



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:31 PM UTC

PDB ID : 9HKU / pdb\_00009hku  
Title : Crystal structure of CREBBP histone acetyltransferase domain in complex with Acetyl-Coenzyme A  
Authors : Mechaly, A.E.; Zhang, W.; Cui, G.; Green, M.R.; Rodrigues-Lima, F.  
Deposited on : 2024-12-04  
Resolution : 2.36 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

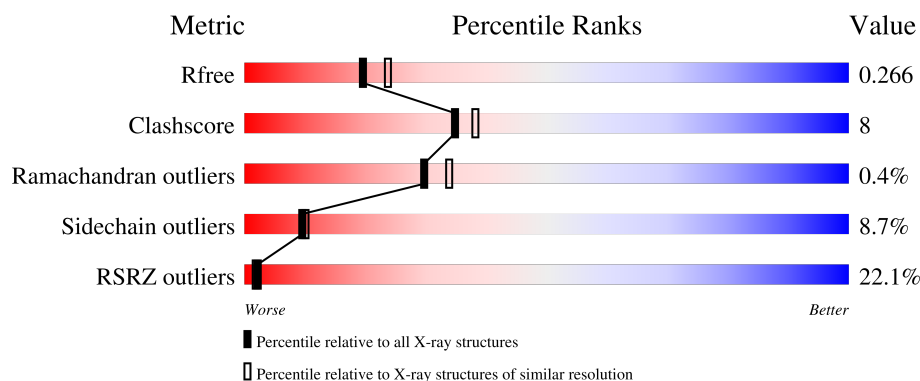
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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  $\geq 3$ , 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	640	<div> <div>16%</div> <div>63%</div> <div>18%</div> <div>•</div> <div>17%</div> </div>
1	B	640	<div> <div>21%</div> <div>62%</div> <div>16%</div> <div>•</div> <div>18%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9160 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 histone acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	1	0
			4426	2833	761	797	35			
1	B	523	Total	C	N	O	S	0	1	0
			4351	2790	745	781	35			

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1055	HIS	-	expression tag	UNP F8VPR5
A	1056	HIS	-	expression tag	UNP F8VPR5
A	1057	HIS	-	expression tag	UNP F8VPR5
A	1058	HIS	-	expression tag	UNP F8VPR5
A	1059	HIS	-	expression tag	UNP F8VPR5
A	1060	HIS	-	expression tag	UNP F8VPR5
A	1061	ASP	-	expression tag	UNP F8VPR5
A	1062	TYR	-	expression tag	UNP F8VPR5
A	1063	ASP	-	expression tag	UNP F8VPR5
A	1064	ILE	-	expression tag	UNP F8VPR5
A	1065	PRO	-	expression tag	UNP F8VPR5
A	1066	THR	-	expression tag	UNP F8VPR5
A	1067	THR	-	expression tag	UNP F8VPR5
A	1068	GLU	-	expression tag	UNP F8VPR5
A	1069	ASN	-	expression tag	UNP F8VPR5
A	1070	LEU	-	expression tag	UNP F8VPR5
A	1071	TYR	-	expression tag	UNP F8VPR5
A	1072	PHE	-	expression tag	UNP F8VPR5
A	1073	GLN	-	expression tag	UNP F8VPR5
A	1074	GLY	-	expression tag	UNP F8VPR5
A	1075	ALA	-	expression tag	UNP F8VPR5
A	1076	MET	-	expression tag	UNP F8VPR5
A	1077	GLY	-	expression tag	UNP F8VPR5
A	1078	SER	-	expression tag	UNP F8VPR5
A	1504	PHE	TYR	engineered mutation	UNP F8VPR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	GLN	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	ARG	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	THR	deletion	UNP F8VPR5
A	?	-	ALA	deletion	UNP F8VPR5
A	?	-	ALA	deletion	UNP F8VPR5
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	THR	deletion	UNP F8VPR5
A	?	-	PRO	deletion	UNP F8VPR5
A	?	-	GLU	deletion	UNP F8VPR5
A	?	-	GLY	deletion	UNP F8VPR5
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	GLN	deletion	UNP F8VPR5
A	?	-	GLY	deletion	UNP F8VPR5
A	?	-	ASP	deletion	UNP F8VPR5
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	ASN	deletion	UNP F8VPR5
A	?	-	ALA	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	ASN	deletion	UNP F8VPR5
A	?	-	ASN	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	THR	deletion	UNP F8VPR5
A	?	-	ASN	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	ASN	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	ILE	deletion	UNP F8VPR5
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	ARG	deletion	UNP F8VPR5
A	?	-	ALA	deletion	UNP F8VPR5
A	?	-	ASN	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	LYS	deletion	UNP F8VPR5
A	?	-	PRO	deletion	UNP F8VPR5
A	?	-	SER	deletion	UNP F8VPR5
A	?	-	MET	deletion	UNP F8VPR5
A	?	-	PRO	deletion	UNP F8VPR5
A	?	-	ASN	deletion	UNP F8VPR5
A	1614	SER	VAL	conflict	UNP F8VPR5
A	1615	GLY	SER	conflict	UNP F8VPR5
A	1616	GLY	ASN	conflict	UNP F8VPR5
A	1617	SER	ASP	conflict	UNP F8VPR5
A	1618	GLY	LEU	conflict	UNP F8VPR5
B	1055	HIS	-	expression tag	UNP F8VPR5
B	1056	HIS	-	expression tag	UNP F8VPR5
B	1057	HIS	-	expression tag	UNP F8VPR5
B	1058	HIS	-	expression tag	UNP F8VPR5
B	1059	HIS	-	expression tag	UNP F8VPR5
B	1060	HIS	-	expression tag	UNP F8VPR5
B	1061	ASP	-	expression tag	UNP F8VPR5
B	1062	TYR	-	expression tag	UNP F8VPR5
B	1063	ASP	-	expression tag	UNP F8VPR5
B	1064	ILE	-	expression tag	UNP F8VPR5
B	1065	PRO	-	expression tag	UNP F8VPR5
B	1066	THR	-	expression tag	UNP F8VPR5
B	1067	THR	-	expression tag	UNP F8VPR5
B	1068	GLU	-	expression tag	UNP F8VPR5
B	1069	ASN	-	expression tag	UNP F8VPR5
B	1070	LEU	-	expression tag	UNP F8VPR5
B	1071	TYR	-	expression tag	UNP F8VPR5
B	1072	PHE	-	expression tag	UNP F8VPR5
B	1073	GLN	-	expression tag	UNP F8VPR5
B	1074	GLY	-	expression tag	UNP F8VPR5
B	1075	ALA	-	expression tag	UNP F8VPR5
B	1076	MET	-	expression tag	UNP F8VPR5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1077	GLY	-	expression tag	UNP F8VPR5
B	1078	SER	-	expression tag	UNP F8VPR5
B	1504	PHE	TYR	engineered mutation	UNP F8VPR5
B	?	-	LEU	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	GLN	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	ARG	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	THR	deletion	UNP F8VPR5
B	?	-	ALA	deletion	UNP F8VPR5
B	?	-	ALA	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	THR	deletion	UNP F8VPR5
B	?	-	PRO	deletion	UNP F8VPR5
B	?	-	GLU	deletion	UNP F8VPR5
B	?	-	GLY	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	GLN	deletion	UNP F8VPR5
B	?	-	GLY	deletion	UNP F8VPR5
B	?	-	ASP	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5
B	?	-	ALA	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	THR	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5

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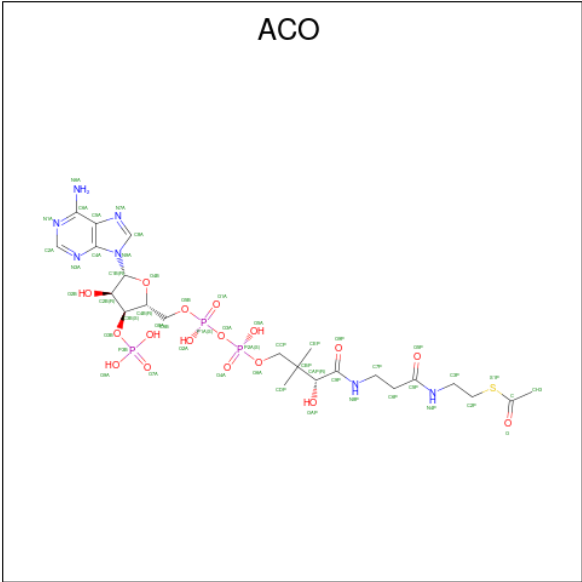
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	ILE	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	ARG	deletion	UNP F8VPR5
B	?	-	ALA	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	PRO	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	MET	deletion	UNP F8VPR5
B	?	-	PRO	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5
B	1614	SER	VAL	conflict	UNP F8VPR5
B	1615	GLY	SER	conflict	UNP F8VPR5
B	1616	GLY	ASN	conflict	UNP F8VPR5
B	1617	SER	ASP	conflict	UNP F8VPR5
B	1618	GLY	LEU	conflict	UNP F8VPR5

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

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

- Molecule 3 is ACETYL COENZYME \*A (CCD ID: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is water.

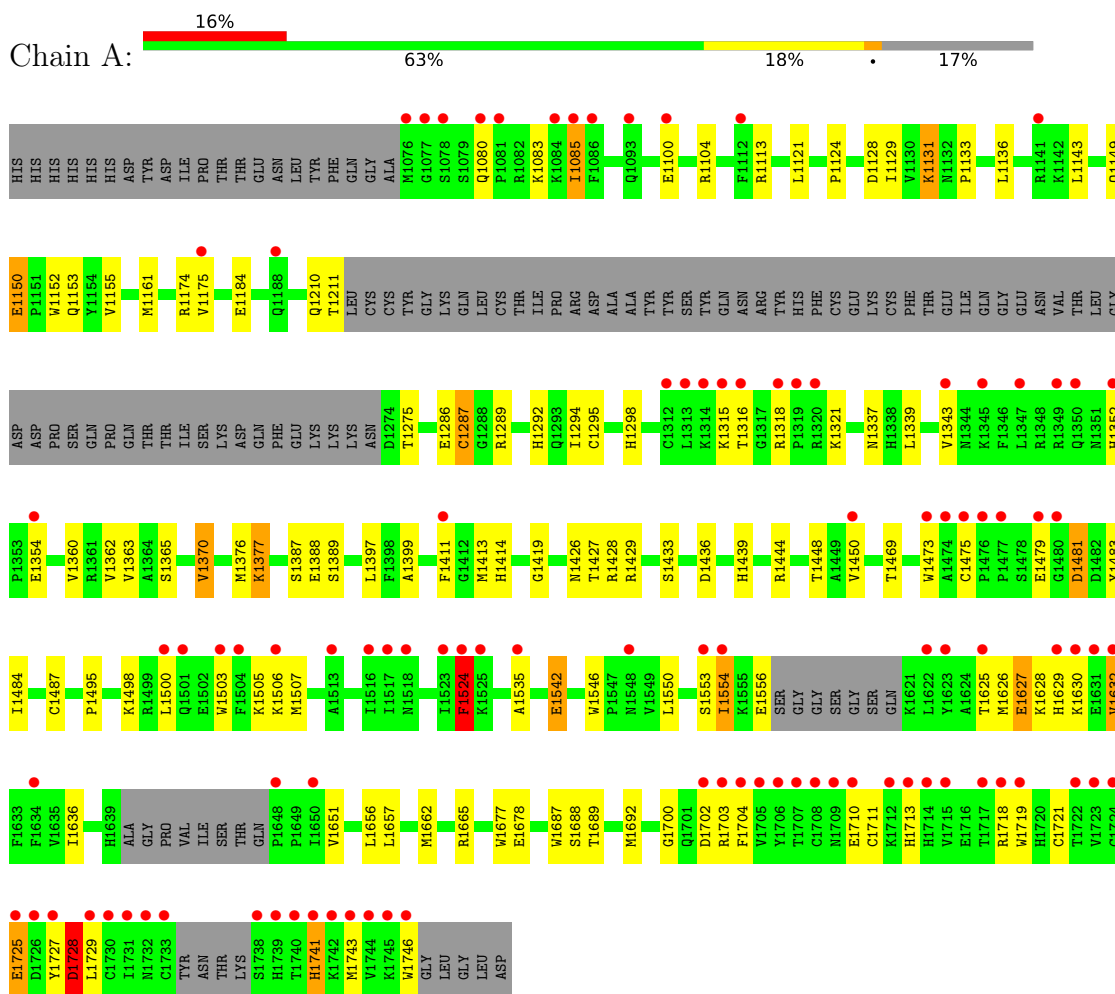
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	111	Total	O	0	0
			111	111		



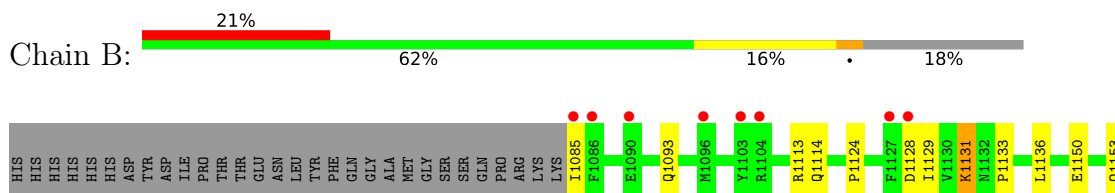
### 3 Residue-property plots [i](#)

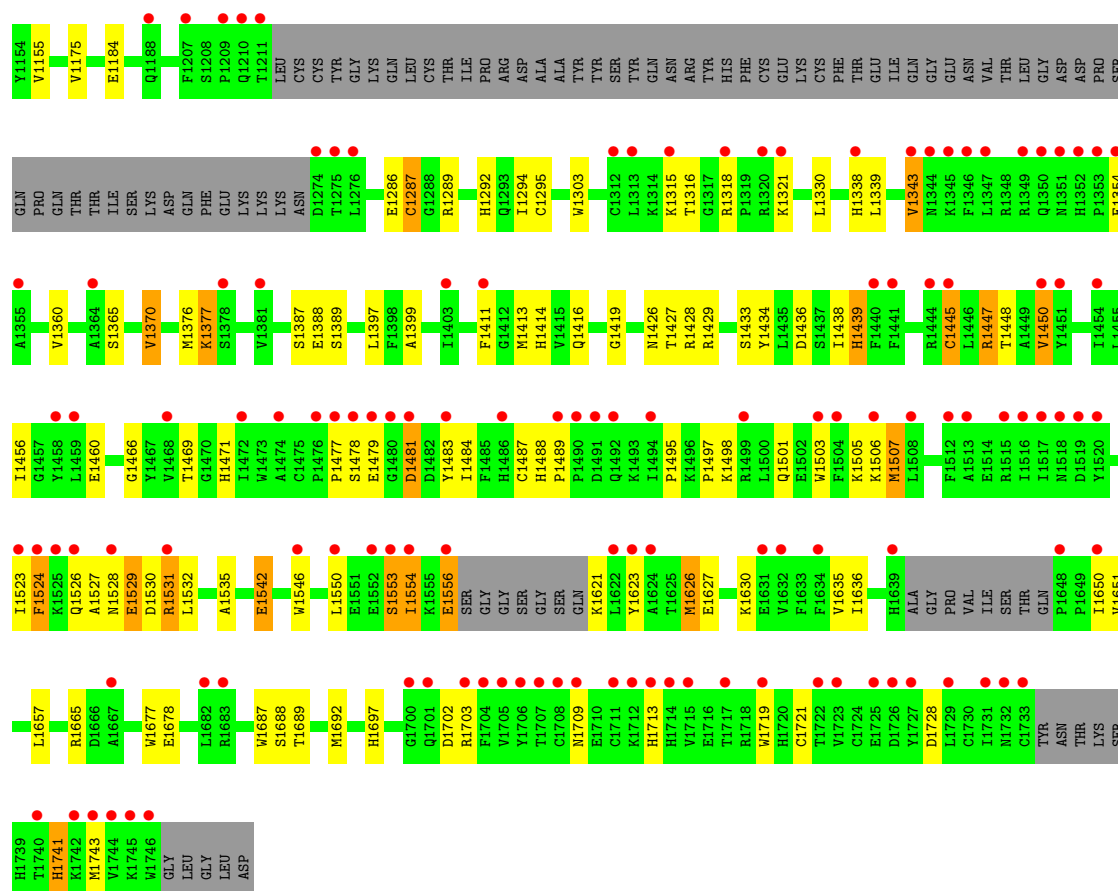
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: histone acetyltransferase



#### • Molecule 1: histone acetyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.62Å 139.93Å 154.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.57 – 2.36 154.57 – 2.36	Depositor EDS
% Data completeness (in resolution range)	51.6 (154.57-2.36) 51.6 (154.57-2.36)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.71 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.245 , 0.287 (Not available) , 0.266	Depositor DCC
$R_{free}$ test set	2017 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9160	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ACO

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	0.70	0/4552	1.14	21/6151 (0.3%)
1	B	0.68	0/4476	1.13	12/6051 (0.2%)
All	All	0.69	0/9028	1.13	33/12202 (0.3%)

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1524	PHE	CA-CB-CG	-8.72	105.08	113.80
1	B	1554	ILE	N-CA-C	-6.50	105.40	111.45
1	B	1286	GLU	CA-C-N	6.22	128.90	120.44
1	B	1286	GLU	C-N-CA	6.22	128.90	120.44
1	A	1665	ARG	CA-C-N	6.15	128.52	120.28

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	4426	0	4294	64	0
1	B	4351	0	4218	71	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	51	0	34	3	0
3	B	51	0	34	6	0
4	A	162	0	0	2	0
4	B	111	0	0	0	0
All	All	9160	0	8580	131	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 8.

The worst 5 of 131 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:1448:THR:HG23	1:B:1503:TRP:HE1	1.09	1.10
1:B:1523:ILE:HG22	1:B:1635:VAL:HG23	1.35	1.06
1:A:1495:PRO:HG3	3:A:1805:ACO:O1A	1.79	0.82
1:B:1553:SER:HA	1:B:1556:GLU:HG2	1.61	0.82
1:B:1495:PRO:HG3	3:B:1805:ACO:O1A	1.83	0.78

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	524/640 (82%)	504 (96%)	19 (4%)	1 (0%)	43	52
1	B	514/640 (80%)	493 (96%)	18 (4%)	3 (1%)	21	24
All	All	1038/1280 (81%)	997 (96%)	37 (4%)	4 (0%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1439	HIS
1	B	1531	ARG
1	B	1626	MET
1	A	1479	GLU

### 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	493/586 (84%)	448 (91%)	45 (9%)	9	9
1	B	484/586 (83%)	443 (92%)	41 (8%)	10	11
All	All	977/1172 (83%)	891 (91%)	86 (9%)	9	10

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1343	VAL
1	B	1506	LYS
1	B	1370	VAL
1	B	1447	ARG
1	B	1542	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1338	HIS
1	B	1709	ASN
1	A	1629	HIS
1	A	1637	HIS
1	A	1639	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACO	A	1805	-	51,53,53	0.53	0	73,79,79	0.52	0
3	ACO	B	1805	-	51,53,53	0.52	1 (1%)	73,79,79	0.61	1 (1%)

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
3	ACO	A	1805	-	-	9/51/67/67	0/3/3/3
3	ACO	B	1805	-	-	11/51/67/67	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1805	ACO	P3B-O3B	2.07	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1805	ACO	P3B-O3B-C3B	-2.09	117.86	123.43

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

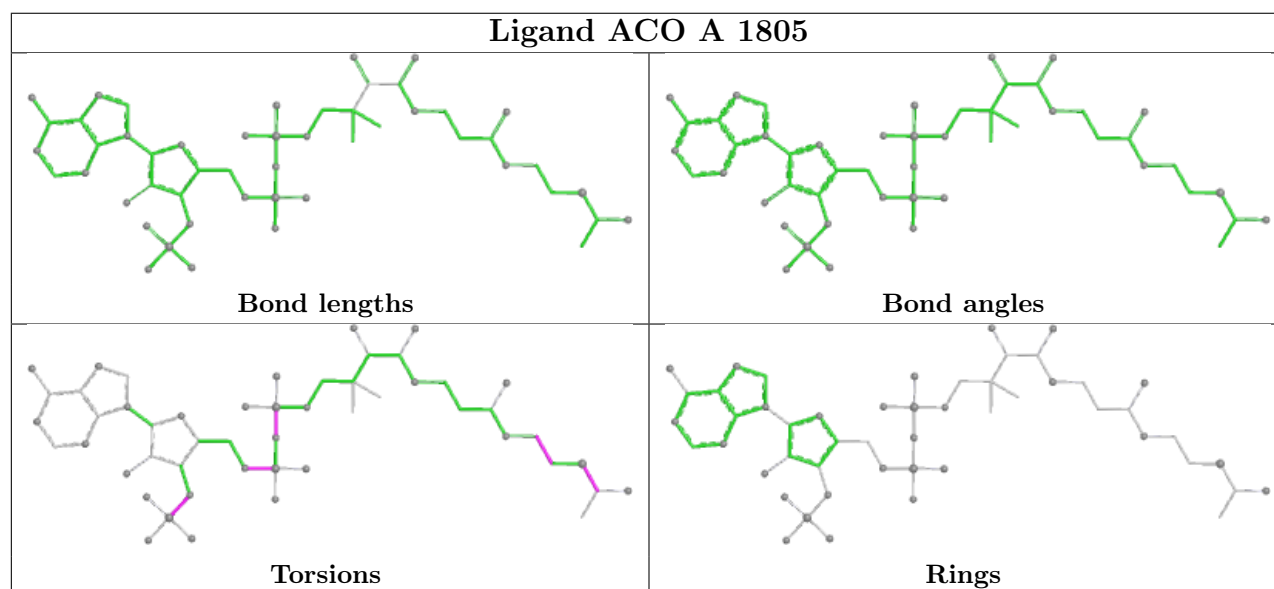
Mol	Chain	Res	Type	Atoms
3	A	1805	ACO	C5B-O5B-P1A-O1A
3	A	1805	ACO	C5B-O5B-P1A-O2A
3	A	1805	ACO	C5B-O5B-P1A-O3A
3	A	1805	ACO	S1P-C2P-C3P-N4P
3	B	1805	ACO	C5B-O5B-P1A-O1A

There are no ring outliers.

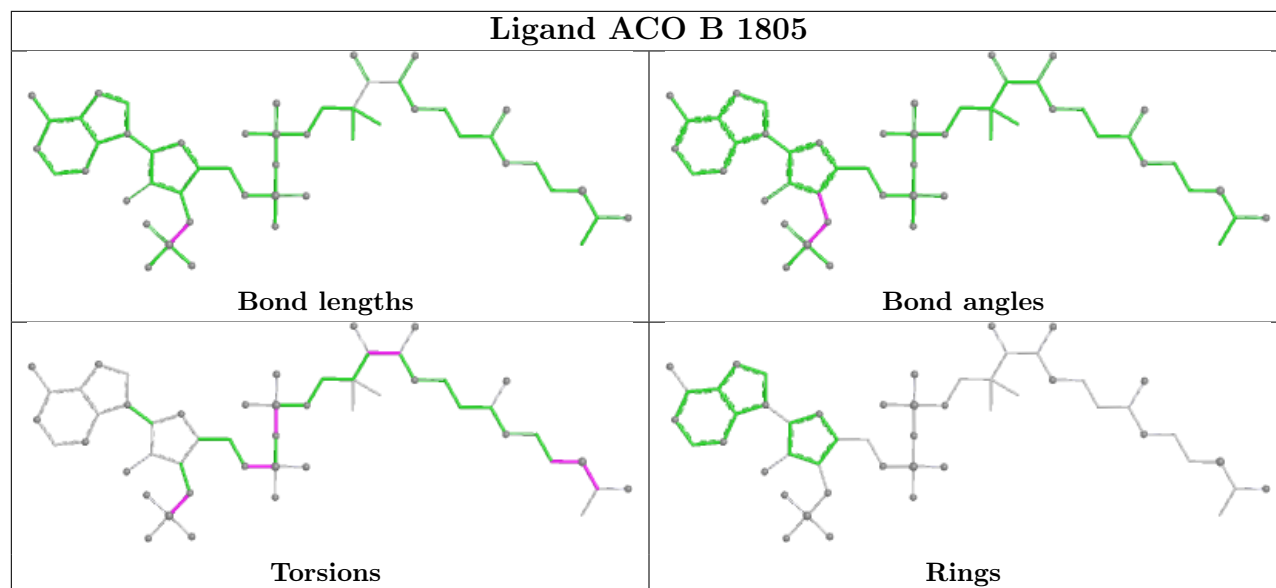
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1805	ACO	3	0
3	B	1805	ACO	6	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	533/640 (83%)	0.95	100 (18%) <b>3</b> <b>3</b>	18, 48, 105, 124	1 (0%)
1	B	523/640 (81%)	1.32	133 (25%) <b>1</b> <b>1</b>	34, 61, 101, 115	1 (0%)
All	All	1056/1280 (82%)	1.14	233 (22%) <b>2</b> <b>2</b>	18, 55, 102, 124	2 (0%)

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1733	CYS	8.1
1	A	1715	VAL	6.8
1	A	1731	ILE	6.4
1	B	1085	ILE	6.2
1	B	1731	ILE	5.8

### 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](#)

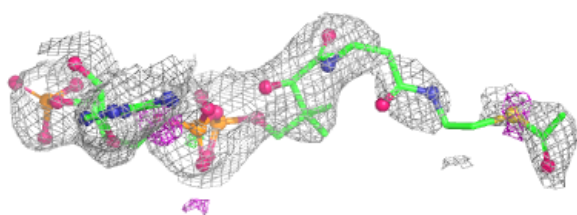
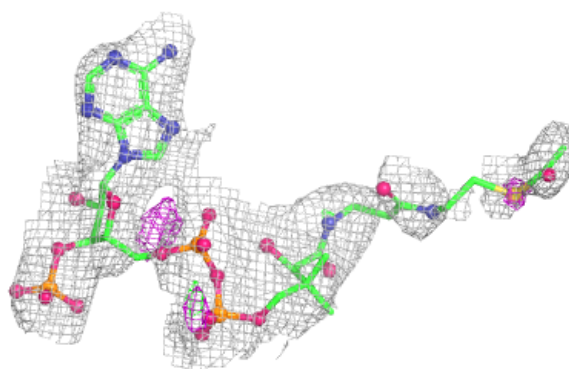
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACO	B	1805	51/51	0.90	0.15	70,75,77,77	0
2	ZN	A	1804	1/1	0.94	0.08	119,119,119,119	0
2	ZN	A	1803	1/1	0.95	0.08	100,100,100,100	0
3	ACO	A	1805	51/51	0.96	0.10	50,52,65,66	0
2	ZN	B	1803	1/1	0.96	0.08	98,98,98,98	0
2	ZN	B	1804	1/1	0.97	0.06	126,126,126,126	0
2	ZN	B	1801	1/1	0.99	0.03	43,43,43,43	0
2	ZN	A	1801	1/1	1.00	0.06	32,32,32,32	0
2	ZN	B	1802	1/1	1.00	0.08	62,62,62,62	0
2	ZN	A	1802	1/1	1.00	0.06	39,39,39,39	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.

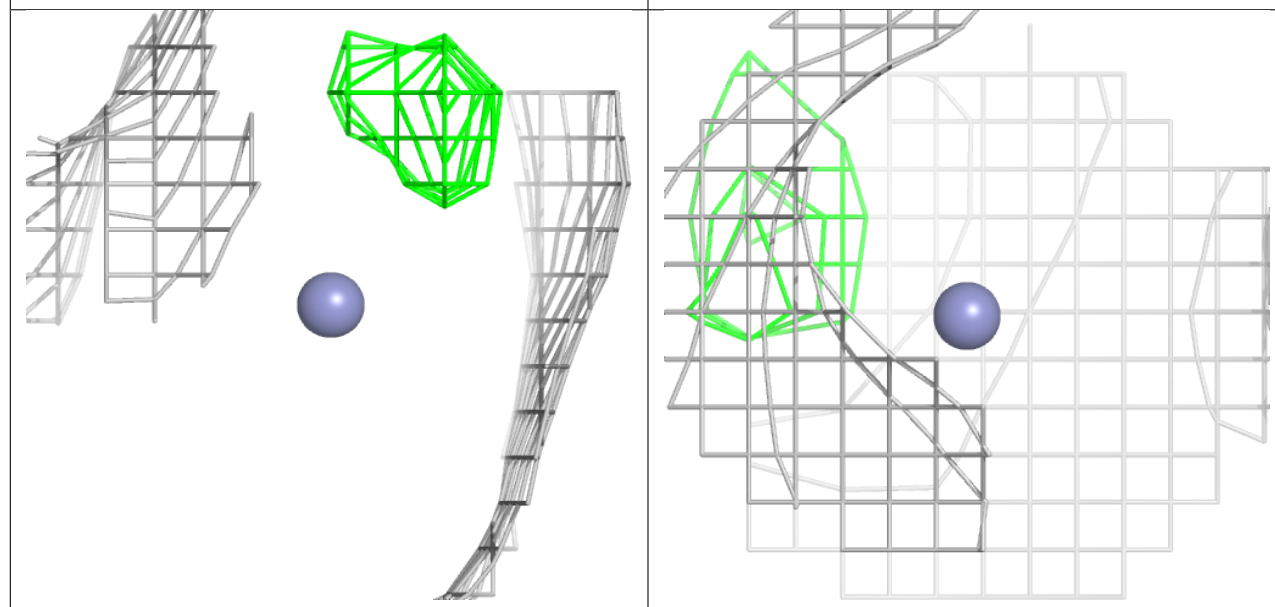
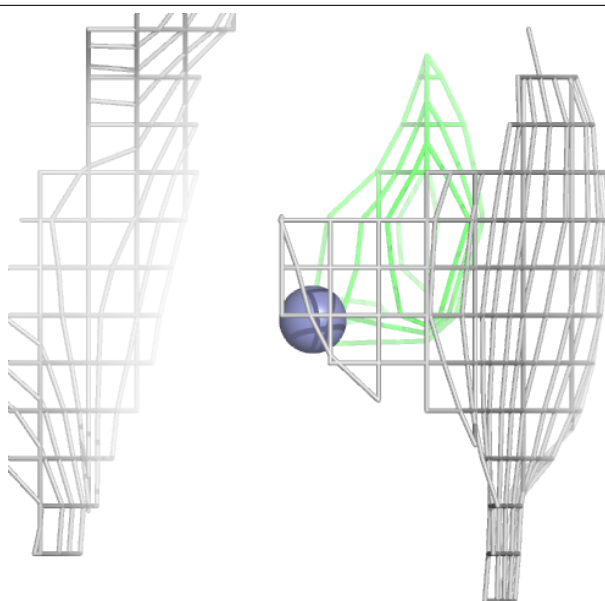
**Electron density around ACO B 1805:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



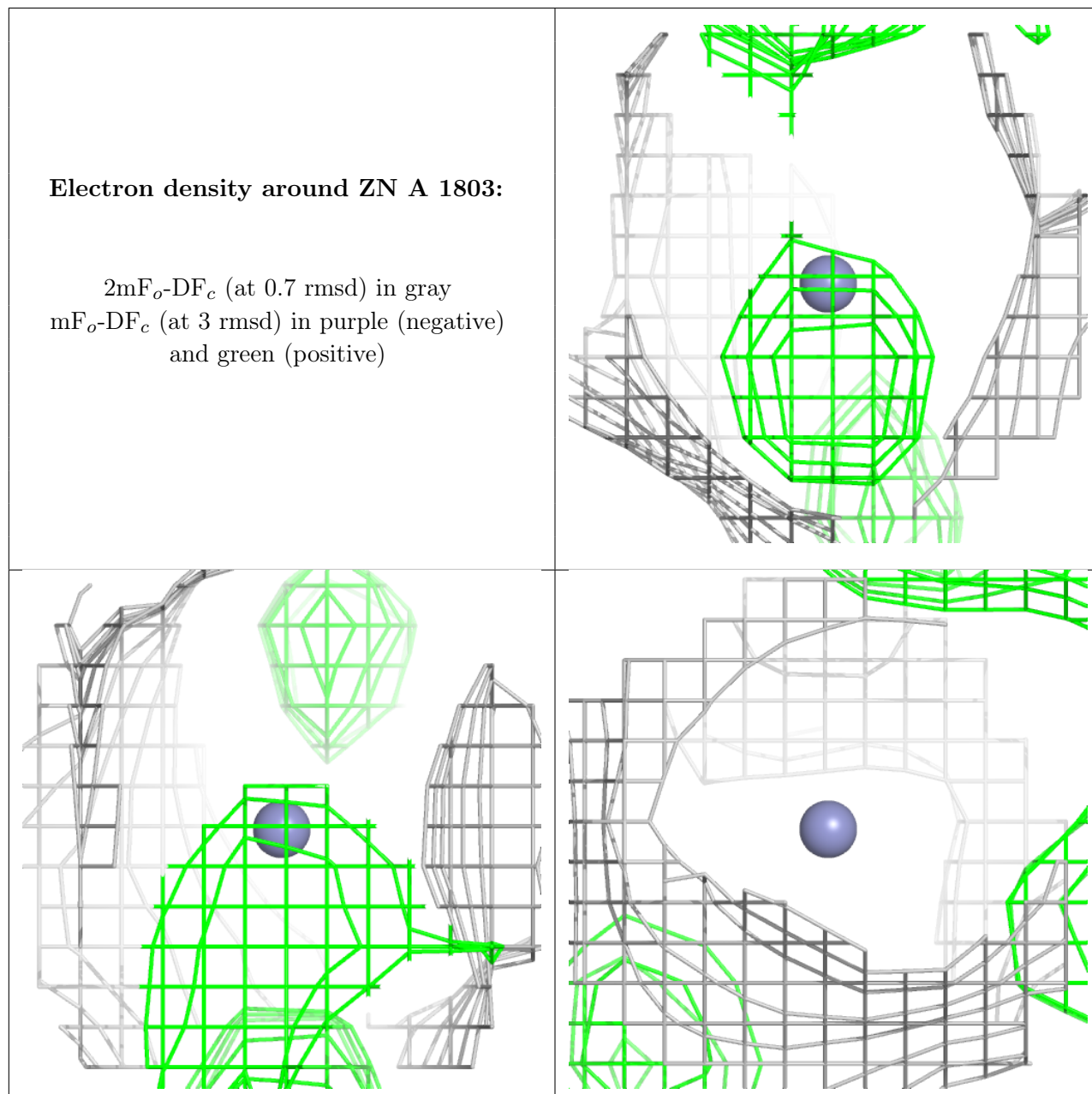
**Electron density around ZN A 1804:**

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



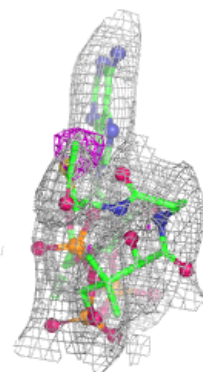
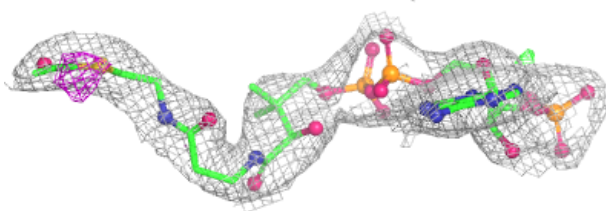
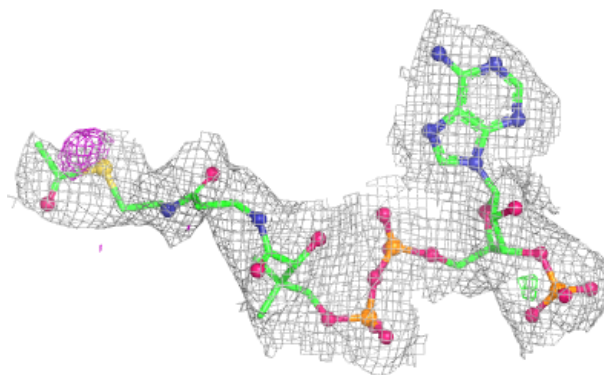
**Electron density around ZN A 1803:**

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



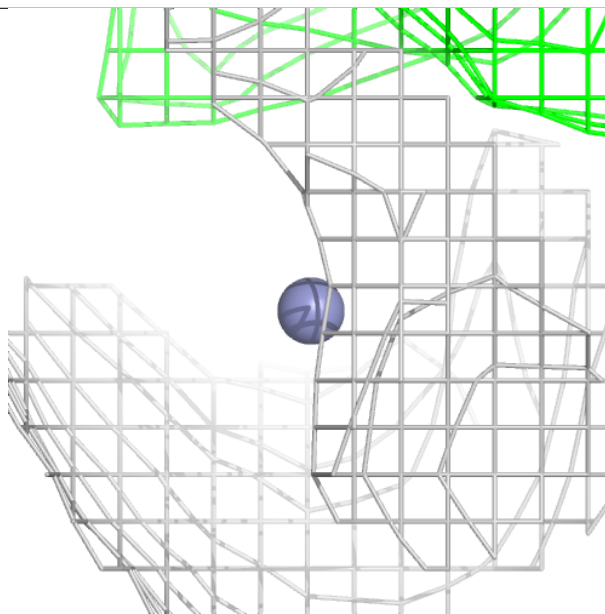
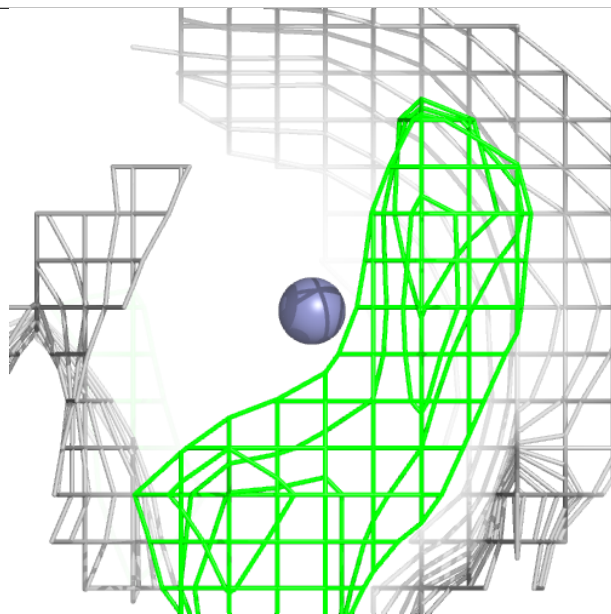
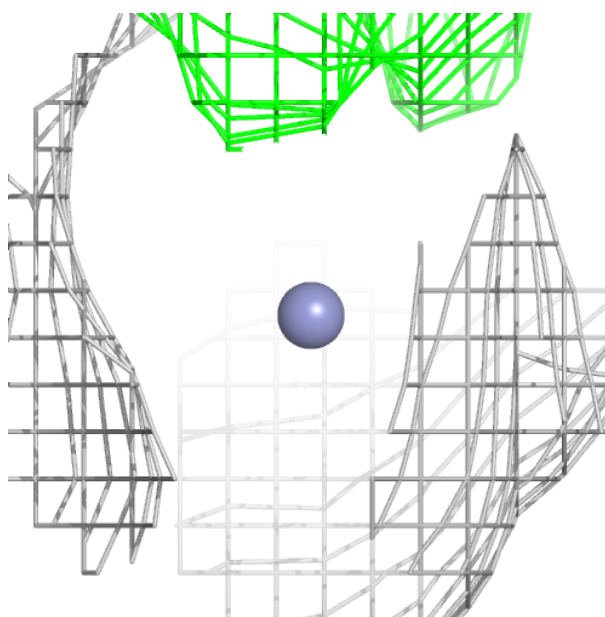
**Electron density around ACO A 1805:**

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



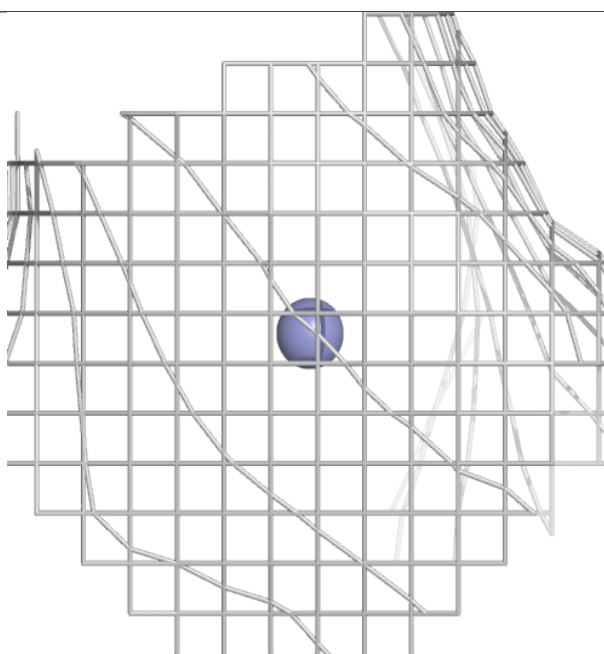
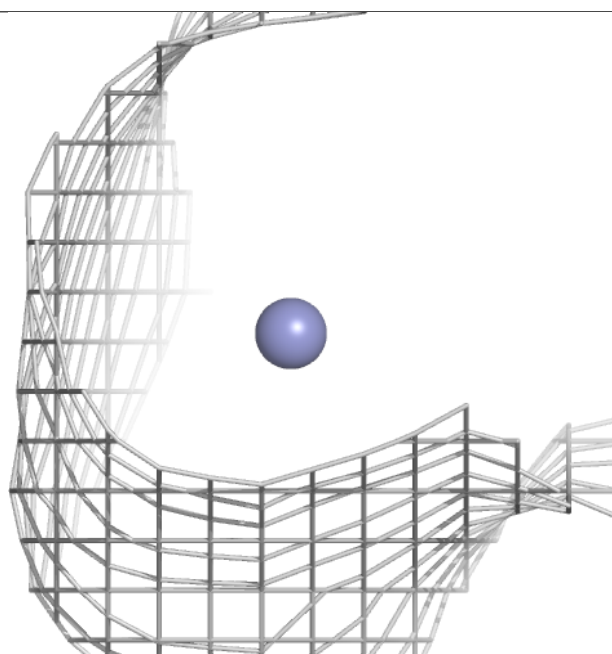
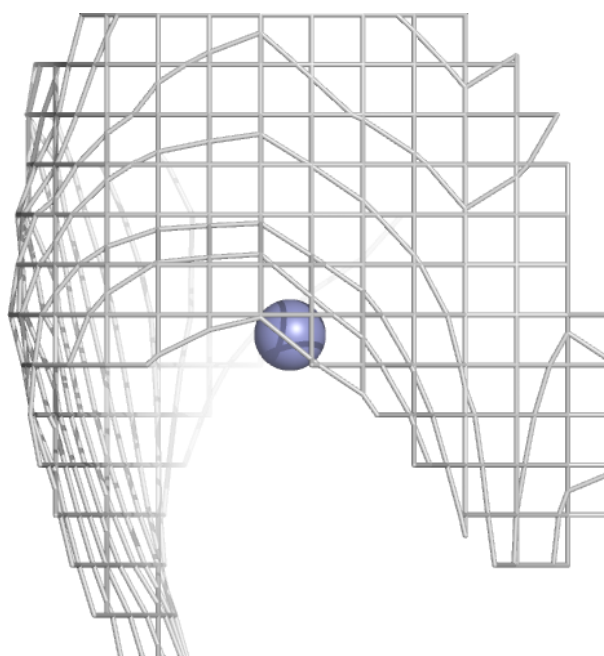
**Electron density around ZN B 1803:**

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



**Electron density around ZN B 1804:**

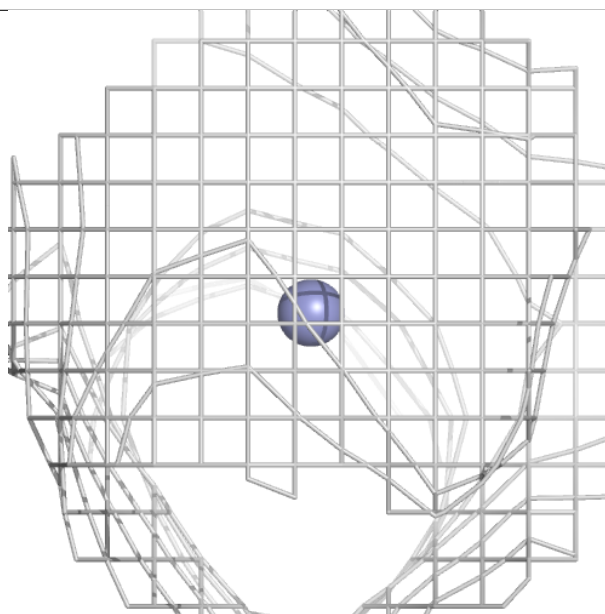
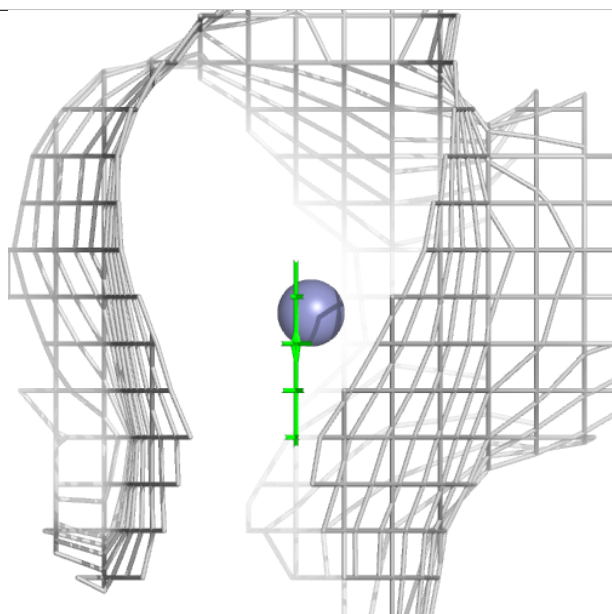
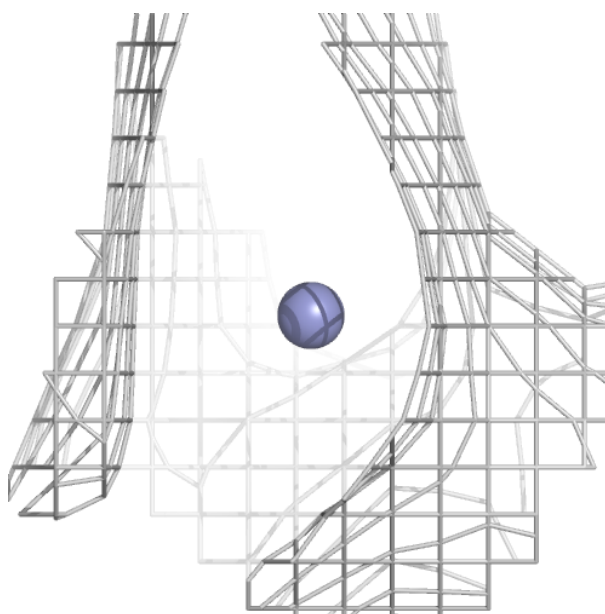
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





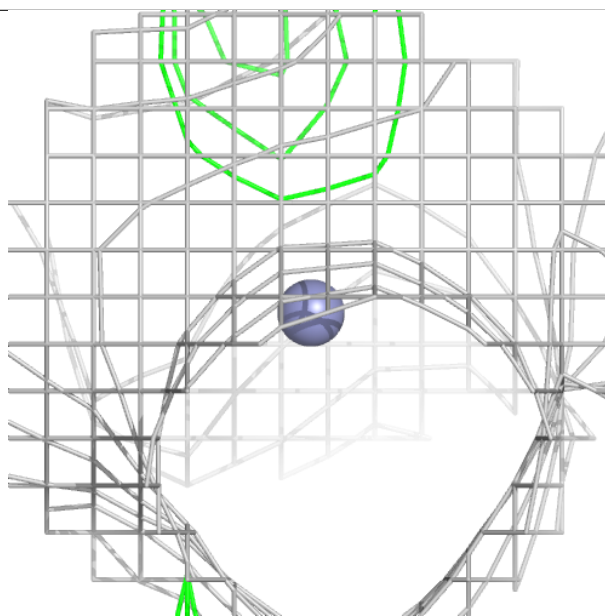
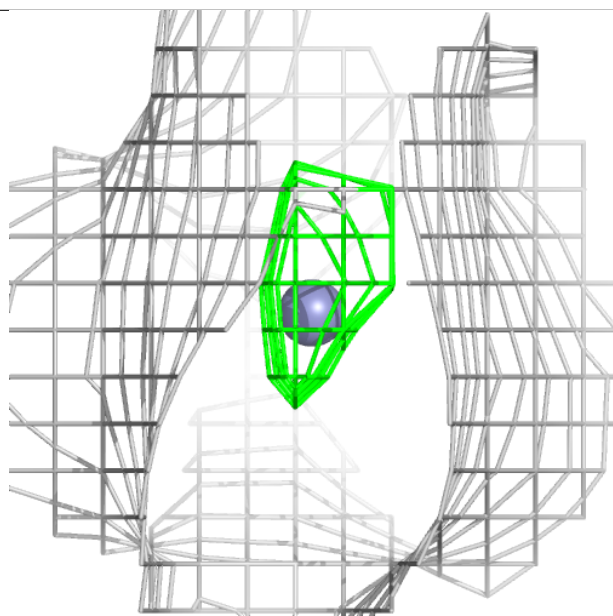
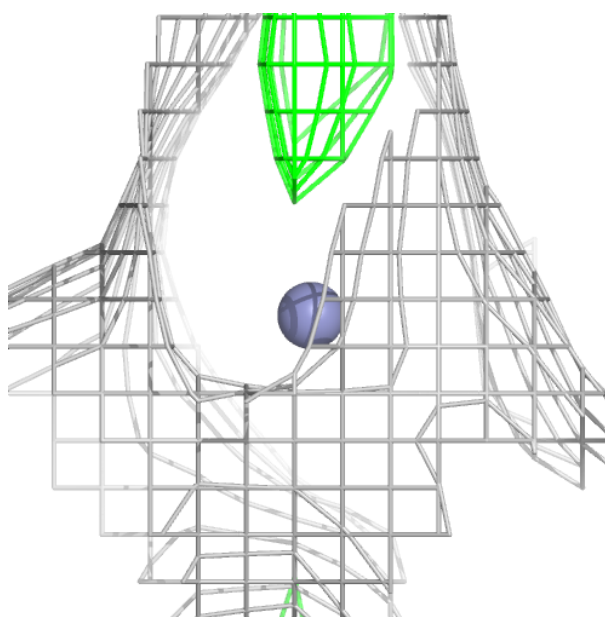
**Electron density around ZN B 1801:**

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



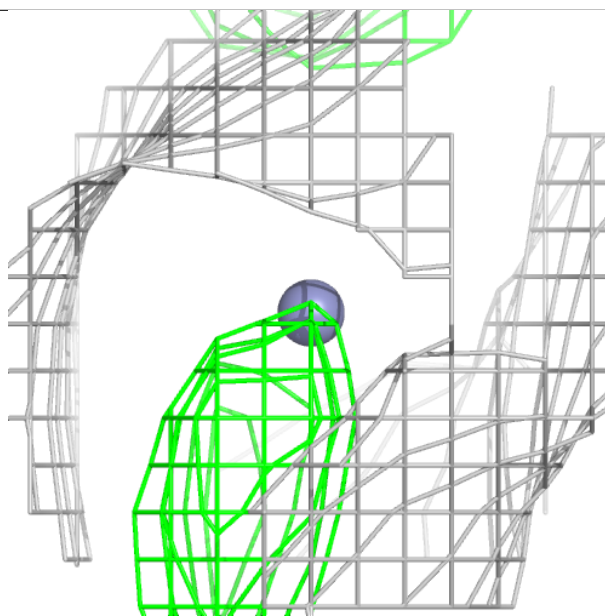
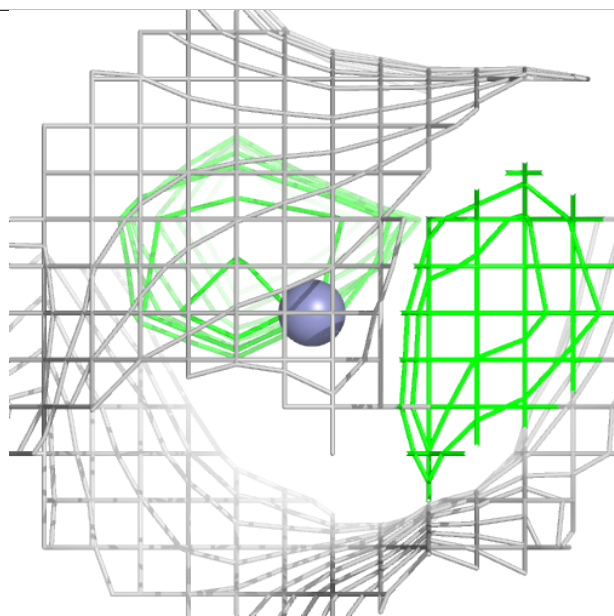
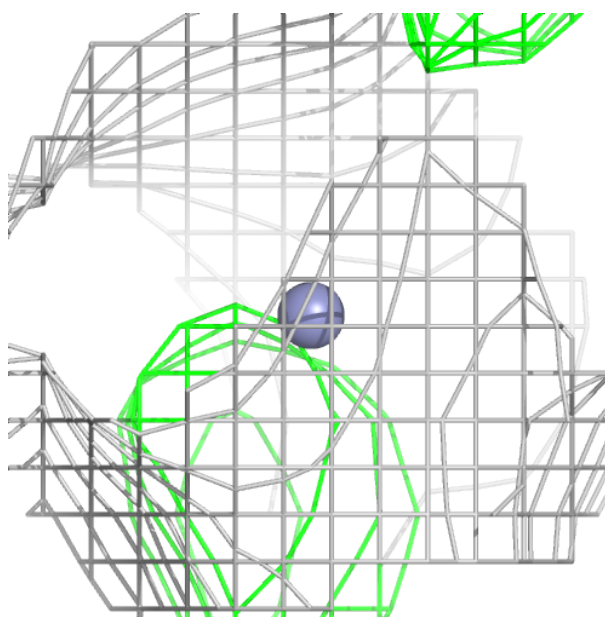
**Electron density around ZN A 1801:**

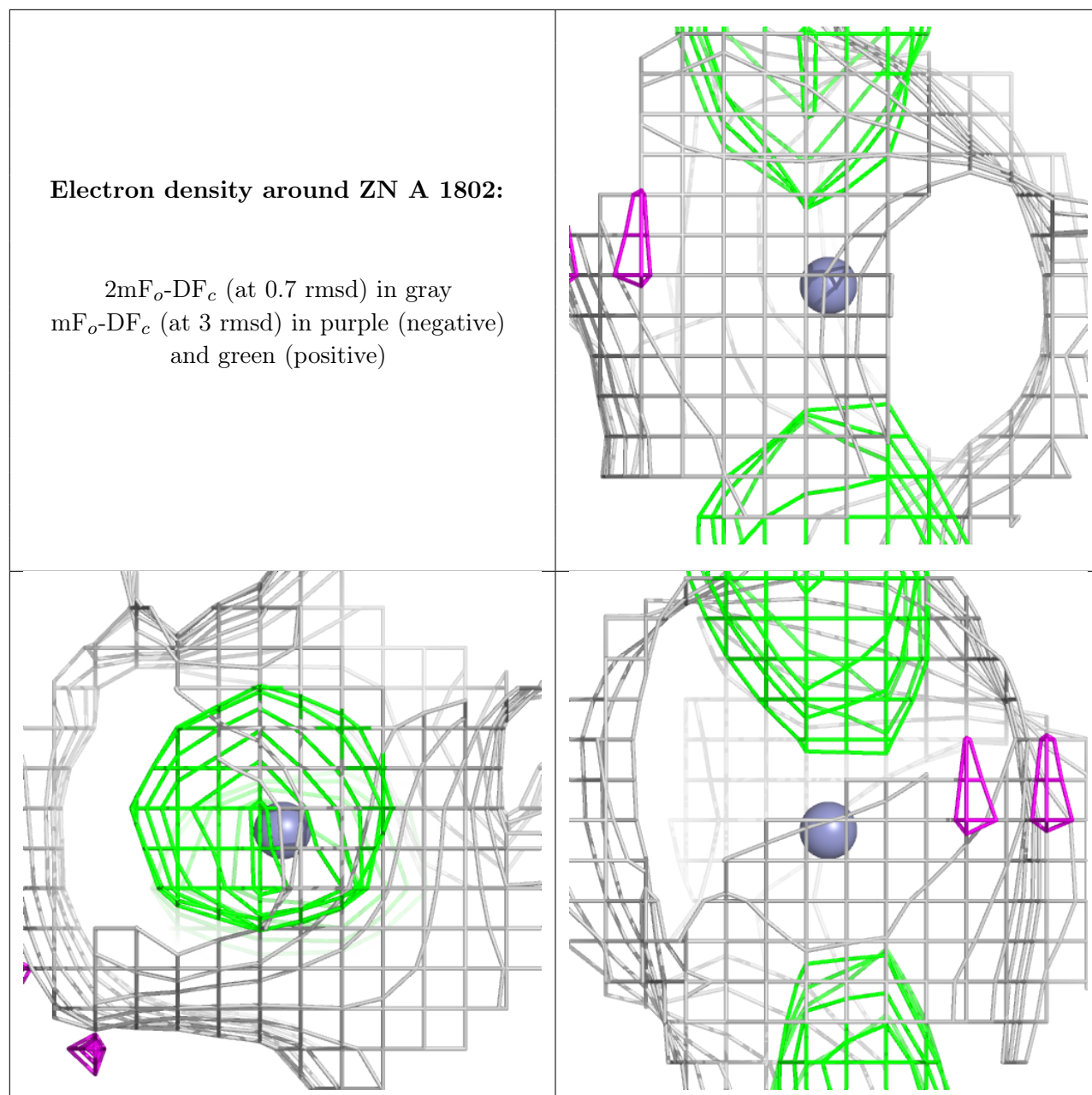
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN B 1802:**

$2mF_o-DF_c$  (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.