



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:06 PM UTC

PDB ID : 6MTW / pdb_00006mtw
Title : Lysosomal Phospholipase A2 in complex with Zinc
Authors : Bouley, R.; Tesmer, J.J.G.
Deposited on : 2018-10-22
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

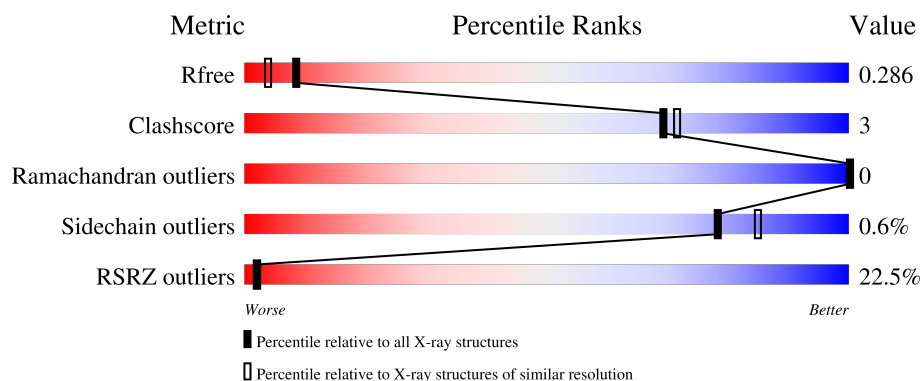
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	380	21% 88% 11%
1	B	380	23% 91% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6446 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 Group XV phospholipase A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			3019	1949	507	550	13			
1	B	376	Total	C	N	O	S	0	0	0
			3019	1949	507	550	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8NCC3
B	0	GLY	-	expression tag	UNP Q8NCC3

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Zn	0	0
			4	4		
4	B	4	Total	Zn	0	0
			4	4		

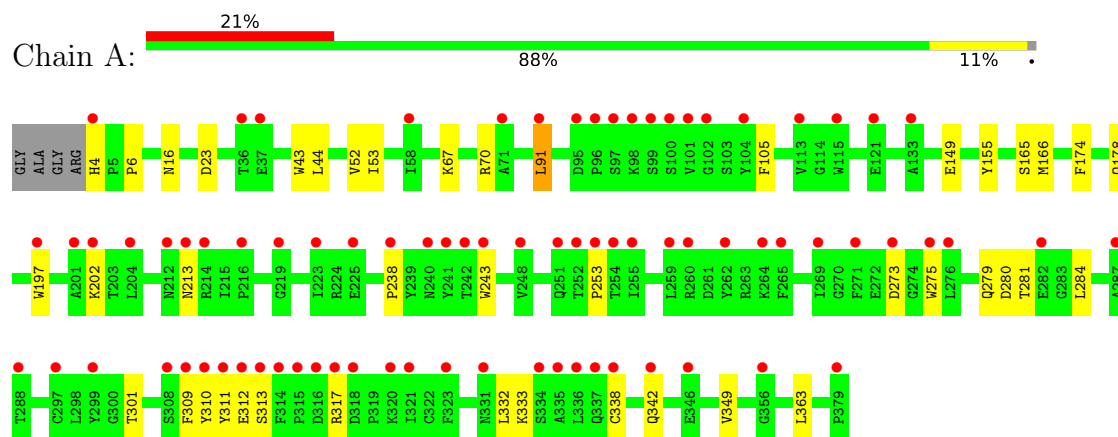
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		
5	B	168	Total	O	0	0
			168	168		

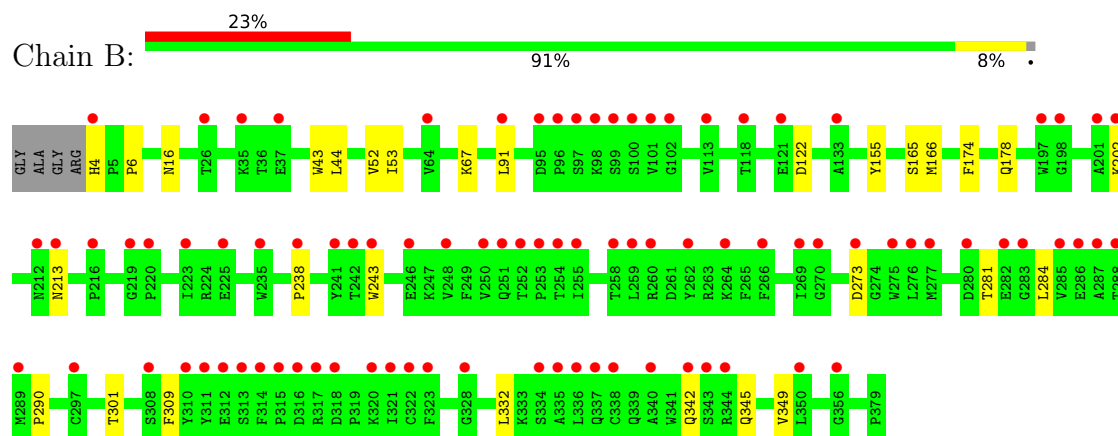
3 Residue-property plots [i](#)

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: Group XV phospholipase A2



• Molecule 1: Group XV phospholipase A2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	84.57Å 84.57Å 321.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 – 2.00 39.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.34-2.00) 89.2 (39.34-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.247 , 0.285 0.248 , 0.286	Depositor DCC
R_{free} test set	1996 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6446	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 28.82 % 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 1.7236e-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: ZN, NAG, CL

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	0.14	0/3108	0.35	0/4236
1	B	0.14	0/3108	0.36	0/4236
All	All	0.14	0/6216	0.36	0/8472

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	3019	0	2954	26	0
1	B	3019	0	2954	16	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	174	0	0	3	0
5	B	168	0	0	2	0
All	All	6446	0	5960	42	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.

All (42) 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:67:LYS:NZ	1:B:273:ASP:OD1	2.31	0.62
1:B:52:VAL:HG13	1:B:53:ILE:HG23	1.82	0.61
1:B:6:PRO:HG3	1:B:155:TYR:HB2	1.85	0.59
1:A:52:VAL:HG13	1:A:53:ILE:HG23	1.84	0.59
1:A:67:LYS:NZ	1:A:273:ASP:OD1	2.33	0.58
1:A:301:THR:HG22	1:A:332:LEU:HD13	1.89	0.55
1:B:202:LYS:NZ	5:B:508:HOH:O	2.42	0.53
1:B:301:THR:HG22	1:B:332:LEU:HD13	1.91	0.53
1:A:23:ASP:OD2	5:A:502:HOH:O	2.19	0.52
1:A:6:PRO:HG3	1:A:155:TYR:HB2	1.90	0.52
1:A:4:HIS:N	5:A:507:HOH:O	2.42	0.52
1:A:197:TRP:NE1	1:A:338:CYS:SG	2.83	0.51
1:A:165:SER:OG	1:A:166:MET:N	2.46	0.49
1:B:213:ASN:ND2	5:B:506:HOH:O	2.45	0.48
1:B:165:SER:OG	1:B:166:MET:N	2.46	0.48
1:A:275:TRP:O	1:A:279:GLN:HG2	2.14	0.47
1:A:202:LYS:HA	1:A:309:PHE:CZ	2.50	0.47
1:A:238:PRO:HB3	1:A:243:TRP:CD1	2.50	0.46
1:B:238:PRO:HB3	1:B:243:TRP:CD1	2.51	0.46
1:A:342:GLN:HG2	1:A:349:VAL:HB	1.97	0.46
1:B:202:LYS:HA	1:B:309:PHE:CZ	2.52	0.45
1:A:310:TYR:HE2	1:A:312:GLU:HG2	1.82	0.45
1:B:4:HIS:NE2	1:B:122:ASP:OD2	2.33	0.44
1:B:281:THR:HA	1:B:284:LEU:HG	1.99	0.44
1:A:91:LEU:HG	1:A:105:PHE:CD2	2.52	0.44
1:A:149:GLU:OE2	5:A:503:HOH:O	2.20	0.43
1:A:70:ARG:NH2	1:A:280:ASP:OD1	2.52	0.43
1:A:333:LYS:HB3	1:A:333:LYS:HE3	1.87	0.43
1:A:43:TRP:HA	1:A:44:LEU:HA	1.72	0.43
1:A:213:ASN:HD22	1:A:213:ASN:HA	1.65	0.42
1:A:91:LEU:O	1:A:105:PHE:HB2	2.19	0.42
1:A:281:THR:HA	1:A:284:LEU:HG	2.01	0.42
1:A:313:SER:HB3	1:A:317:ARG:HG3	2.01	0.42
1:B:202:LYS:HB2	1:B:202:LYS:HE3	1.59	0.42
1:A:253:PRO:HD3	1:A:311:TYR:O	2.20	0.42
1:A:174:PHE:O	1:A:178:GLN:HG2	2.20	0.41
1:A:202:LYS:HA	1:A:309:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.89	0.41
1:B:43:TRP:HA	1:B:44:LEU:HA	1.72	0.41
1:B:342:GLN:HG2	1:B:349:VAL:HB	2.04	0.40
1:B:174:PHE:O	1:B:178:GLN:HG2	2.22	0.40
1:B:290:PRO:HB2	1:B:345:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/380 (98%)	364 (97%)	10 (3%)	0	100	100
1	B	374/380 (98%)	364 (97%)	10 (3%)	0	100	100
All	All	748/760 (98%)	728 (97%)	20 (3%)	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	328/329 (100%)	326 (99%)	2 (1%)	78	85
1	B	328/329 (100%)	326 (99%)	2 (1%)	78	85
All	All	656/658 (100%)	652 (99%)	4 (1%)	78	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	91	LEU
1	B	16	ASN
1	B	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	B	106	HIS
1	B	180	GLN
1	B	342	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 14 ligands modelled in this entry, 10 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
2	NAG	A	402	1	14,14,15	1.68	3 (21%)	17,19,21	1.55	3 (17%)
2	NAG	B	402	1	14,14,15	1.72	3 (21%)	17,19,21	1.53	4 (23%)
2	NAG	A	401	1	14,14,15	1.60	2 (14%)	17,19,21	1.56	4 (23%)
2	NAG	B	401	1	14,14,15	1.64	2 (14%)	17,19,21	1.54	4 (23%)

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
2	NAG	A	402	1	-	0/6/23/26	0/1/1/1
2	NAG	B	402	1	-	0/6/23/26	0/1/1/1
2	NAG	A	401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	401	1	-	1/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAG	C1-C2	4.33	1.58	1.52
2	B	402	NAG	C1-C2	3.75	1.57	1.52
2	A	401	NAG	C1-C2	3.71	1.57	1.52
2	A	402	NAG	C1-C2	3.60	1.57	1.52
2	B	402	NAG	O5-C5	-2.90	1.37	1.43
2	A	402	NAG	O5-C5	-2.61	1.38	1.43
2	A	401	NAG	O5-C5	-2.46	1.38	1.43
2	A	402	NAG	C3-C2	2.24	1.57	1.52
2	B	401	NAG	O5-C5	-2.10	1.39	1.43
2	B	402	NAG	C3-C2	2.06	1.56	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	NAG	C2-N2-C7	-3.49	118.22	122.90
2	B	402	NAG	C2-N2-C7	-3.22	118.58	122.90
2	A	401	NAG	C2-N2-C7	-3.17	118.65	122.90
2	B	401	NAG	C2-N2-C7	-3.09	118.75	122.90
2	A	401	NAG	C6-C5-C4	-2.94	105.79	113.02
2	B	402	NAG	C1-C2-N2	-2.77	106.08	110.43
2	B	401	NAG	C6-C5-C4	-2.76	106.25	113.02
2	A	401	NAG	O4-C4-C3	-2.41	104.69	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	NAG	C1-C2-N2	-2.41	106.64	110.43
2	A	401	NAG	C1-C2-N2	-2.37	106.70	110.43
2	A	402	NAG	C6-C5-C4	-2.23	107.55	113.02
2	B	401	NAG	C1-C2-N2	-2.20	106.97	110.43
2	B	402	NAG	C6-C5-C4	-2.17	107.68	113.02
2	B	401	NAG	O4-C4-C3	-2.15	105.30	110.38
2	B	402	NAG	O4-C4-C3	-2.02	105.61	110.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAG	O5-C5-C6-O6

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	376/380 (98%)	1.26	80 (21%) 2 2	19, 32, 53, 83	0
1	B	376/380 (98%)	1.32	89 (23%) 2 2	20, 32, 56, 76	0
All	All	752/760 (98%)	1.29	169 (22%) 2 2	19, 32, 54, 83	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	VAL	5.3
1	B	336	LEU	5.1
1	B	99	SER	5.0
1	A	338	CYS	4.5
1	B	338	CYS	4.5
1	A	99	SER	4.5
1	B	287	ALA	4.5
1	A	101	VAL	4.4
1	A	255	ILE	4.2
1	B	275	TRP	4.1
1	B	91	LEU	4.0
1	B	334	SER	4.0
1	A	259	LEU	3.9
1	B	335	ALA	3.9
1	B	337	GLN	3.8
1	B	95	ASP	3.7
1	A	275	TRP	3.7
1	B	243	TRP	3.7
1	A	243	TRP	3.7
1	A	95	ASP	3.7
1	A	312	GLU	3.5
1	A	100	SER	3.4
1	B	255	ILE	3.3
1	A	98	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	313	SER	3.3
1	A	253	PRO	3.3
1	B	316	ASP	3.3
1	A	133	ALA	3.3
1	A	334	SER	3.3
1	B	314	PHE	3.2
1	B	282	GLU	3.2
1	B	259	LEU	3.2
1	A	252	THR	3.1
1	B	98	LYS	3.1
1	B	254	THR	3.1
1	B	4	HIS	3.1
1	A	314	PHE	3.1
1	A	238	PRO	3.1
1	A	91	LEU	3.1
1	A	201	ALA	3.1
1	B	213	ASN	3.0
1	B	100	SER	3.0
1	A	335	ALA	3.0
1	B	343	SER	2.9
1	B	285	VAL	2.9
1	A	225	GLU	2.9
1	B	238	PRO	2.9
1	A	287	ALA	2.9
1	A	276	LEU	2.9
1	B	312	GLU	2.9
1	A	316	ASP	2.9
1	A	315	PRO	2.8
1	A	37	GLU	2.8
1	A	202	LYS	2.8
1	A	254	THR	2.8
1	B	286	GLU	2.8
1	B	310	TYR	2.7
1	B	342	GLN	2.7
1	B	322	CYS	2.7
1	A	288	THR	2.7
1	B	276	LEU	2.7
1	A	321	ILE	2.7
1	A	379	PRO	2.7
1	B	220	PRO	2.7
1	A	4	HIS	2.7
1	A	309	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	344	ARG	2.7
1	A	356	GLY	2.6
1	B	317	ARG	2.6
1	B	201	ALA	2.6
1	A	337	GLN	2.6
1	A	241	TYR	2.6
1	B	252	THR	2.6
1	B	297	CYS	2.6
1	B	320	LYS	2.6
1	B	251	GLN	2.6
1	A	213	ASN	2.6
1	A	242	THR	2.6
1	A	308	SER	2.6
1	B	26	THR	2.6
1	B	241	TYR	2.6
1	A	216	PRO	2.6
1	B	216	PRO	2.6
1	A	336	LEU	2.6
1	A	223	ILE	2.6
1	A	318	ASP	2.6
1	A	262	TYR	2.5
1	B	289	MET	2.5
1	A	104	TYR	2.5
1	A	313	SER	2.5
1	B	340	ALA	2.5
1	A	36	THR	2.5
1	B	253	PRO	2.5
1	B	315	PRO	2.5
1	A	320	LYS	2.5
1	B	266	PHE	2.5
1	B	242	THR	2.5
1	A	282	GLU	2.4
1	B	248	VAL	2.4
1	A	346	GLU	2.4
1	B	225	GLU	2.4
1	B	102	GLY	2.4
1	B	219	GLY	2.4
1	B	328	GLY	2.4
1	B	356	GLY	2.4
1	B	269	ILE	2.4
1	B	37	GLU	2.4
1	B	96	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	212	ASN	2.4
1	B	198	GLY	2.4
1	B	270	GLY	2.4
1	B	280	ASP	2.3
1	A	299	TYR	2.3
1	A	323	PHE	2.3
1	A	273	ASP	2.3
1	B	118	THR	2.3
1	A	251	GLN	2.3
1	A	96	PRO	2.3
1	B	133	ALA	2.3
1	A	214	ARG	2.3
1	A	97	SER	2.3
1	B	308	SER	2.3
1	B	64	VAL	2.3
1	A	240	ASN	2.3
1	A	297	CYS	2.3
1	B	350	LEU	2.3
1	A	311	TYR	2.2
1	B	323	PHE	2.2
1	B	321	ILE	2.2
1	B	202	LYS	2.2
1	A	102	GLY	2.2
1	A	115	TRP	2.2
1	A	197	TRP	2.2
1	B	212	ASN	2.2
1	B	311	TYR	2.2
1	B	223	ILE	2.2
1	B	197	TRP	2.2
1	A	317	ARG	2.2
1	B	260	ARG	2.2
1	A	342	GLN	2.2
1	B	273	ASP	2.2
1	A	271	PHE	2.1
1	A	310	TYR	2.1
1	B	262	TYR	2.1
1	B	97	SER	2.1
1	A	219	GLY	2.1
1	B	283	GLY	2.1
1	A	260	ARG	2.1
1	B	277	MET	2.1
1	A	331	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	318	ASP	2.1
1	B	35	LYS	2.1
1	A	71	ALA	2.1
1	A	58	ILE	2.1
1	A	269	ILE	2.1
1	A	264	LYS	2.1
1	B	288	THR	2.1
1	A	248	VAL	2.1
1	B	113	VAL	2.1
1	B	235	TRP	2.1
1	A	121	GLU	2.0
1	B	258	THR	2.0
1	A	204	LEU	2.0
1	B	121	GLU	2.0
1	B	246	GLU	2.0
1	B	264	LYS	2.0
1	A	265	PHE	2.0
1	A	113	VAL	2.0
1	B	250	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	402	14/15	0.86	0.12	33,37,46,47	0
2	NAG	B	402	14/15	0.86	0.13	35,38,52,55	0
2	NAG	B	401	14/15	0.88	0.12	34,40,43,47	0
2	NAG	A	401	14/15	0.89	0.12	29,34,36,41	0

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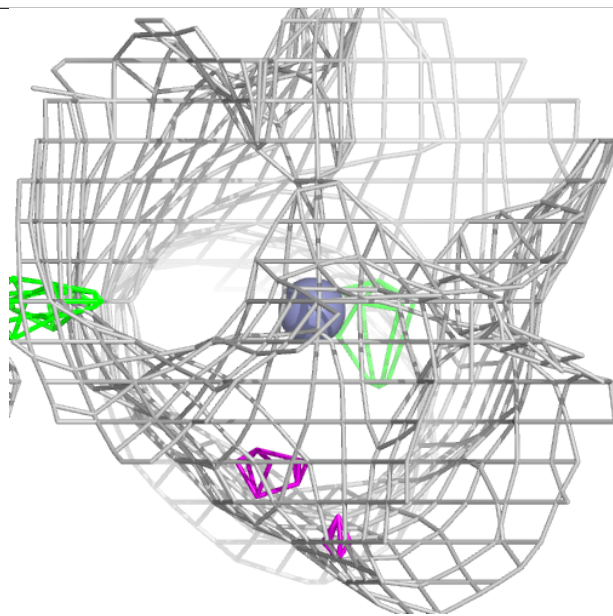
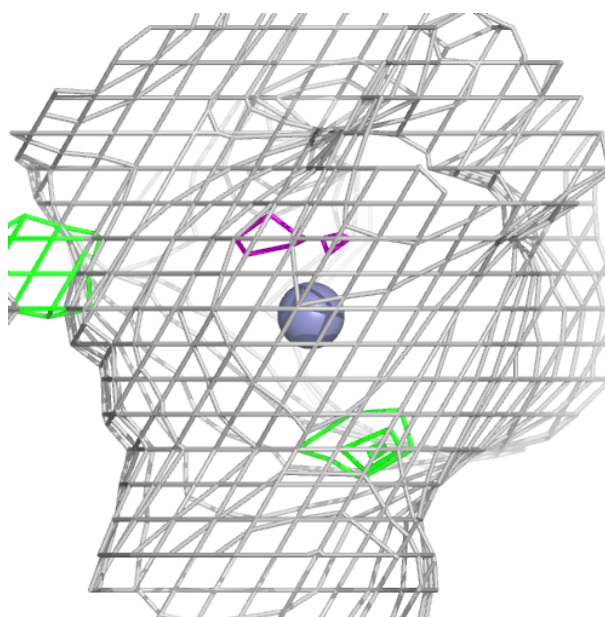
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	403	1/1	0.94	0.11	56,56,56,56	0
3	CL	A	403	1/1	0.96	0.15	48,48,48,48	0
4	ZN	A	406	1/1	0.97	0.05	39,39,39,39	0
4	ZN	B	406	1/1	0.97	0.04	38,38,38,38	0
4	ZN	B	405	1/1	0.98	0.04	37,37,37,37	0
4	ZN	A	405	1/1	0.98	0.04	38,38,38,38	0
4	ZN	A	407	1/1	0.99	0.04	51,51,51,51	0
4	ZN	B	404	1/1	0.99	0.02	33,33,33,33	0
4	ZN	B	407	1/1	0.99	0.03	47,47,47,47	0
4	ZN	A	404	1/1	1.00	0.01	32,32,32,32	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.

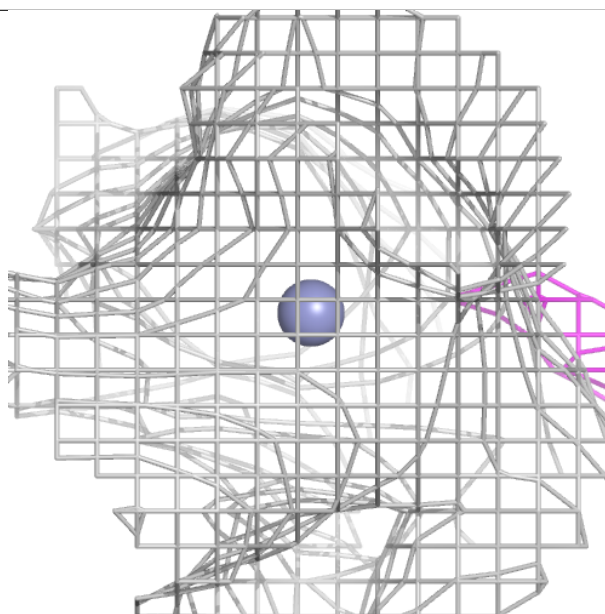
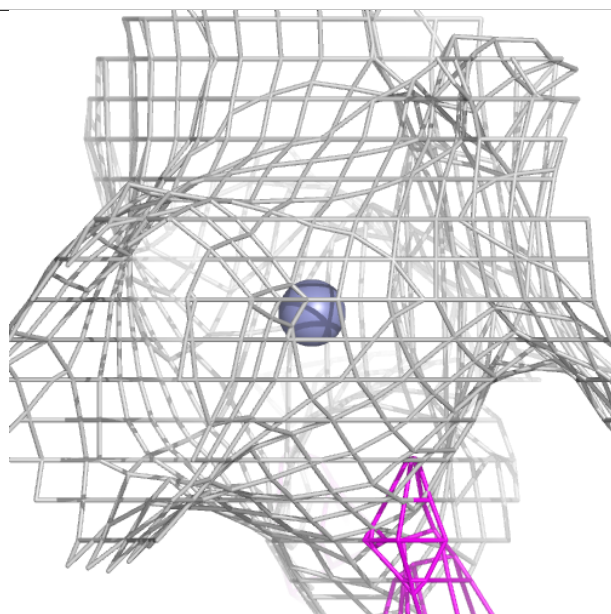
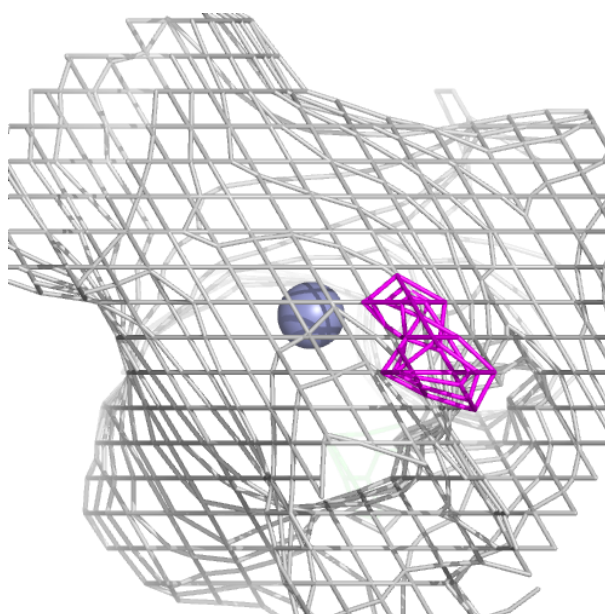
Electron density around ZN A 406:

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



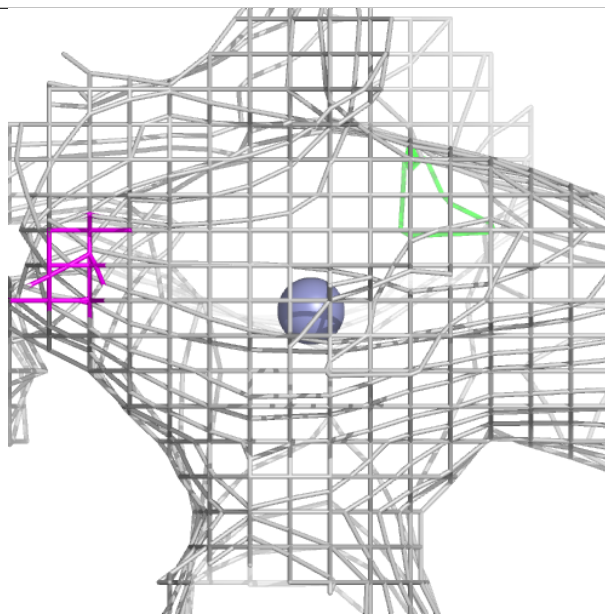
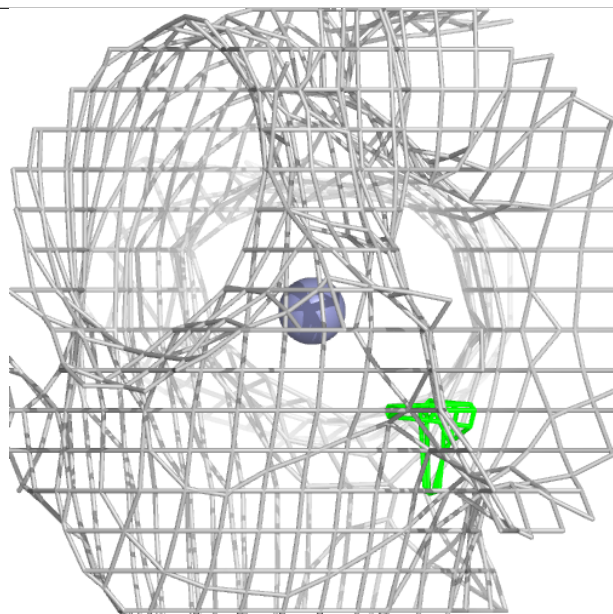
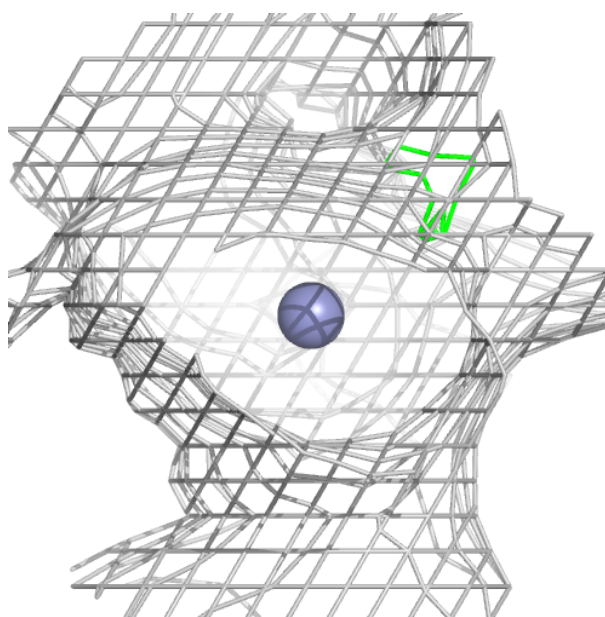
Electron density around ZN B 406:

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



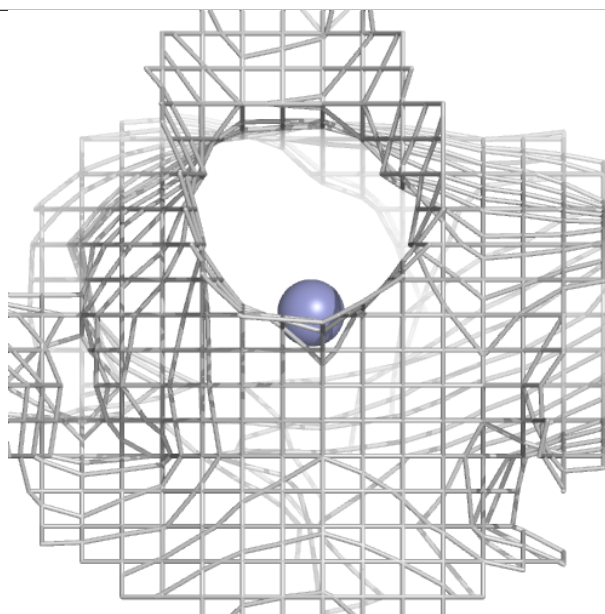
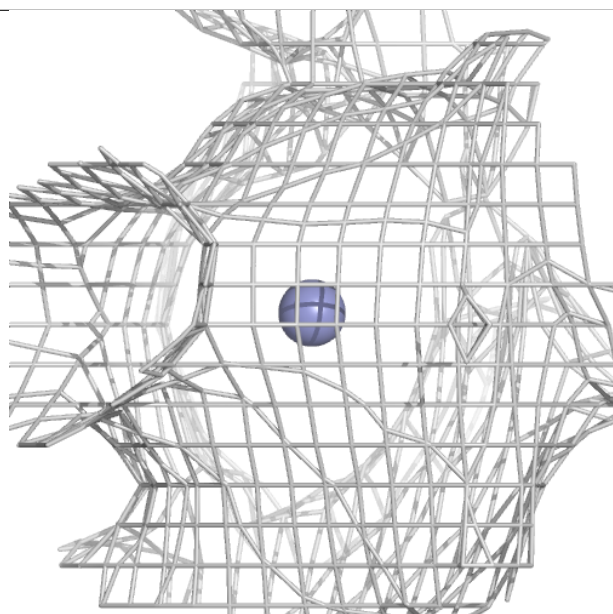
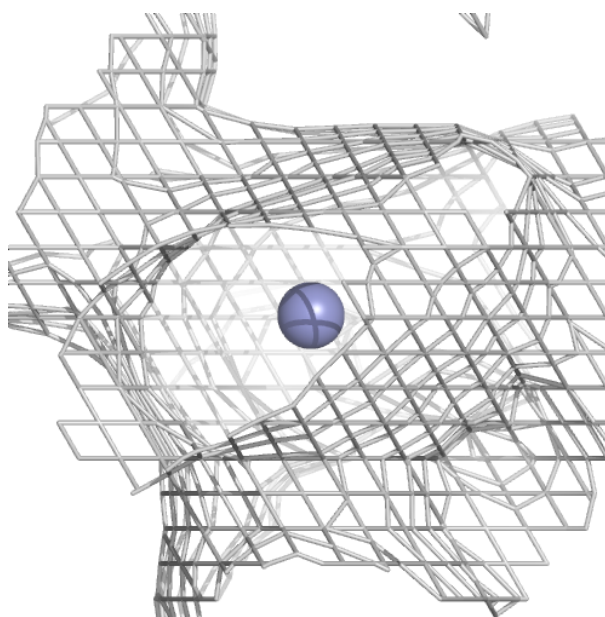
Electron density around ZN B 405:

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and green (positive)



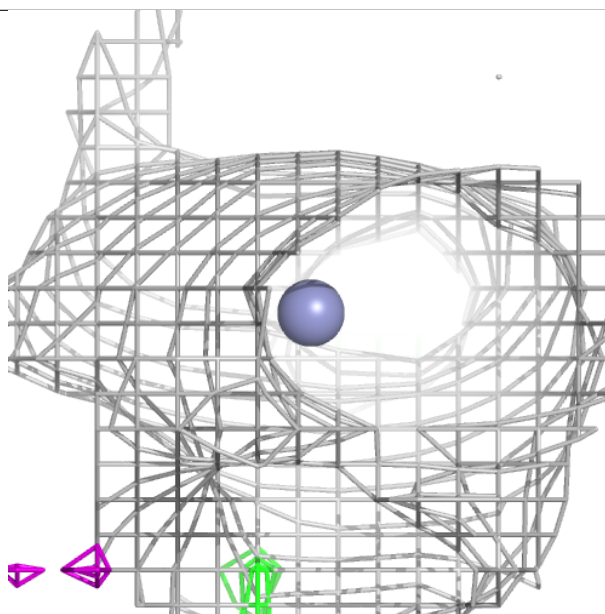
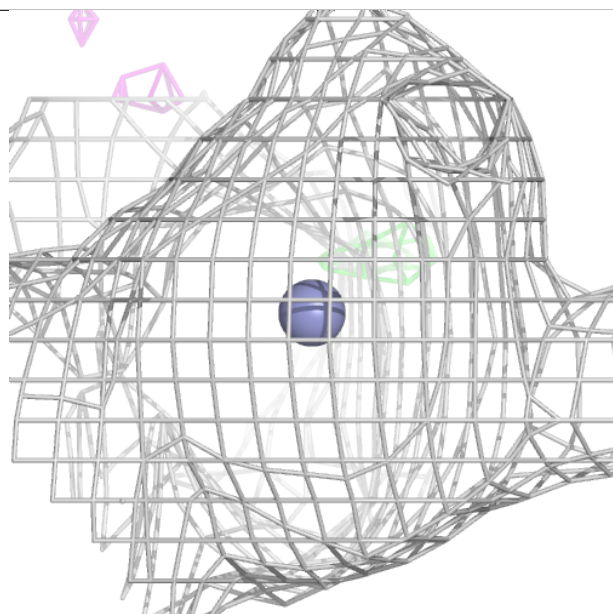
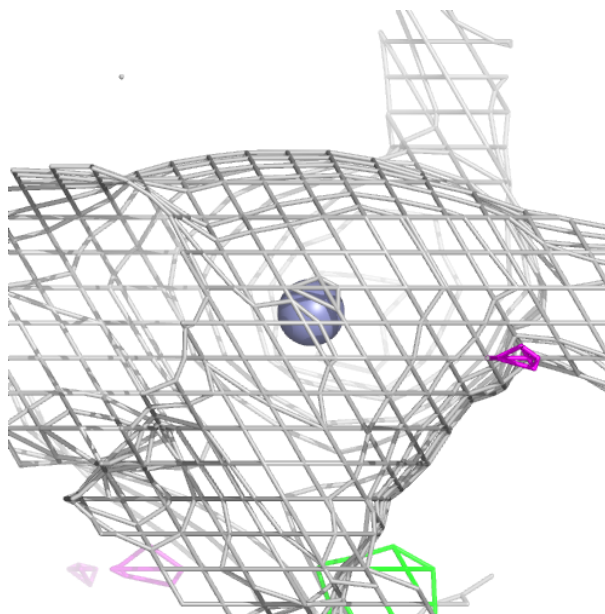
Electron density around ZN A 405:

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and green (positive)



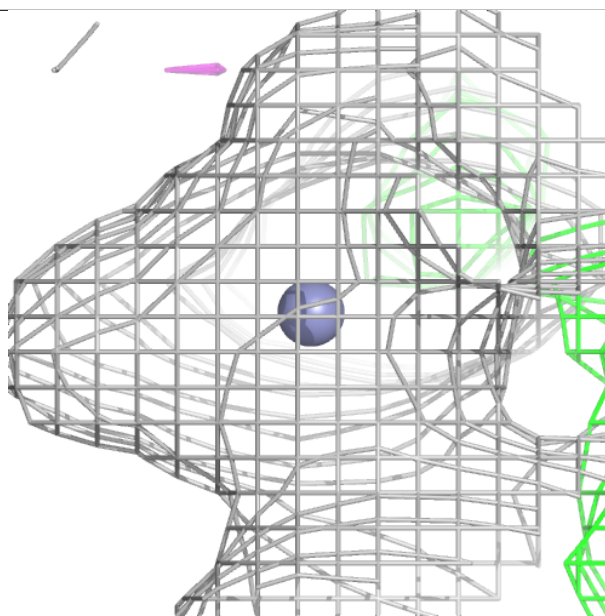
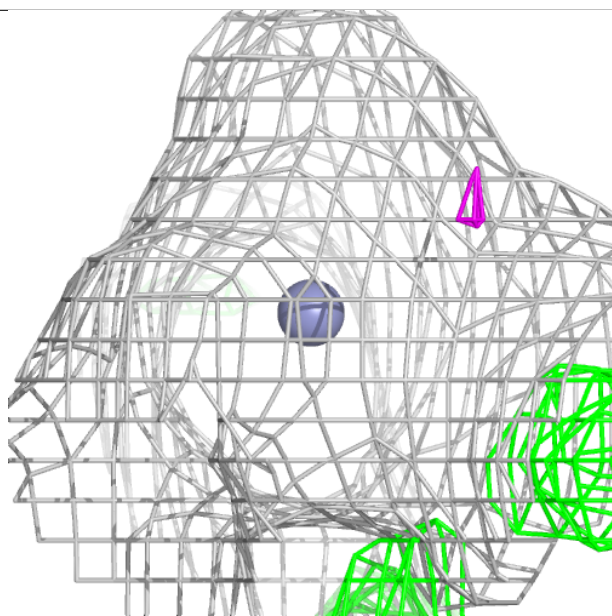
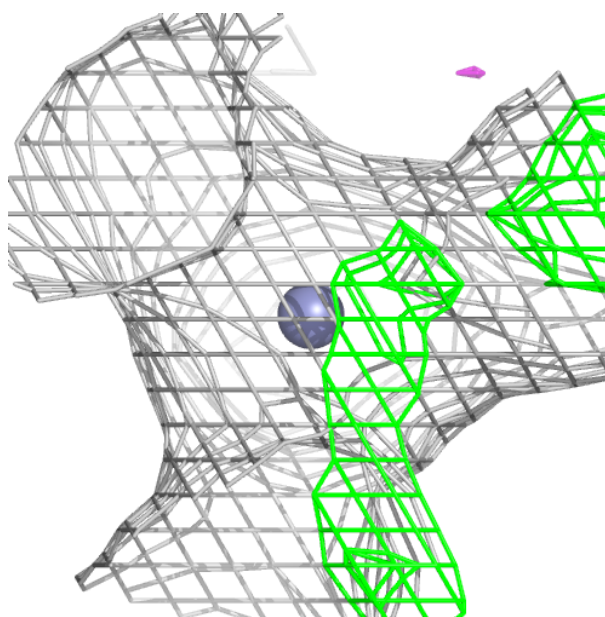
Electron density around ZN A 407:

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



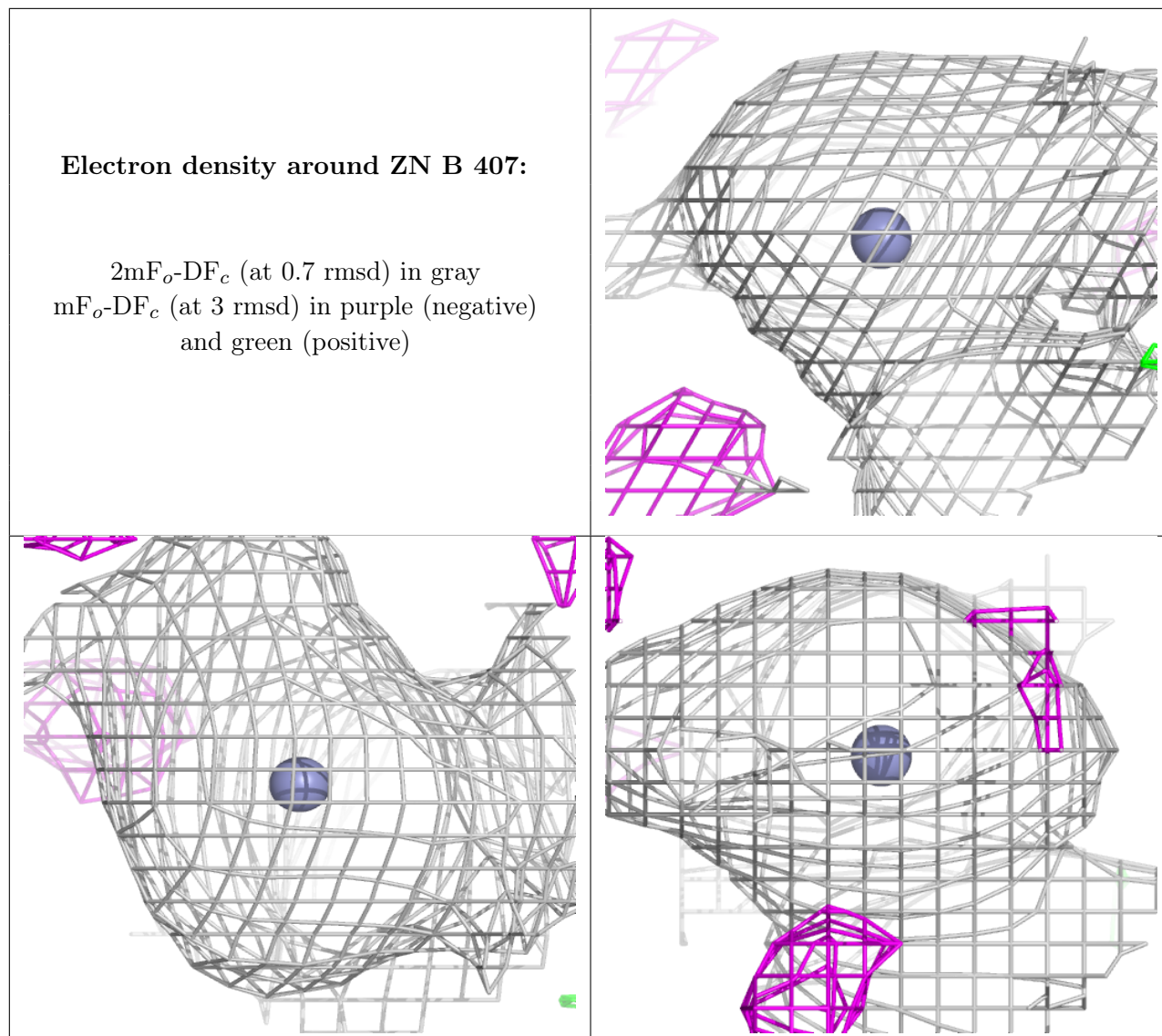
Electron density around ZN B 404:

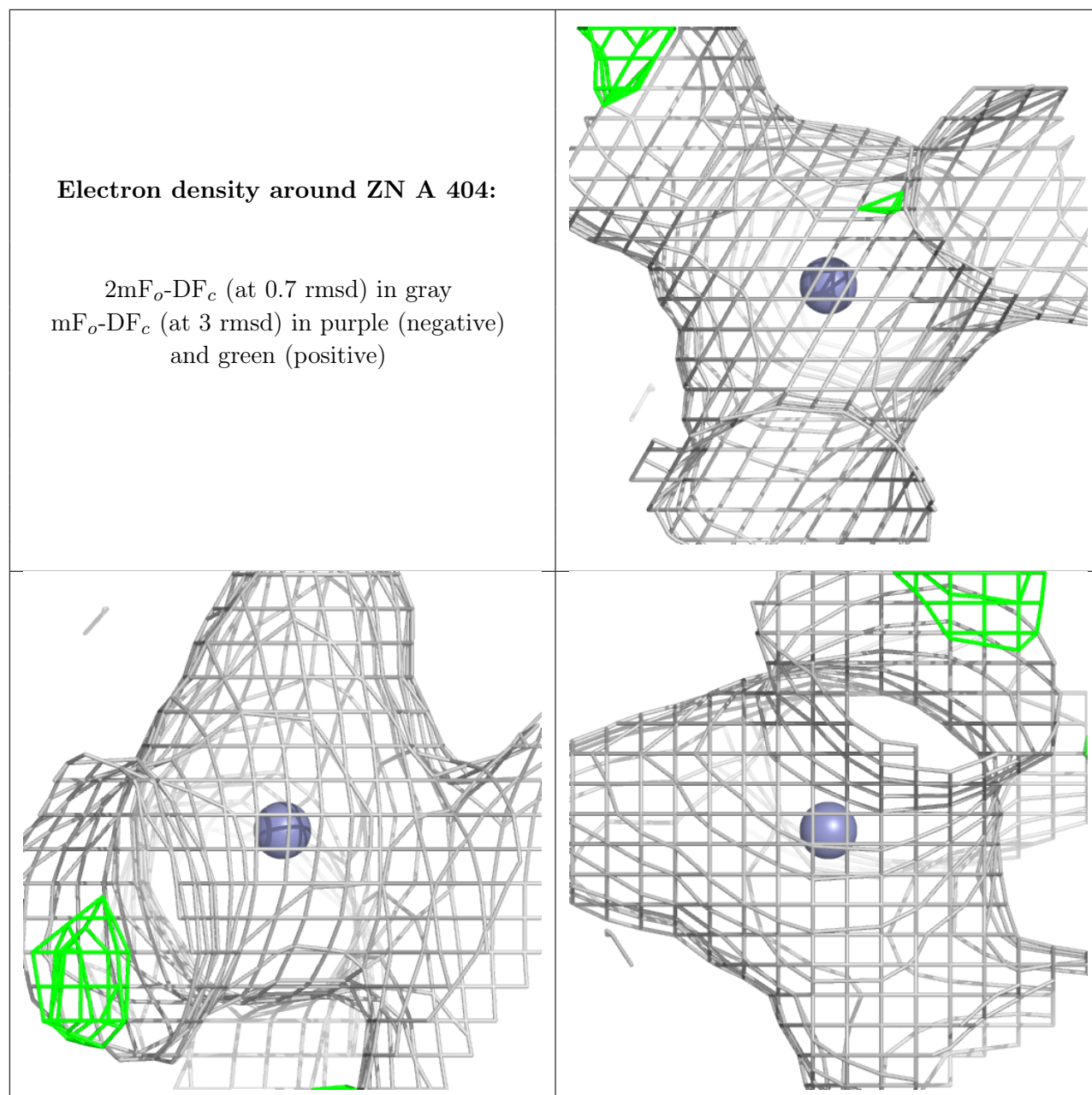
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 407:

$2mF_o-DF_c$ (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.