



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:32 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 Full wwPDB X-ray Structure Validation 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

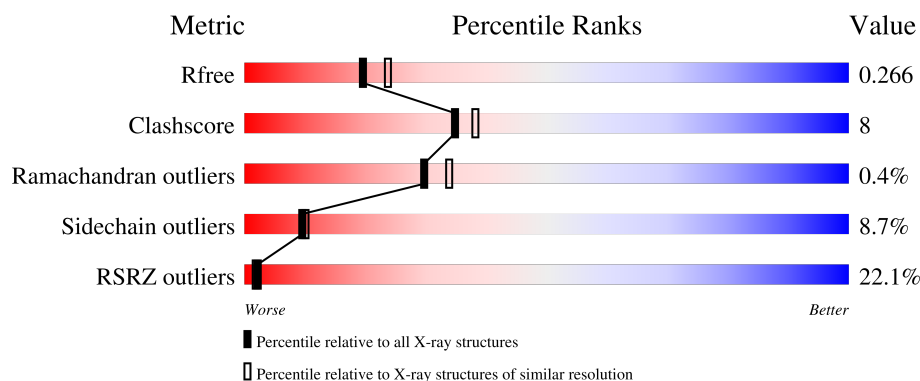
# 1 Overall quality at a glance

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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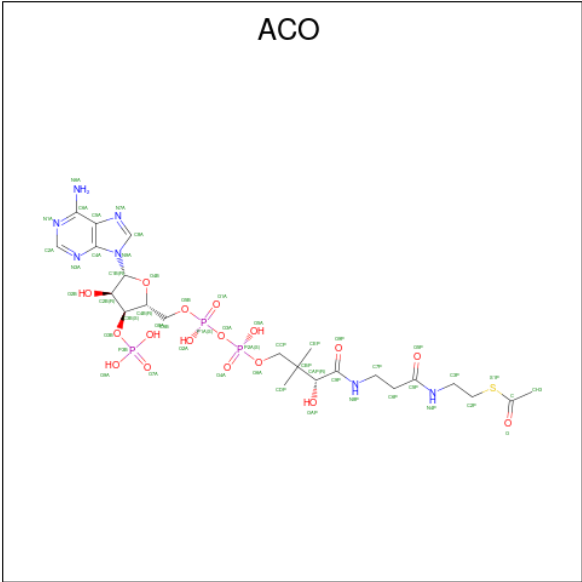
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	ASN	deletion	UNP F8VPR5
B	?	-	LYS	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP F8VPR5
B	?	-	ILE	deletion	UNP F8VPR5
B	?	-	SER	deletion	UNP 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.

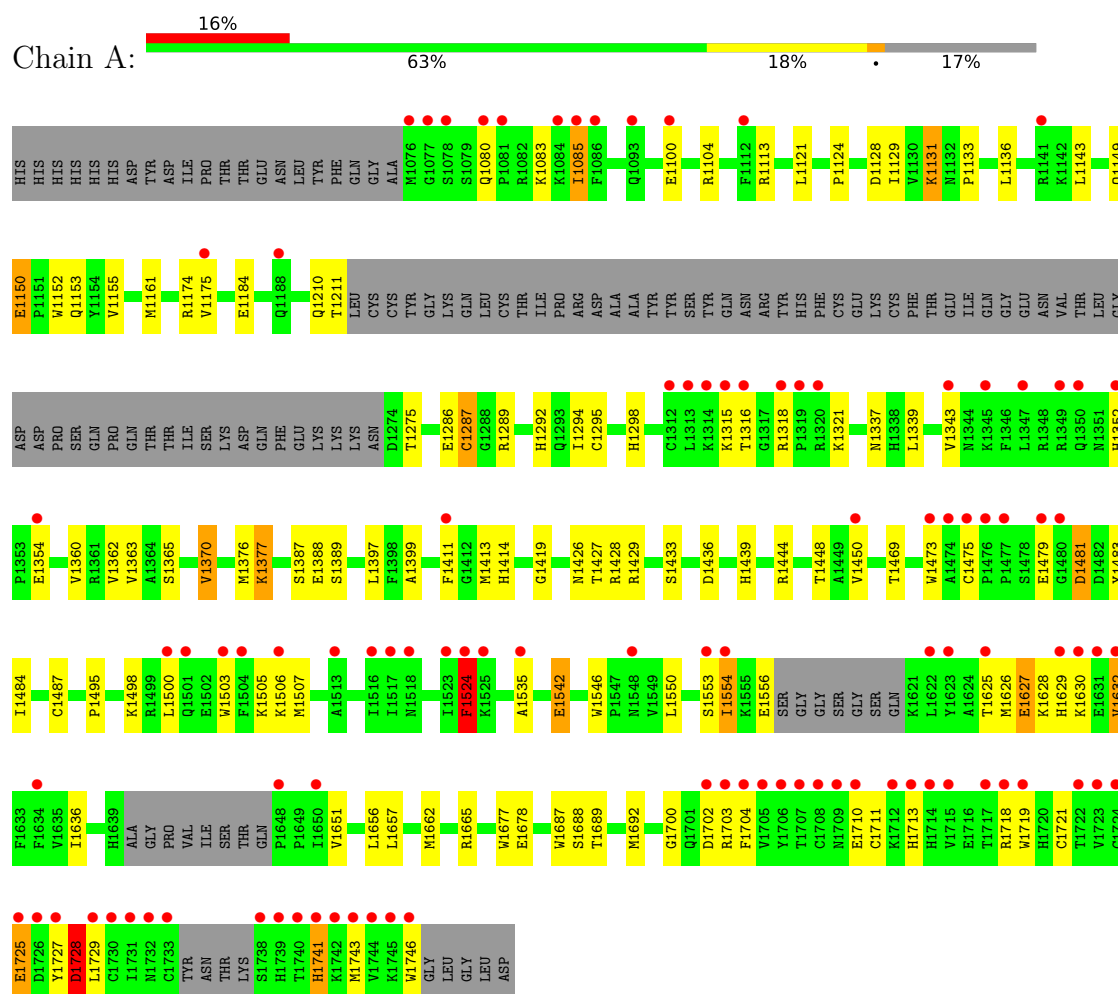
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	111	Total	O	0	0
			111	111		



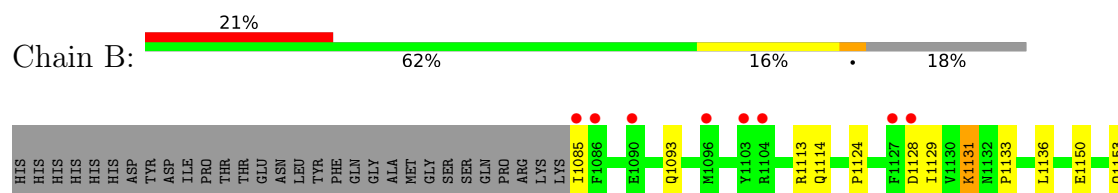
### 3 Residue-property plots [i](#)

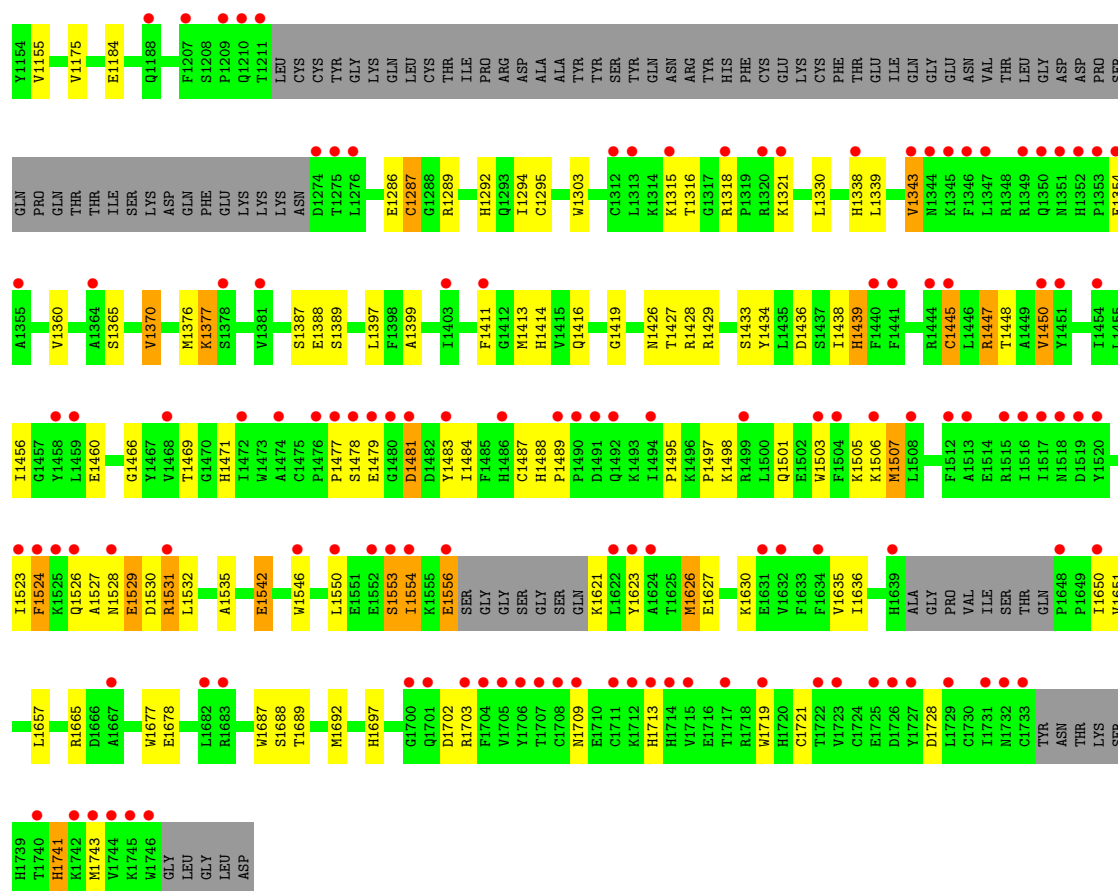
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

All (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
1	A	1665	ARG	C-N-CA	6.15	128.52	120.28
1	A	1524	PHE	CA-CB-CG	6.13	119.94	113.80
1	B	1665	ARG	CA-C-N	6.12	128.48	120.28
1	B	1665	ARG	C-N-CA	6.12	128.48	120.28
1	A	1700	GLY	CA-C-N	6.08	128.93	120.29
1	A	1700	GLY	C-N-CA	6.08	128.93	120.29
1	B	1528	ASN	CA-C-N	6.07	133.13	121.54
1	B	1528	ASN	C-N-CA	6.07	133.13	121.54
1	A	1629	HIS	CA-C-N	6.04	131.09	121.66
1	A	1629	HIS	C-N-CA	6.04	131.09	121.66
1	A	1286	GLU	CA-C-N	5.82	128.36	120.44
1	A	1286	GLU	C-N-CA	5.82	128.36	120.44
1	A	1129	ILE	N-CA-C	-5.63	106.21	111.45
1	A	1481	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	1419	GLY	N-CA-C	5.58	121.07	111.98
1	A	1419	GLY	N-CA-C	5.56	121.05	111.98
1	A	1124	PRO	CA-C-N	5.48	127.89	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1124	PRO	C-N-CA	5.48	127.89	120.38
1	A	1321	LYS	CA-C-N	5.30	128.30	120.82
1	A	1321	LYS	C-N-CA	5.30	128.30	120.82
1	B	1124	PRO	CA-C-N	5.30	127.64	120.38
1	B	1124	PRO	C-N-CA	5.30	127.64	120.38
1	A	1554	ILE	N-CA-C	-5.27	105.71	110.82
1	A	1143	LEU	CA-C-N	5.15	127.18	120.28
1	A	1143	LEU	C-N-CA	5.15	127.18	120.28
1	A	1629	HIS	CA-CB-CG	-5.15	108.65	113.80
1	B	1129	ILE	N-CA-C	-5.13	106.68	111.45
1	A	1728	ASP	CA-CB-CG	5.04	117.64	112.60

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
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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1448:THR:HG23	1:B:1503:TRP:NE1	1.94	0.77
1:B:1448:THR:CG2	1:B:1503:TRP:HE1	1.95	0.76
1:B:1447:ARG:HD2	3:B:1805:ACO:O4A	1.89	0.71
1:B:1483:TYR:HE2	3:B:1805:ACO:H22	1.57	0.70
1:B:1438:ILE:HD13	1:B:1488:HIS:CD2	2.32	0.64
1:B:1526:GLN:NE2	1:B:1530:ASP:OD2	2.31	0.64
1:A:1448:THR:HG23	1:A:1503:TRP:HE1	1.62	0.64
1:A:1473:TRP:CD1	1:A:1632:VAL:HG23	2.32	0.63
1:A:1524:PHE:HB3	1:A:1627:GLU:OE2	1.99	0.62
1:A:1427:THR:HG22	1:A:1428:ARG:HG3	1.82	0.62
1:B:1427:THR:HG22	1:B:1428:ARG:HG3	1.82	0.62
1:A:1625:THR:HA	1:A:1628:LYS:HD2	1.81	0.61
1:B:1447:ARG:NH1	3:B:1805:ACO:O4A	2.33	0.61
1:A:1718:ARG:HH11	1:A:1728:ASP:HB3	1.67	0.59
1:B:1287:CYS:HB3	1:B:1289:ARG:HG2	1.85	0.59
1:A:1365:SER:HB3	1:A:1657:LEU:H	1.69	0.58
1:B:1365:SER:HB3	1:B:1657:LEU:H	1.68	0.58
1:A:1414:HIS:HD2	4:A:1925:HOH:O	1.86	0.58
1:A:1436:ASP:HB3	1:A:1484:ILE:HB	1.86	0.58
1:A:1448:THR:HG23	1:A:1503:TRP:NE1	2.18	0.57
1:B:1523:ILE:HG13	1:B:1524:PHE:CZ	2.39	0.57
1:A:1710:GLU:HG2	1:A:1729:LEU:HD22	1.87	0.57
1:B:1526:GLN:HG2	1:B:1635:VAL:HG11	1.87	0.56
1:A:1377:LYS:HE2	1:A:1388:GLU:HG2	1.86	0.56
1:A:1718:ARG:NH1	1:A:1728:ASP:HB3	2.20	0.56
1:A:1429:ARG:HG2	1:A:1469:THR:HB	1.88	0.56
1:B:1546:TRP:HH2	1:B:1626:MET:HA	1.71	0.56
1:A:1625:THR:HA	1:A:1628:LYS:CD	2.36	0.55
1:B:1377:LYS:HE2	1:B:1388:GLU:HG2	1.89	0.55
1:B:1709:ASN:ND2	1:B:1728:ASP:H	2.04	0.55
1:B:1477:PRO:HA	1:B:1483:TYR:CZ	2.41	0.54
1:B:1436:ASP:HB3	1:B:1484:ILE:HB	1.87	0.54
1:B:1623:TYR:O	1:B:1626:MET:HB2	2.06	0.54
1:B:1487:CYS:HB3	1:B:1678:GLU:HB3	1.90	0.54
1:B:1523:ILE:HG22	1:B:1635:VAL:CG2	2.25	0.54
1:B:1429:ARG:HG2	1:B:1469:THR:HB	1.90	0.54
1:B:1439:HIS:CE1	1:B:1489:PRO:HG2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1524:PHE:CE1	1:B:1626:MET:HB3	2.43	0.54
1:A:1352:HIS:CE1	1:B:1445[A]:CYS:HG	2.25	0.53
1:A:1080:GLN:CG	1:A:1083:LYS:HB2	2.39	0.53
1:A:1689:THR:HA	1:A:1692:MET:HE2	1.90	0.53
1:B:1399:ALA:HB3	1:B:1411:PHE:HB3	1.91	0.53
1:B:1376:MET:HE1	1:B:1535:ALA:HB1	1.91	0.52
1:B:1689:THR:HA	1:B:1692:MET:HE2	1.90	0.52
1:B:1527:ALA:HB1	1:B:1532:LEU:HD22	1.91	0.52
1:B:1113:ARG:HA	1:B:1136:LEU:HB2	1.90	0.52
1:A:1399:ALA:HB3	1:A:1411:PHE:HB3	1.92	0.52
1:A:1287:CYS:SG	1:A:1289:ARG:NH1	2.78	0.52
1:A:1376:MET:HE1	1:A:1535:ALA:HB1	1.92	0.52
1:A:1473:TRP:HD1	1:A:1632:VAL:HG23	1.75	0.52
1:A:1397:LEU:HD11	1:A:1413:MET:HE2	1.93	0.51
1:A:1656:LEU:O	1:A:1703:ARG:NH1	2.44	0.51
1:A:1113:ARG:HA	1:A:1136:LEU:HB2	1.93	0.51
1:B:1397:LEU:HD11	1:B:1413:MET:HE2	1.93	0.51
1:B:1469:THR:CG2	1:B:1471:HIS:NE2	2.74	0.50
1:A:1487:CYS:HB3	1:A:1678:GLU:HB3	1.93	0.50
1:B:1524:PHE:CE1	1:B:1626:MET:SD	3.04	0.50
1:A:1711:CYS:HB3	1:A:1713:HIS:CD2	2.46	0.50
1:A:1718:ARG:NH2	1:A:1746:TRP:CE3	2.80	0.49
1:A:1292:HIS:HB2	1:A:1295:CYS:HB2	1.95	0.49
1:B:1469:THR:HG22	1:B:1471:HIS:NE2	2.27	0.49
1:B:1376:MET:HE2	1:B:1550:LEU:HD13	1.94	0.48
1:B:1703:ARG:HA	1:B:1703:ARG:HE	1.77	0.48
1:B:1524:PHE:HE1	1:B:1626:MET:SD	2.37	0.48
1:B:1524:PHE:HD2	1:B:1630:LYS:HB3	1.79	0.48
1:B:1438:ILE:CD1	1:B:1488:HIS:CD2	2.97	0.48
1:A:1376:MET:HE2	1:A:1550:LEU:HD13	1.94	0.48
1:A:1475:CYS:O	1:A:1483:TYR:OH	2.29	0.48
1:A:1500:LEU:HD21	3:A:1805:ACO:H32	1.97	0.47
1:A:1080:GLN:HG3	1:A:1083:LYS:HB2	1.96	0.47
1:A:1316:THR:HG22	1:A:1318:ARG:H	1.80	0.47
1:A:1546:TRP:HH2	1:A:1626:MET:HA	1.80	0.47
1:A:1524:PHE:CZ	1:A:1630:LYS:HA	2.50	0.46
1:B:1292:HIS:HB2	1:B:1295:CYS:HB2	1.97	0.46
1:A:1352:HIS:NE2	1:B:1445[B]:CYS:SG	2.88	0.46
1:A:1370:VAL:HB	1:A:1542:GLU:HG2	1.98	0.46
1:B:1370:VAL:HB	1:B:1542:GLU:HG2	1.98	0.46
1:B:1414:HIS:HB2	1:B:1434:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1316:THR:HG22	1:B:1318:ARG:H	1.80	0.46
1:B:1721:CYS:SG	1:B:1741:HIS:ND1	2.89	0.45
1:A:1711:CYS:HB3	1:A:1713:HIS:HD2	1.81	0.45
1:B:1343:VAL:HG22	1:B:1450:VAL:HG22	1.98	0.45
1:B:1719:TRP:HB3	1:B:1743:MET:HB3	1.98	0.45
1:B:1294:ILE:HG23	1:B:1687:TRP:HB2	2.00	0.44
1:B:1478:SER:O	1:B:1481:ASP:HB2	2.18	0.44
1:A:1436:ASP:CB	1:A:1484:ILE:HB	2.48	0.44
3:B:1805:ACO:O1A	3:B:1805:ACO:H8A	2.18	0.44
1:A:1294:ILE:HG23	1:A:1687:TRP:HB2	2.00	0.43
1:A:1426:ASN:HA	1:A:1429:ARG:HD2	2.00	0.43
1:A:1448:THR:OG1	3:A:1805:ACO:O5A	2.26	0.43
1:A:1721:CYS:SG	1:A:1741:HIS:ND1	2.92	0.43
1:B:1330:LEU:HD23	1:B:1697:HIS:CE1	2.53	0.43
1:B:1447:ARG:HG3	1:B:1448:THR:H	1.83	0.43
1:A:1298:HIS:HD2	4:A:1961:HOH:O	2.02	0.43
1:A:1352:HIS:CE1	1:B:1445[B]:CYS:SG	3.11	0.43
1:A:1719:TRP:HB3	1:A:1743:MET:HB3	1.99	0.43
1:B:1456:ILE:CG1	1:B:1507:MET:HE3	2.49	0.43
1:B:1483:TYR:CE2	3:B:1805:ACO:H22	2.45	0.43
1:B:1426:ASN:HA	1:B:1429:ARG:HD2	2.01	0.43
1:B:1131:LYS:O	1:B:1133:PRO:HD3	2.19	0.42
1:A:1721:CYS:HB3	1:A:1727:TYR:HB3	2.00	0.42
1:B:1416:GLN:HE21	1:B:1433:SER:HB3	1.83	0.42
1:B:1456:ILE:HG13	1:B:1507:MET:HE3	2.01	0.42
1:A:1630:LYS:HB2	1:A:1630:LYS:HE2	1.90	0.42
1:B:1466:GLY:HA3	1:B:1650:ILE:HG22	2.02	0.42
1:A:1352:HIS:CE1	1:B:1445[A]:CYS:SG	3.11	0.42
1:A:1524:PHE:CB	1:A:1627:GLU:OE2	2.67	0.42
1:A:1718:ARG:NH2	1:A:1746:TRP:HE3	2.16	0.42
1:A:1131:LYS:O	1:A:1133:PRO:HD3	2.20	0.41
1:B:1703:ARG:HA	1:B:1703:ARG:NE	2.35	0.41
1:A:1339:LEU:HD12	1:A:1360:VAL:HG11	2.02	0.41
1:B:1527:ALA:C	1:B:1529:GLU:H	2.28	0.41
1:A:1337:ASN:ND2	1:A:1725:GLU:HG3	2.35	0.41
1:A:1085:ILE:HD12	1:A:1085:ILE:HA	1.95	0.41
1:A:1677:TRP:HB3	1:A:1688:SER:HB3	2.03	0.41
1:A:1161:MET:HE2	1:A:1161:MET:HB3	1.97	0.41
1:A:1150:GLU:CD	1:A:1152:TRP:HB2	2.46	0.41
1:A:1362:VAL:HG22	1:A:1397:LEU:HB3	2.03	0.41
1:B:1338:HIS:HE1	1:B:1460:GLU:OE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:GLU:O	1:A:1104:ARG:HG3	2.22	0.40
1:B:1677:TRP:HB3	1:B:1688:SER:HB3	2.03	0.40
1:A:1352:HIS:CE1	1:B:1445[B]:CYS:HG	2.38	0.40
1:A:1363:VAL:CG2	1:A:1662:MET:HG3	2.51	0.40
1:B:1303:TRP:CD1	1:B:1321:LYS:HG2	2.56	0.40
1:B:1339:LEU:HD12	1:B:1360:VAL:HG11	2.02	0.40
1:B:1497:PRO:O	1:B:1501:GLN:HG3	2.22	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	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

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1085	ILE
1	A	1121	LEU
1	A	1128	ASP
1	A	1131	LYS
1	A	1149	GLN
1	A	1150	GLU
1	A	1153	GLN
1	A	1155	VAL
1	A	1174	ARG
1	A	1175	VAL
1	A	1184	GLU
1	A	1210	GLN
1	A	1211	THR
1	A	1275	THR
1	A	1287	CYS
1	A	1315	LYS
1	A	1343	VAL
1	A	1354	GLU
1	A	1370	VAL
1	A	1377	LYS
1	A	1387	SER
1	A	1389	SER
1	A	1433	SER
1	A	1439	HIS
1	A	1444	ARG
1	A	1450	VAL
1	A	1481	ASP
1	A	1498	LYS
1	A	1505	LYS
1	A	1506	LYS
1	A	1507	MET
1	A	1524	PHE
1	A	1542	GLU

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Mol	Chain	Res	Type
1	A	1553	SER
1	A	1554	ILE
1	A	1556	GLU
1	A	1627	GLU
1	A	1632	VAL
1	A	1636	ILE
1	A	1651	VAL
1	A	1702	ASP
1	A	1704	PHE
1	A	1725	GLU
1	A	1728	ASP
1	A	1741	HIS
1	B	1085	ILE
1	B	1093	GLN
1	B	1114	GLN
1	B	1128	ASP
1	B	1131	LYS
1	B	1150	GLU
1	B	1153	GLN
1	B	1155	VAL
1	B	1175	VAL
1	B	1184	GLU
1	B	1287	CYS
1	B	1315	LYS
1	B	1343	VAL
1	B	1354	GLU
1	B	1370	VAL
1	B	1377	LYS
1	B	1387	SER
1	B	1389	SER
1	B	1445[A]	CYS
1	B	1445[B]	CYS
1	B	1447	ARG
1	B	1450	VAL
1	B	1479	GLU
1	B	1481	ASP
1	B	1498	LYS
1	B	1505	LYS
1	B	1506	LYS
1	B	1507	MET
1	B	1529	GLU
1	B	1531	ARG

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Mol	Chain	Res	Type
1	B	1542	GLU
1	B	1553	SER
1	B	1554	ILE
1	B	1556	GLU
1	B	1621	LYS
1	B	1627	GLU
1	B	1636	ILE
1	B	1651	VAL
1	B	1702	ASP
1	B	1713	HIS
1	B	1741	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1163	ASN
1	A	1293	GLN
1	A	1298	HIS
1	A	1337	ASN
1	A	1338	HIS
1	A	1350	GLN
1	A	1414	HIS
1	A	1629	HIS
1	A	1637	HIS
1	A	1639	HIS
1	A	1713	HIS
1	B	1114	GLN
1	B	1119	GLN
1	B	1331	GLN
1	B	1338	HIS
1	B	1350	GLN
1	B	1709	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

All (20) torsion outliers are listed below:

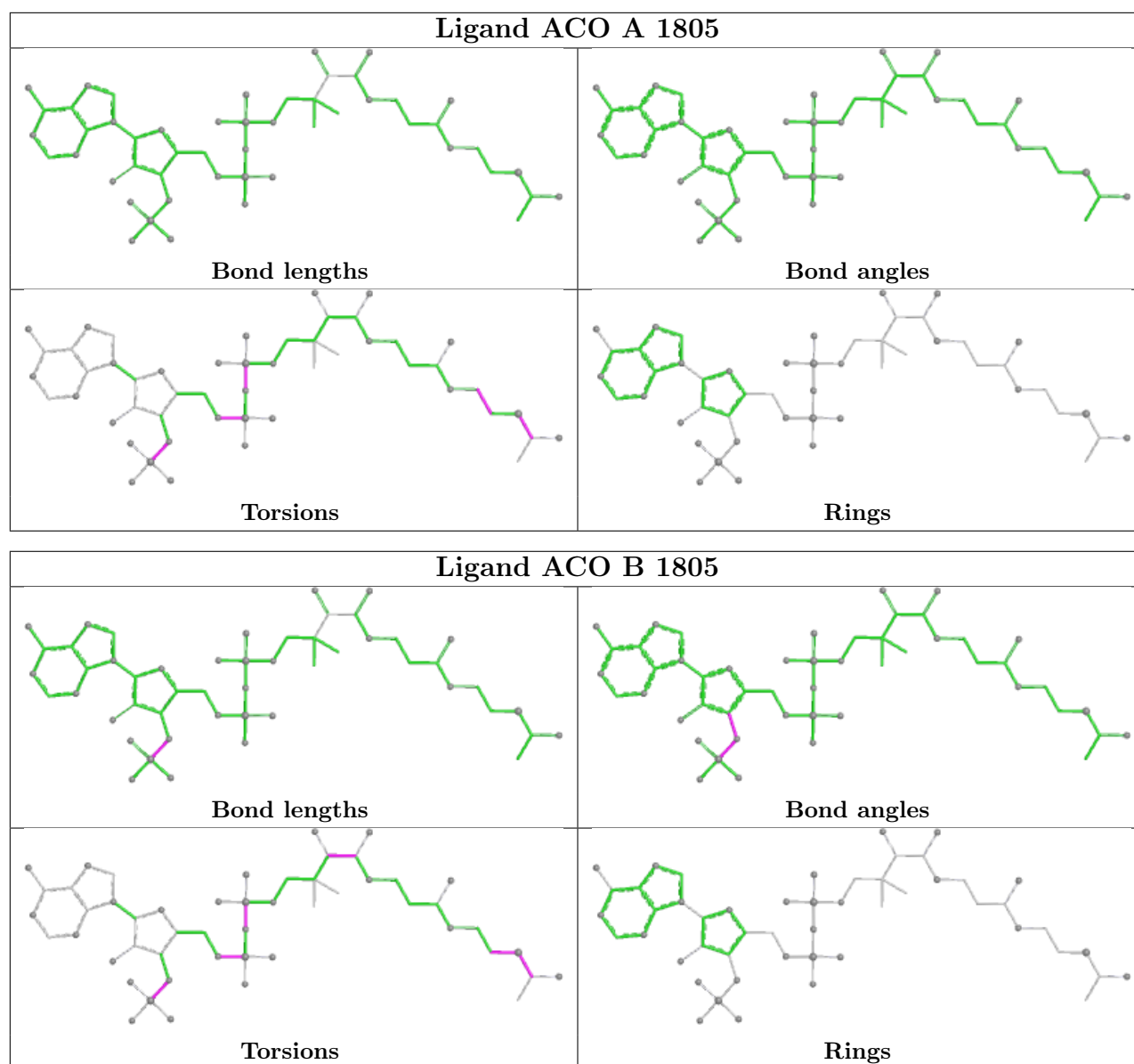
Mol	Chain	Res	Type	Atoms
3	A	1805	ACO	C5B-O5B-P1A-O1A
3	A	1805	ACO	C5B-O5B-P1A-O2A
3	A	1805	ACO	C5B-O5B-P1A-O3A
3	A	1805	ACO	S1P-C2P-C3P-N4P
3	B	1805	ACO	C5B-O5B-P1A-O1A
3	B	1805	ACO	C5B-O5B-P1A-O2A
3	B	1805	ACO	C5B-O5B-P1A-O3A
3	B	1805	ACO	N8P-C9P-CAP-OAP
3	B	1805	ACO	C3P-C2P-S1P-C
3	B	1805	ACO	O-C-S1P-C2P
3	B	1805	ACO	CH3-C-S1P-C2P
3	B	1805	ACO	O9P-C9P-CAP-OAP
3	A	1805	ACO	C3B-O3B-P3B-O7A
3	B	1805	ACO	C3B-O3B-P3B-O7A
3	B	1805	ACO	P1A-O3A-P2A-O5A
3	A	1805	ACO	C3B-O3B-P3B-O8A
3	A	1805	ACO	O-C-S1P-C2P
3	A	1805	ACO	P1A-O3A-P2A-O4A
3	A	1805	ACO	P1A-O3A-P2A-O5A
3	B	1805	ACO	P1A-O3A-P2A-O4A

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

### 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, 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%)

All (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
1	B	1520	TYR	5.5
1	B	1474	ALA	5.4
1	A	1704	PHE	5.4
1	B	1445[A]	CYS	5.0
1	B	1523	ILE	4.9
1	A	1632	VAL	4.9
1	A	1729	LEU	4.8
1	B	1525	LYS	4.7
1	B	1275	THR	4.6
1	B	1554	ILE	4.6
1	A	1723	VAL	4.4
1	B	1744	VAL	4.4
1	B	1476	PRO	4.4
1	B	1714	HIS	4.4
1	B	1712	LYS	4.4
1	B	1746	TRP	4.4
1	A	1479	GLU	4.3
1	A	1746	TRP	4.3
1	B	1622	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	1524	PHE	4.3
1	B	1704	PHE	4.2
1	A	1703	ARG	4.2
1	A	1648	PRO	4.2
1	B	1729	LEU	4.2
1	B	1745	LYS	4.2
1	B	1477	PRO	4.1
1	B	1468	VAL	4.1
1	A	1354	GLU	4.0
1	A	1631	GLU	3.9
1	B	1648	PRO	3.9
1	B	1733	CYS	3.8
1	B	1700	GLY	3.8
1	A	1738	SER	3.7
1	B	1347	LEU	3.7
1	A	1744	VAL	3.7
1	B	1318	ARG	3.7
1	A	1722	THR	3.7
1	B	1411	PHE	3.7
1	A	1474	ALA	3.7
1	B	1450	VAL	3.6
1	A	1718	ARG	3.6
1	A	1707	THR	3.6
1	B	1274	ASP	3.6
1	A	1740	THR	3.6
1	A	1714	HIS	3.6
1	B	1353	PRO	3.6
1	A	1727	TYR	3.6
1	A	1706	TYR	3.5
1	A	1742	LYS	3.5
1	B	1723	VAL	3.5
1	A	1312	CYS	3.5
1	A	1725	GLU	3.5
1	B	1211	THR	3.4
1	A	1730	CYS	3.4
1	A	1726	ASP	3.4
1	B	1742	LYS	3.4
1	B	1086	PHE	3.4
1	B	1632	VAL	3.4
1	B	1491	ASP	3.4
1	A	1629	HIS	3.3
1	A	1112	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1546	TRP	3.3
1	B	1483	TYR	3.3
1	B	1472	ILE	3.2
1	B	1444	ARG	3.2
1	B	1528	ASN	3.2
1	B	1550	LEU	3.2
1	B	1727	TYR	3.2
1	A	1313	LEU	3.2
1	A	1717	THR	3.2
1	B	1515	ARG	3.2
1	B	1480	GLY	3.2
1	A	1076	MET	3.1
1	B	1479	GLU	3.1
1	B	1631	GLU	3.1
1	B	1732	ASN	3.1
1	B	1343	VAL	3.1
1	B	1517	ILE	3.1
1	A	1719	TRP	3.1
1	A	1081	PRO	3.1
1	A	1712	LYS	3.1
1	A	1745	LYS	3.0
1	A	1517	ILE	3.0
1	A	1554	ILE	3.0
1	B	1312	CYS	3.0
1	A	1743	MET	3.0
1	B	1381	VAL	3.0
1	B	1531	ARG	3.0
1	A	1630	LYS	2.9
1	A	1501	GLN	2.9
1	A	1622	LEU	2.9
1	B	1707	THR	2.9
1	A	1078	SER	2.9
1	A	1506	LYS	2.9
1	B	1209	PRO	2.9
1	A	1318	ARG	2.9
1	B	1210	GLN	2.9
1	B	1518	ASN	2.9
1	B	1313	LEU	2.8
1	B	1440	PHE	2.8
1	B	1715	VAL	2.8
1	B	1740	THR	2.8
1	B	1345	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1732	ASN	2.8
1	B	1743	MET	2.8
1	A	1713	HIS	2.8
1	A	1315	LYS	2.8
1	A	1625	THR	2.8
1	A	1724	CYS	2.8
1	B	1458	TYR	2.8
1	A	1705	VAL	2.8
1	A	1516	ILE	2.7
1	B	1516	ILE	2.7
1	A	1708	CYS	2.7
1	B	1486	HIS	2.7
1	A	1343	VAL	2.7
1	A	1518	ASN	2.7
1	A	1480	GLY	2.7
1	B	1320	ARG	2.7
1	B	1276	LEU	2.7
1	B	1624	ALA	2.7
1	B	1494	ILE	2.7
1	B	1096	MET	2.7
1	A	1741	HIS	2.6
1	A	1086	PHE	2.6
1	B	1441	PHE	2.6
1	A	1085	ILE	2.6
1	A	1477	PRO	2.6
1	B	1708	CYS	2.6
1	A	1710	GLU	2.6
1	B	1351	ASN	2.6
1	B	1709	ASN	2.6
1	A	1077	GLY	2.6
1	B	1127	PHE	2.6
1	B	1623	TYR	2.6
1	A	1349	ARG	2.5
1	A	1080	GLN	2.5
1	A	1504	PHE	2.5
1	B	1650	ILE	2.5
1	B	1556	GLU	2.4
1	B	1346	PHE	2.4
1	A	1503	TRP	2.4
1	B	1503	TRP	2.4
1	A	1084	LYS	2.4
1	A	1320	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1473	TRP	2.4
1	A	1623	TYR	2.4
1	B	1639	HIS	2.4
1	A	1702	ASP	2.4
1	B	1364	ALA	2.4
1	B	1490	PRO	2.4
1	B	1513	ALA	2.4
1	A	1316	THR	2.4
1	B	1722	THR	2.4
1	B	1634	PHE	2.4
1	B	1703	ARG	2.4
1	A	1524	PHE	2.4
1	B	1354	GLU	2.4
1	B	1481	ASP	2.3
1	B	1506	LYS	2.3
1	B	1705	VAL	2.3
1	A	1141	ARG	2.3
1	A	1475	CYS	2.3
1	B	1713	HIS	2.3
1	B	1701	GLN	2.3
1	A	1709	ASN	2.3
1	A	1100	GLU	2.3
1	A	1450	VAL	2.3
1	B	1188	GLN	2.3
1	A	1347	LEU	2.3
1	B	1478	SER	2.3
1	A	1352	HIS	2.3
1	B	1352	HIS	2.3
1	B	1350	GLN	2.3
1	B	1492	GLN	2.3
1	A	1634	PHE	2.3
1	B	1344	ASN	2.3
1	B	1726	ASP	2.3
1	A	1319	PRO	2.3
1	A	1739	HIS	2.3
1	B	1090	GLU	2.3
1	B	1504	PHE	2.2
1	B	1349	ARG	2.2
1	B	1683	ARG	2.2
1	B	1706	TYR	2.2
1	A	1350	GLN	2.2
1	A	1650	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1175	VAL	2.2
1	B	1207	PHE	2.2
1	A	1476	PRO	2.2
1	A	1525	LYS	2.2
1	B	1103	TYR	2.2
1	B	1378	SER	2.2
1	B	1403	ILE	2.2
1	B	1338	HIS	2.2
1	B	1711	CYS	2.2
1	B	1355	ALA	2.2
1	B	1454	ILE	2.1
1	B	1508	LEU	2.1
1	A	1535	ALA	2.1
1	A	1553	SER	2.1
1	A	1523	ILE	2.1
1	B	1321	LYS	2.1
1	A	1548	ASN	2.1
1	B	1552	GLU	2.1
1	B	1719	TRP	2.1
1	A	1188	GLN	2.1
1	A	1411	PHE	2.1
1	B	1512	PHE	2.1
1	B	1104	ARG	2.1
1	B	1499	ARG	2.1
1	A	1513	ALA	2.1
1	B	1667	ALA	2.1
1	B	1451	TYR	2.1
1	B	1315	LYS	2.1
1	A	1093	GLN	2.1
1	B	1553	SER	2.0
1	B	1526	GLN	2.0
1	B	1128	ASP	2.0
1	B	1459	LEU	2.0
1	A	1345	LYS	2.0
1	B	1717	THR	2.0
1	B	1725	GLU	2.0
1	A	1500	LEU	2.0
1	B	1519	ASP	2.0
1	B	1682	LEU	2.0
1	B	1489	PRO	2.0
1	A	1314	LYS	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](#)

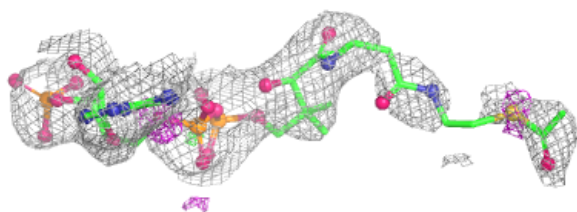
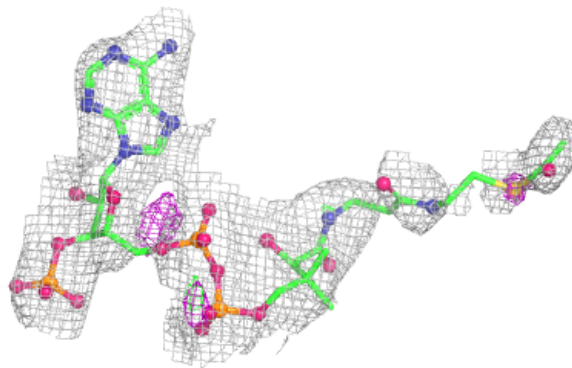
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

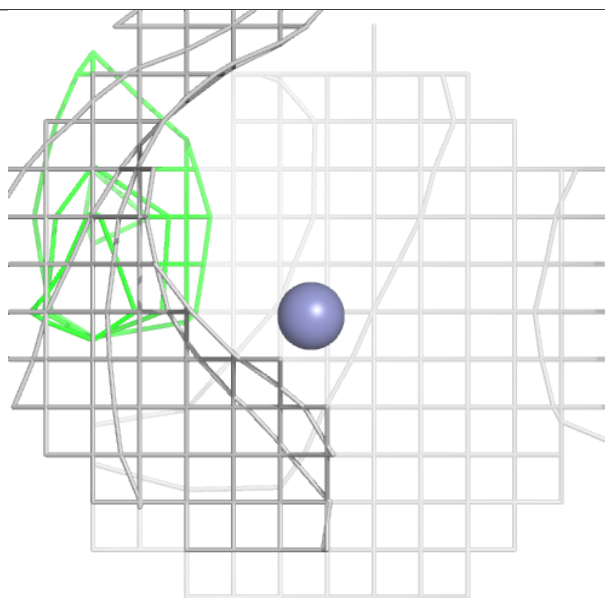
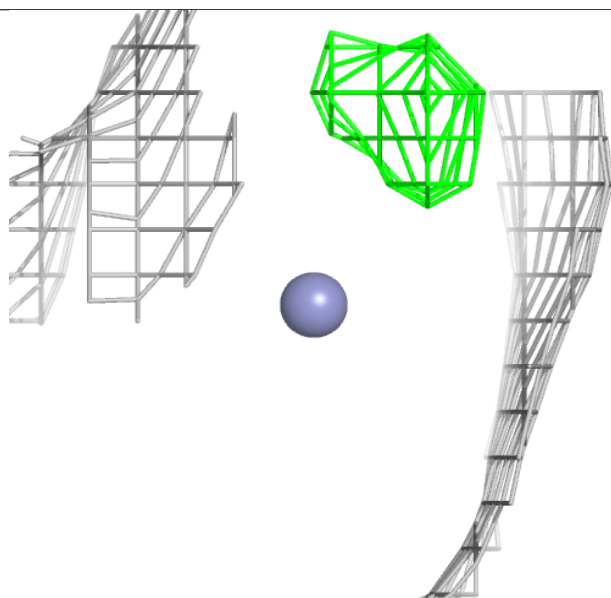
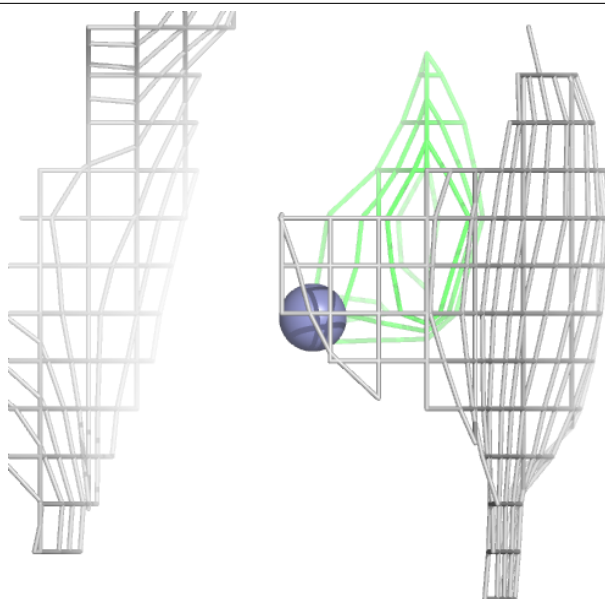
**Electron density around ACO B 1805:**

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



**Electron density around ZN A 1804:**

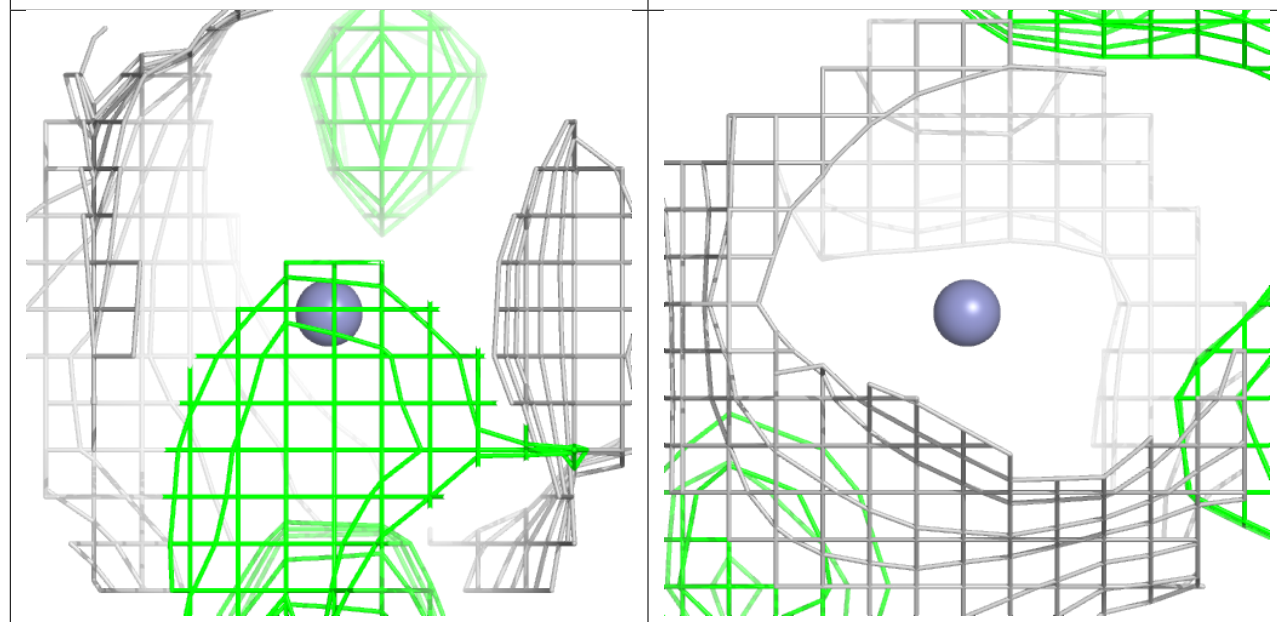
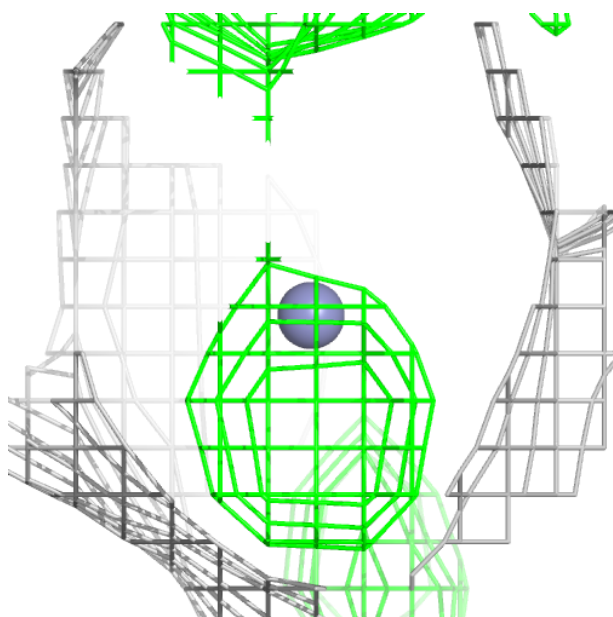
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





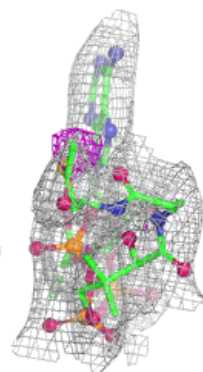
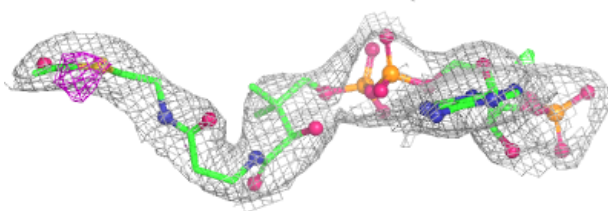
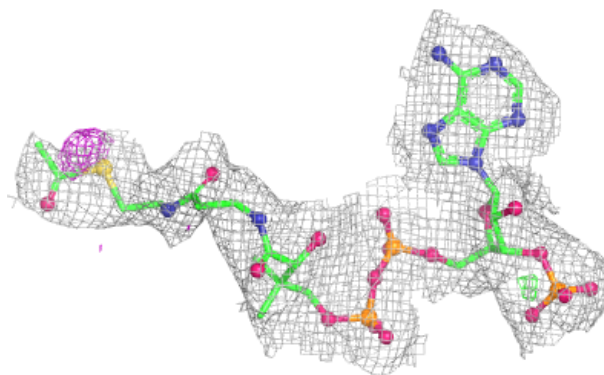
**Electron density around ZN A 1803:**

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



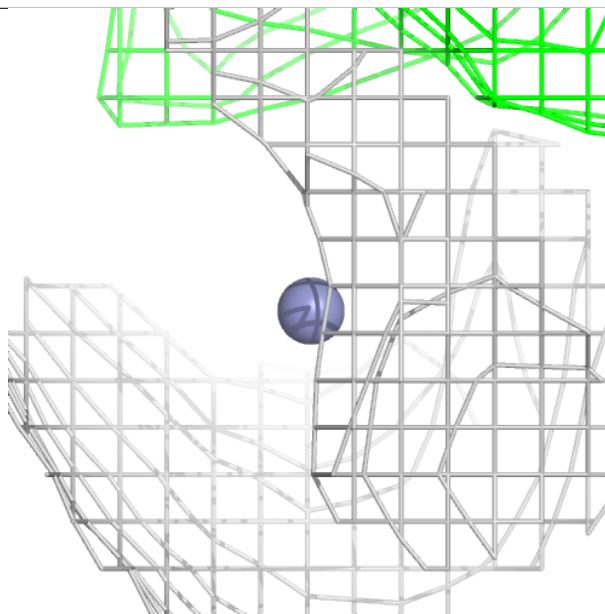
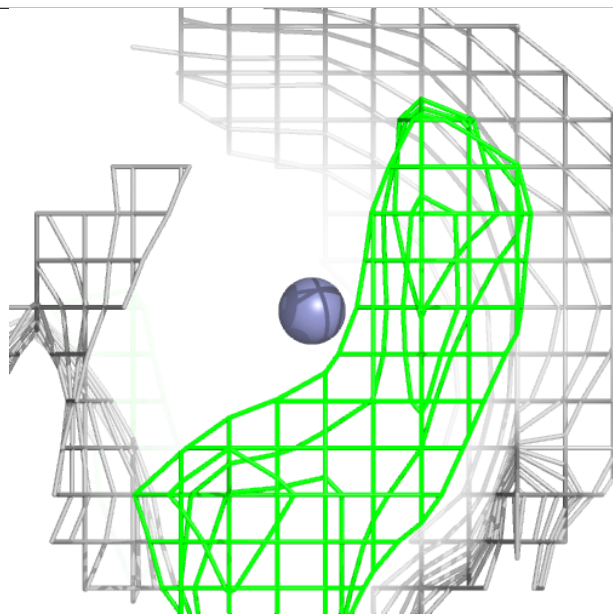
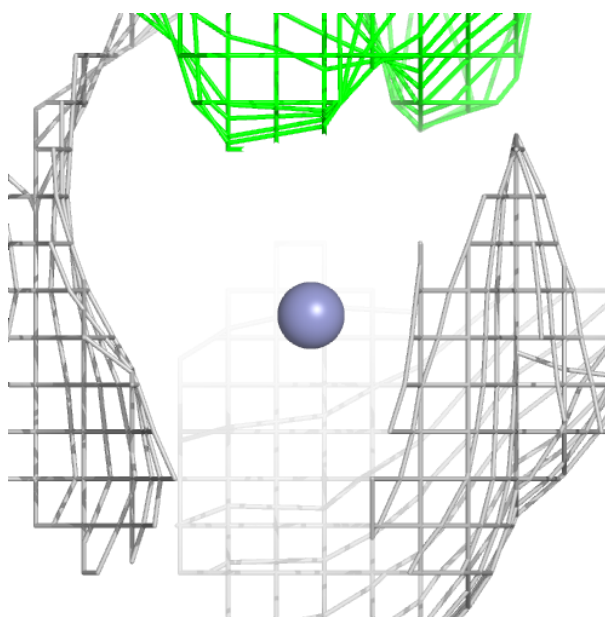
**Electron density around ACO A 1805:**

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



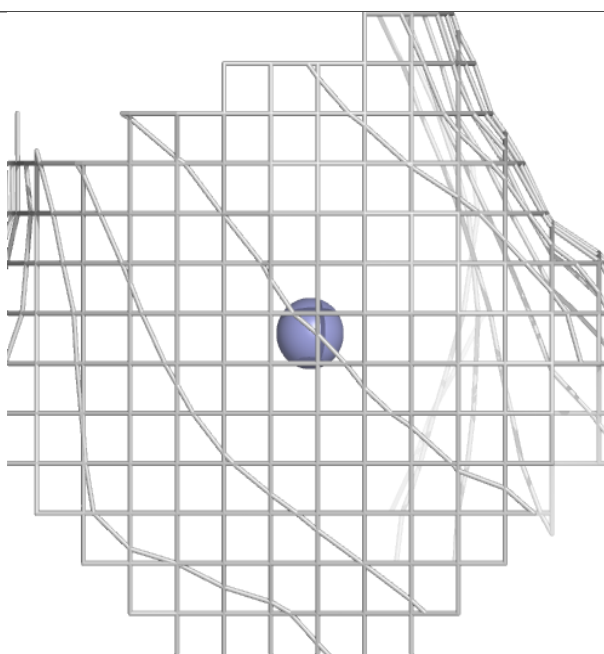
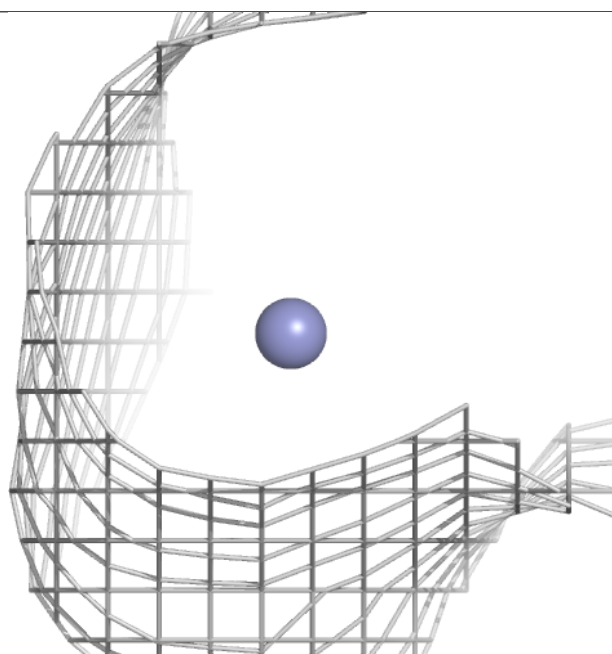
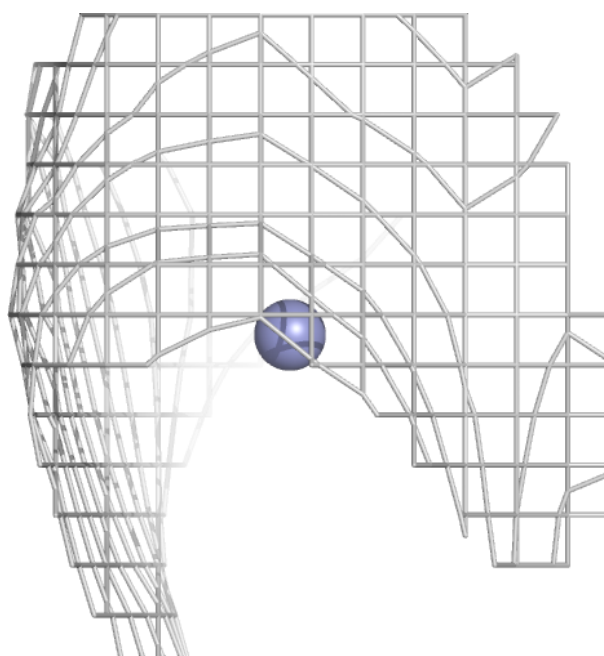
**Electron density around ZN B 1803:**

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



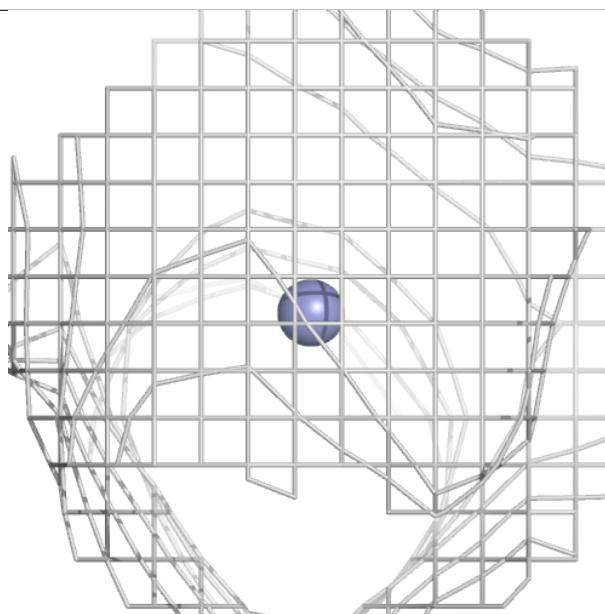
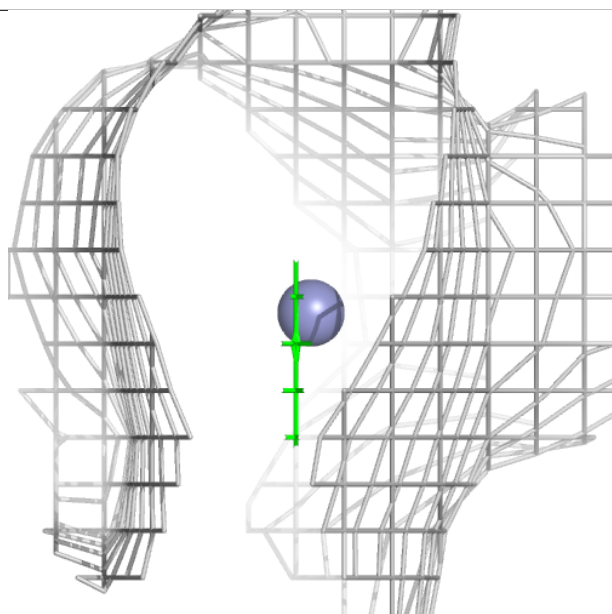
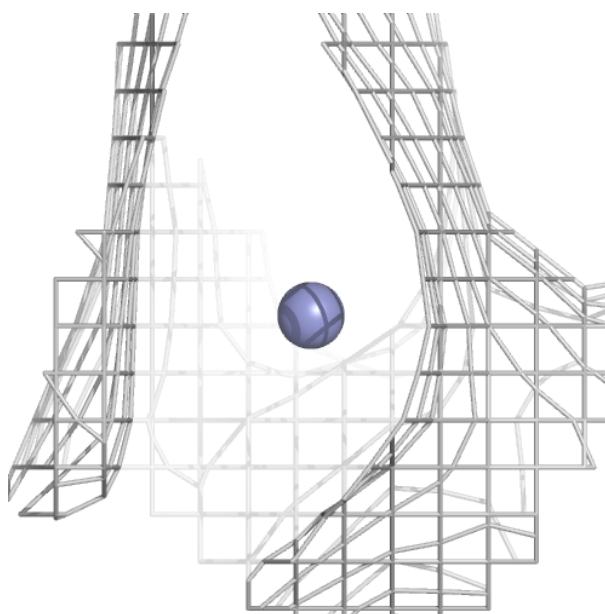
**Electron density around ZN B 1804:**

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



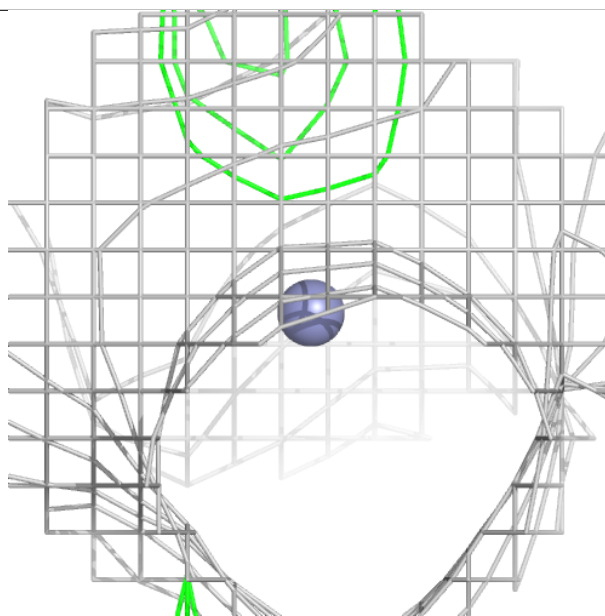
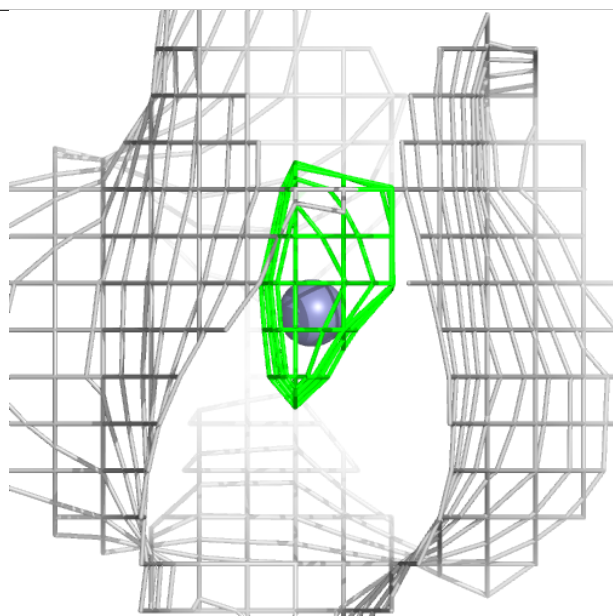
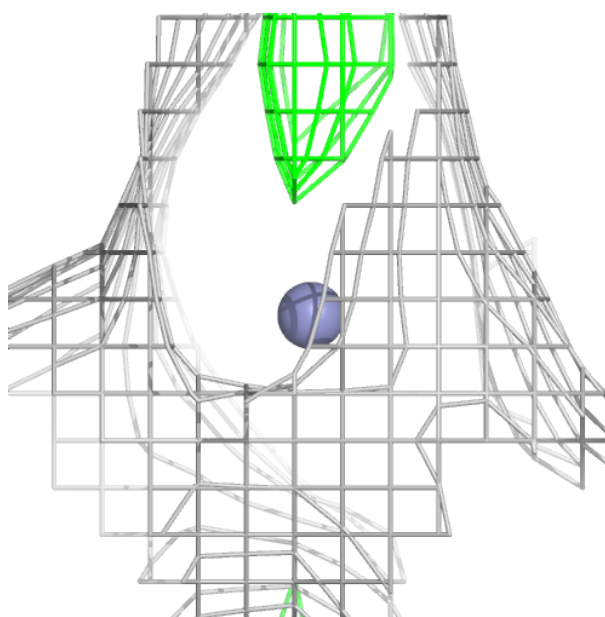
**Electron density around ZN B 1801:**

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



**Electron density around ZN A 1801:**

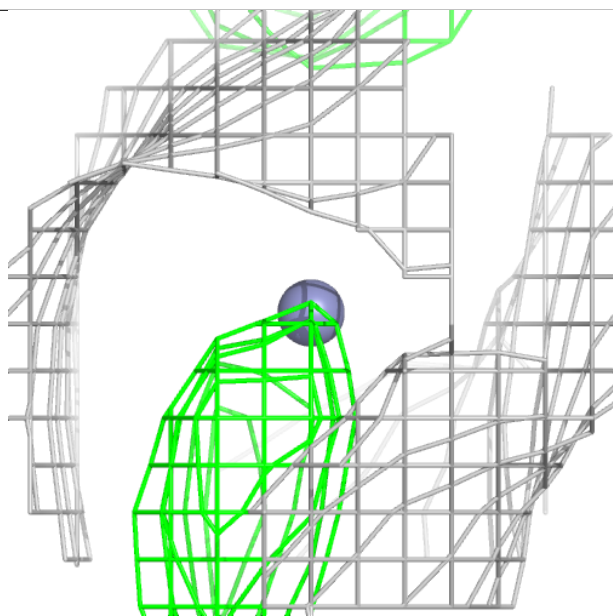
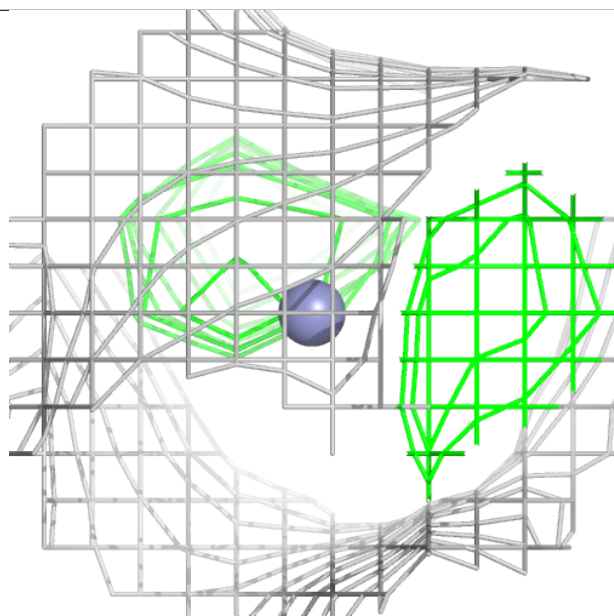
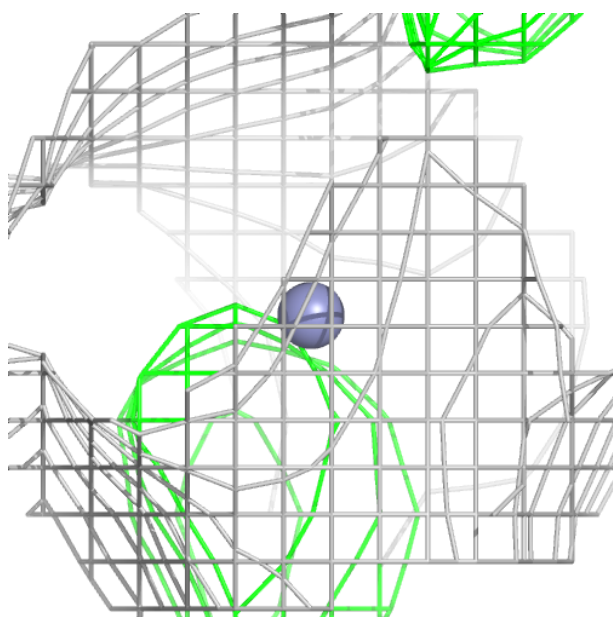
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

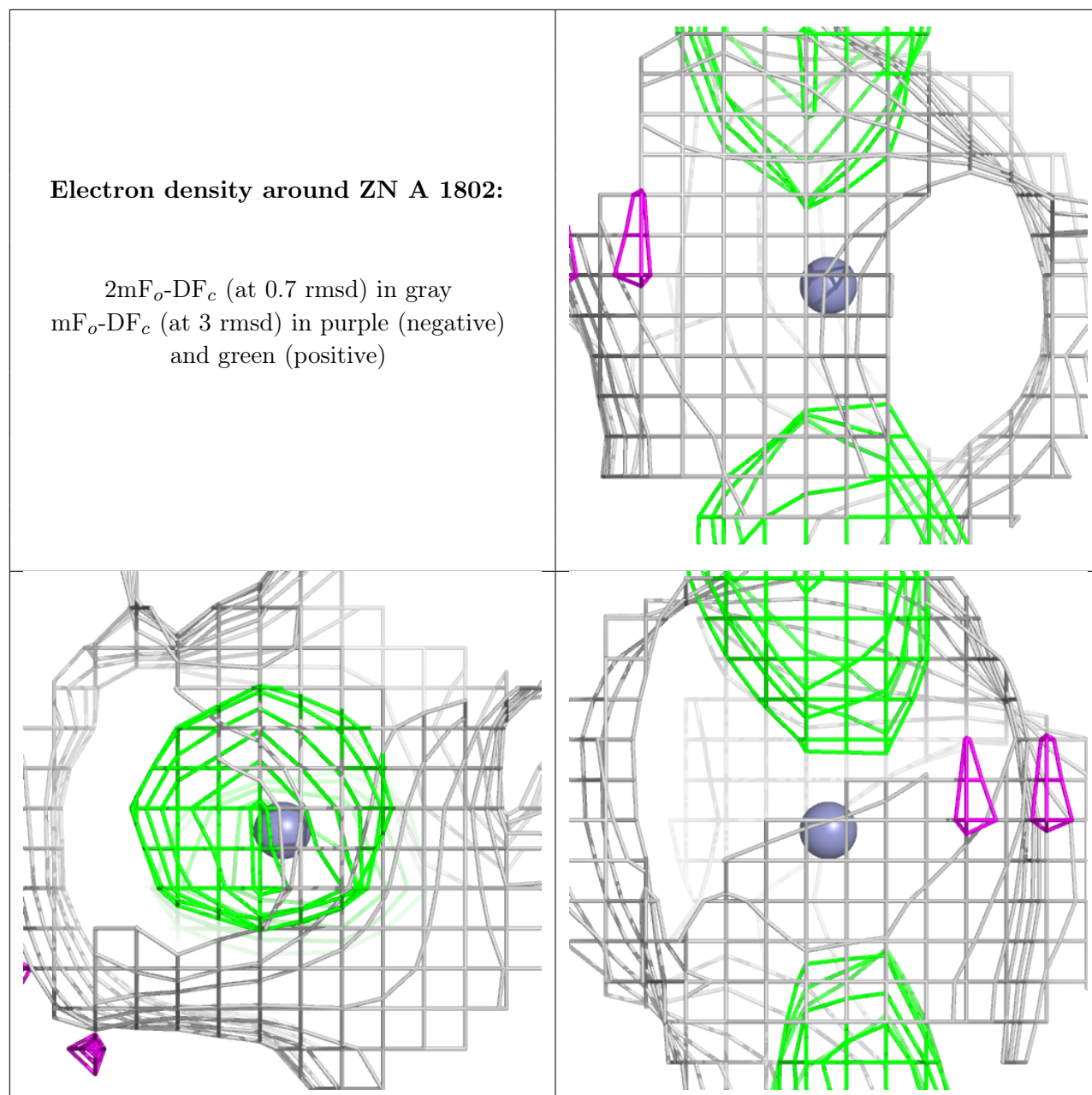




**Electron density around ZN B 1802:**

$2mF_o-DF_c$  (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.