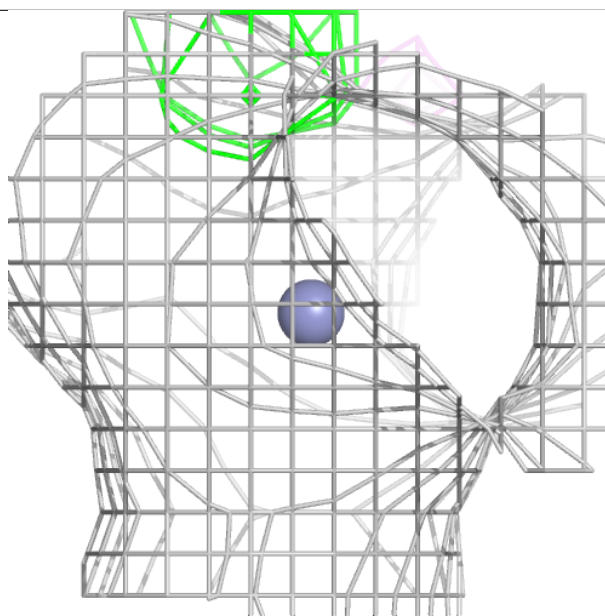
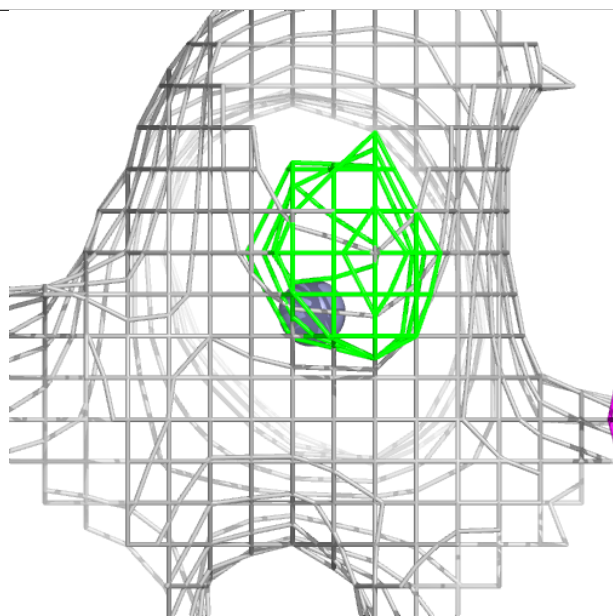
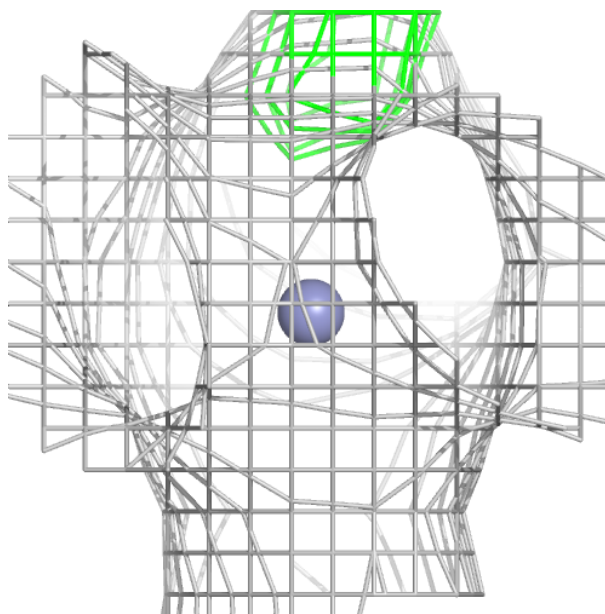
Electron density around ZN E 201:

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and green (positive)



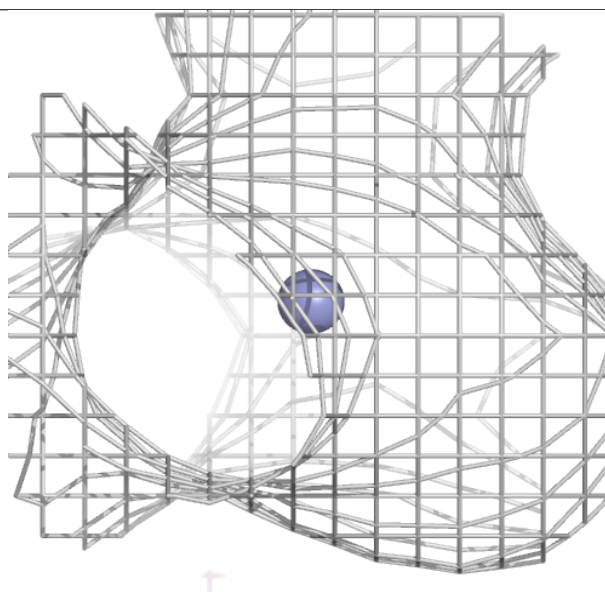
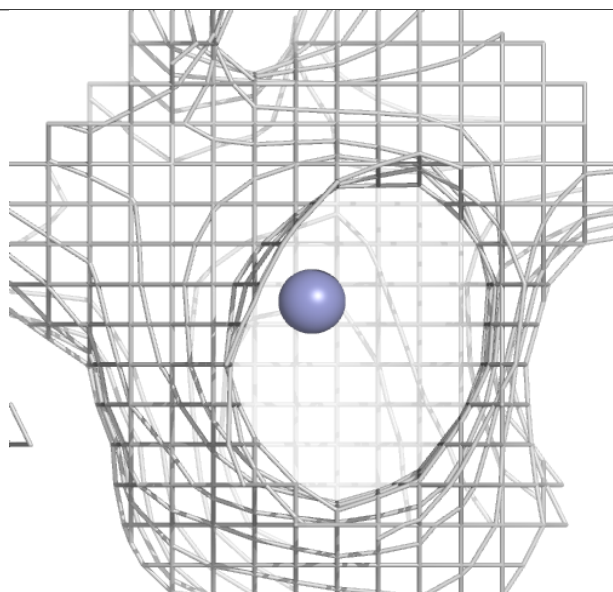
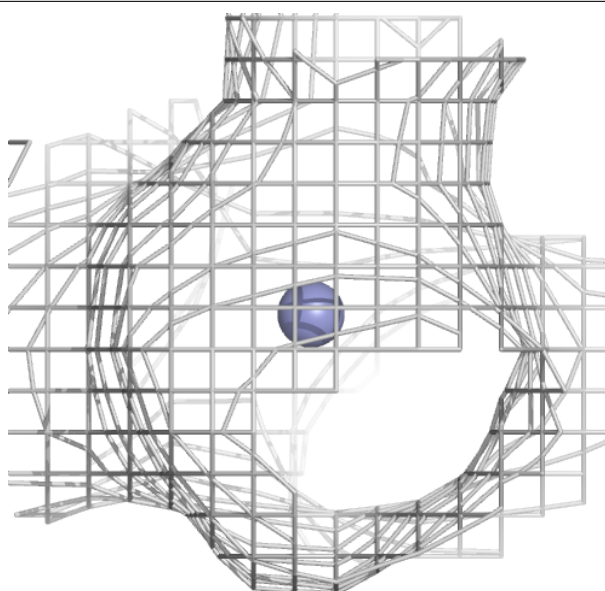
Electron density around ZN G 201:

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



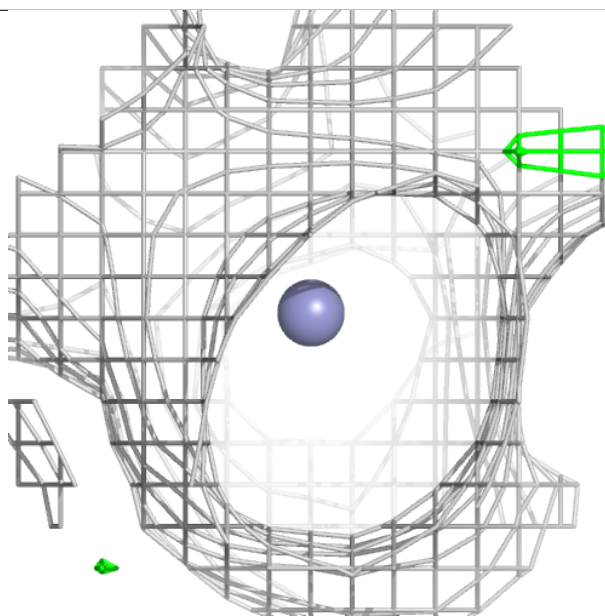
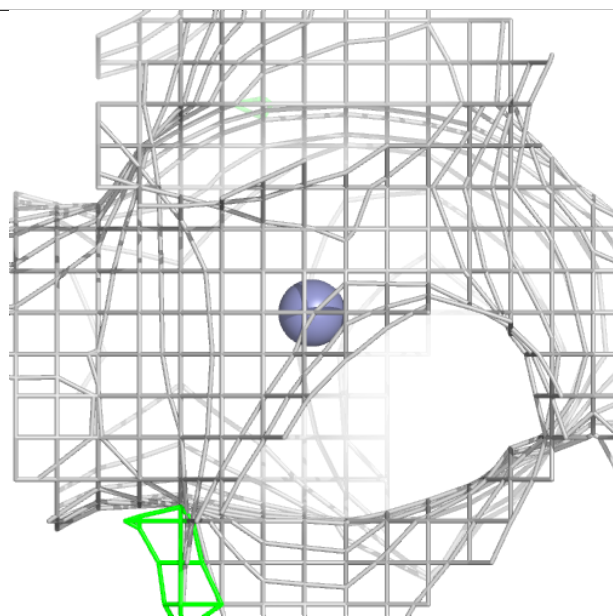
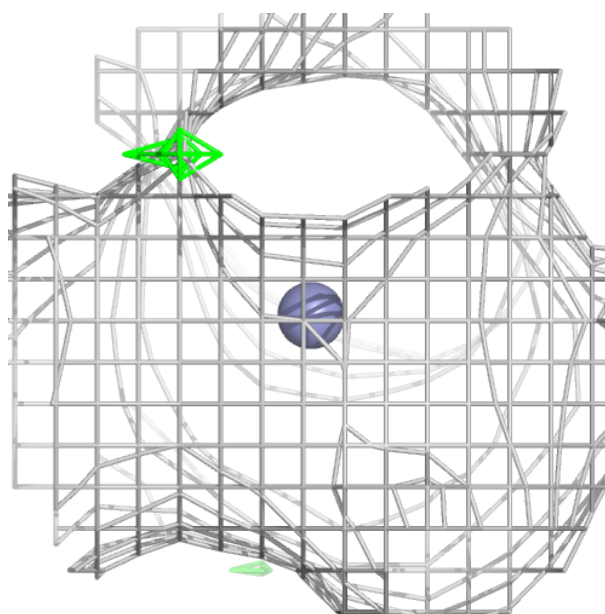
Electron density around ZN D 201:

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



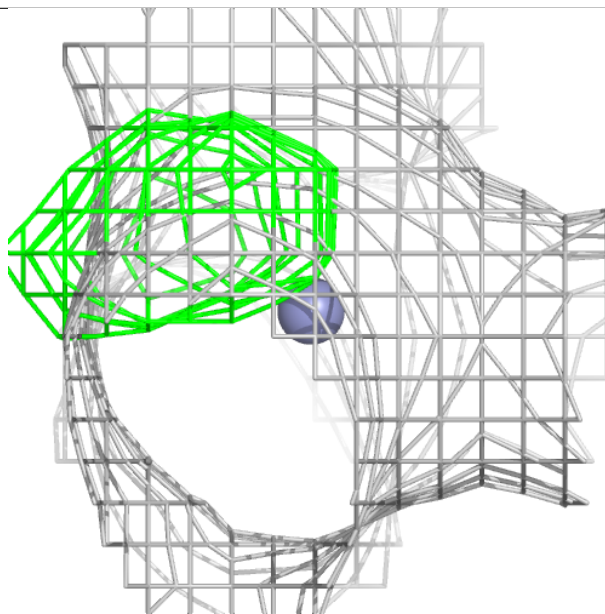
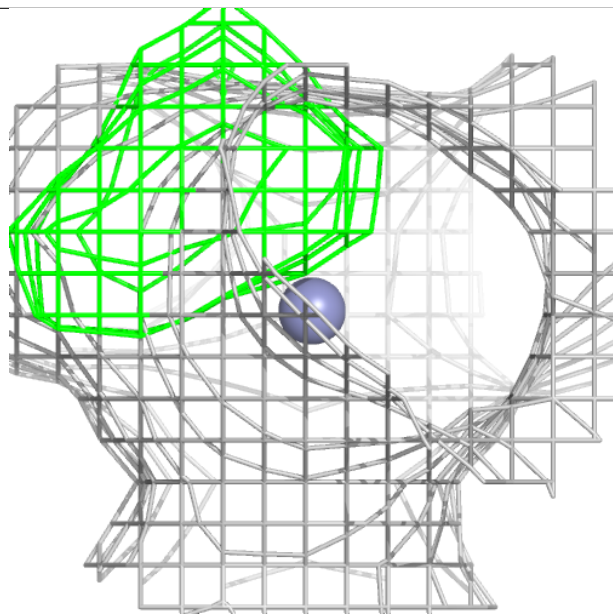
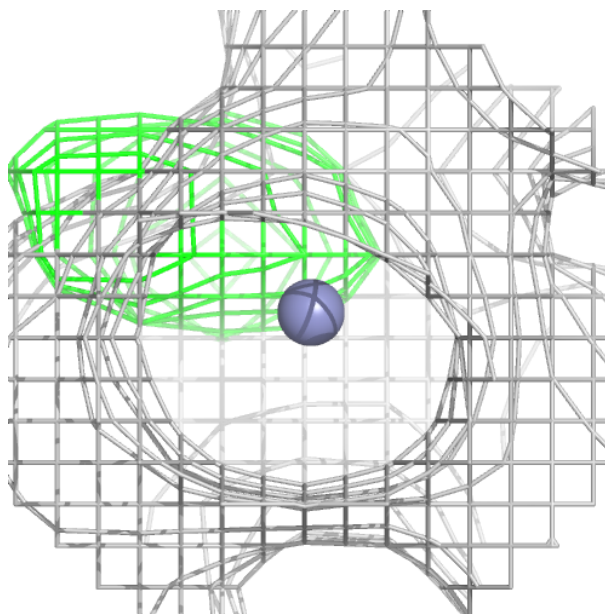
Electron density around ZN H 201:

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



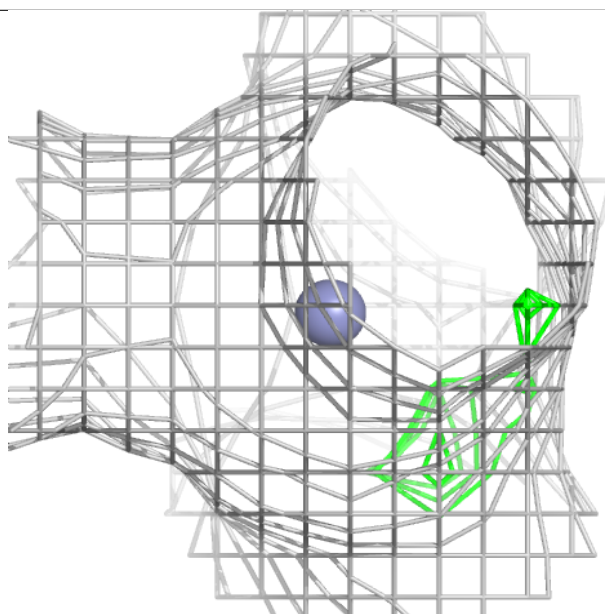
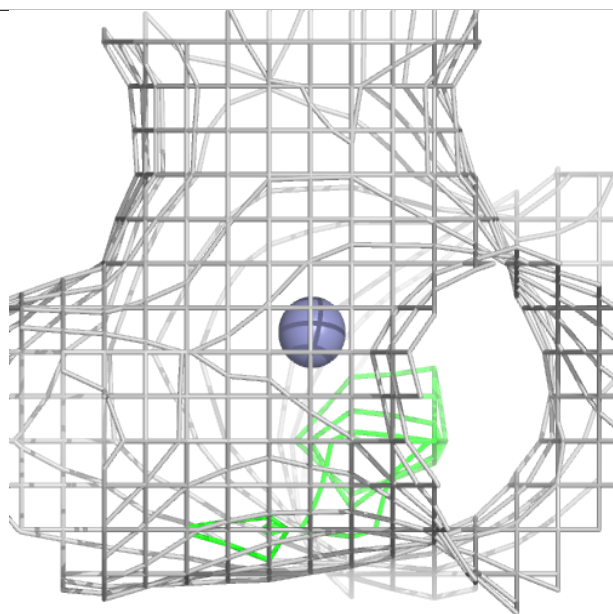
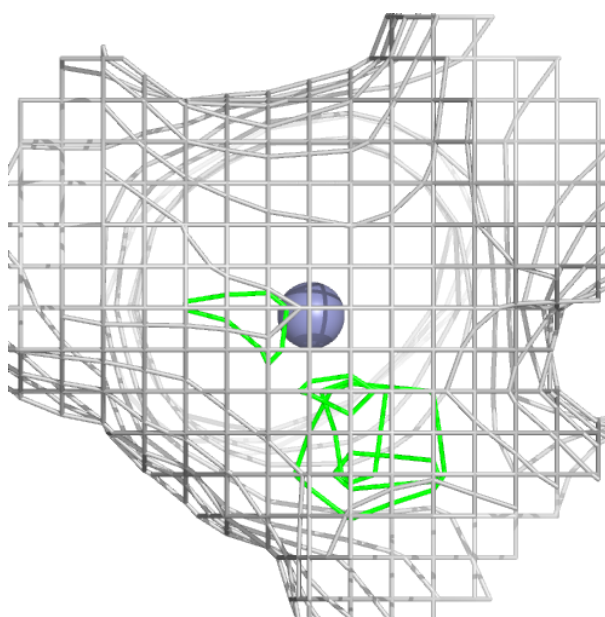
Electron density around ZN I 201:

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



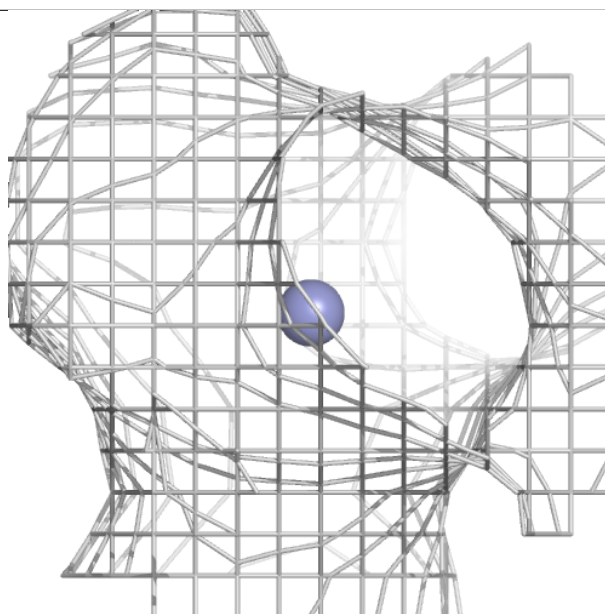
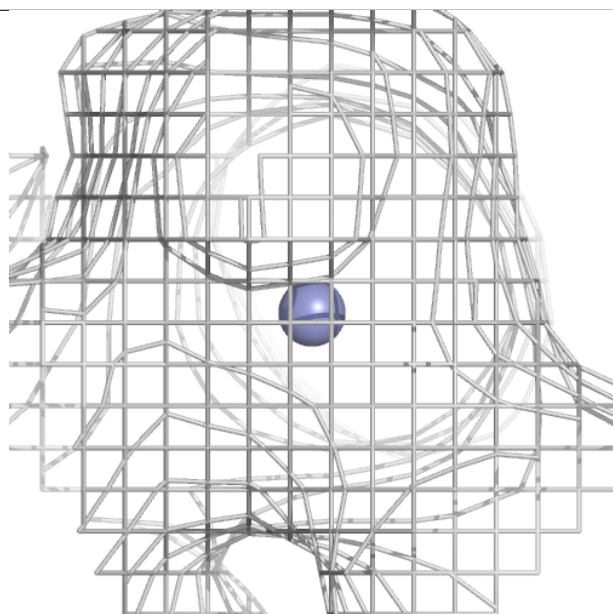
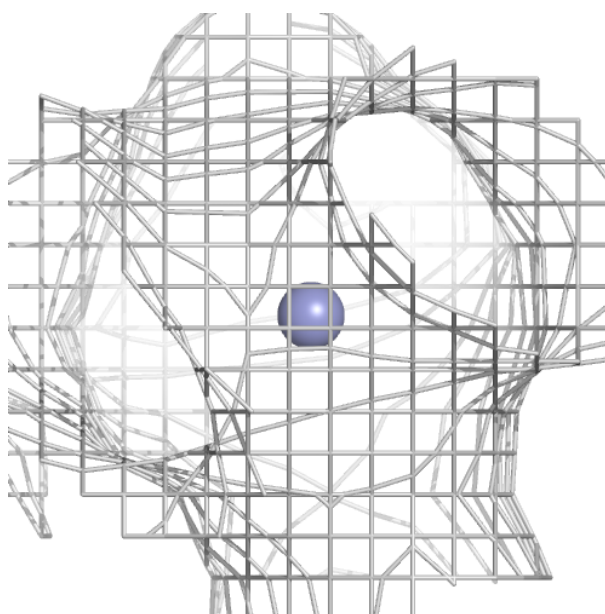
Electron density around ZN F 201:

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



Electron density around ZN C 201:

$2mF_o-DF_c$ (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.