



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2025 – 06:26 PM EST

PDB ID : 9OER / pdb\_00009oer  
Title : HalA with lysine, Fe(II), chloride, and a peroxyhemiketal intermediate  
Authors : Kissman, E.N.; Yang, A.Y.; Chang, M.C.Y.  
Deposited on : 2025-04-29  
Resolution : 1.72 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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

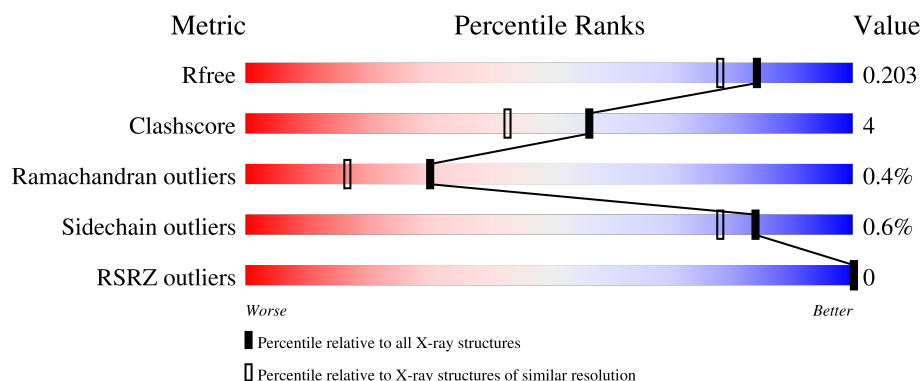
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*






The reported resolution of this entry is 1.72 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

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	258	
1	B	258	
1	C	258	
1	D	258	
1	E	258	

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Mol	Chain	Length	Quality of chain
1	F	258	 87% 10% •
1	G	258	 86% 11% •
1	H	258	 87% 11% •

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16420 atoms, of which 0 are hydrogens and 0 are deuteriums.

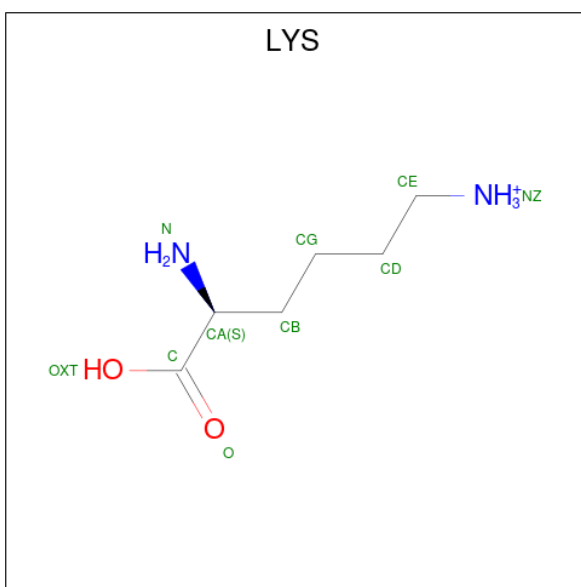
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lysine halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1956	1232	354	364	6			
1	B	252	Total	C	N	O	S	0	0	0
			1960	1234	354	366	6			
1	C	253	Total	C	N	O	S	0	0	0
			1947	1225	353	363	6			
1	D	252	Total	C	N	O	S	0	0	0
			1933	1215	348	364	6			
1	E	250	Total	C	N	O	S	0	0	0
			1944	1225	349	364	6			
1	F	250	Total	C	N	O	S	0	0	0
			1935	1220	351	358	6			
1	G	252	Total	C	N	O	S	0	0	0
			1946	1225	353	362	6			
1	H	252	Total	C	N	O	S	0	0	0
			1931	1216	347	362	6			

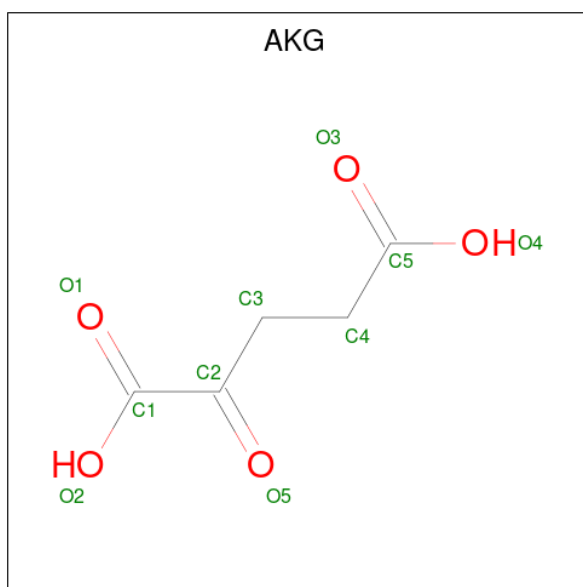
- Molecule 2 is LYSINE (CCD ID: LYS) (formula:  $C_6H_{15}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	E	1	Total	C	N	O	0	0
			10	6	2	2		
2	F	1	Total	C	N	O	0	0
			10	6	2	2		
2	H	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

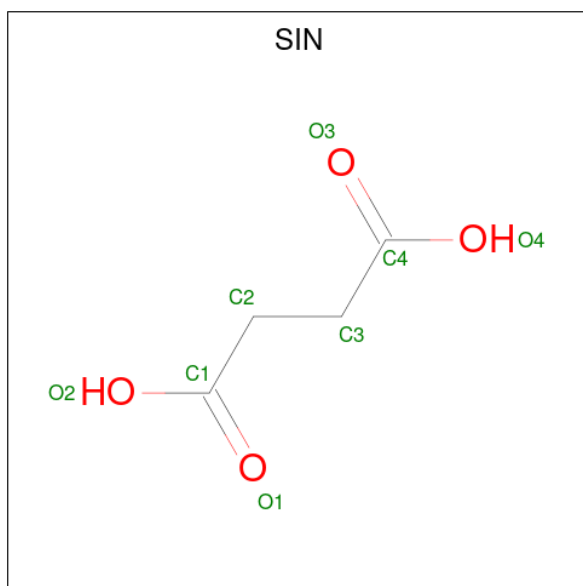
- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		
4	B	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		
4	D	1	Total	Fe	0	0
			1	1		
4	E	1	Total	Fe	0	0
			1	1		
4	F	1	Total	Fe	0	0
			1	1		
4	G	1	Total	Fe	0	0
			1	1		
4	H	1	Total	Fe	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0

- Molecule 6 is SUCCINIC ACID (CCD ID: SIN) (formula:  $C_4H_6O_4$ ) (labeled as "Ligand of Interest" by depositor).



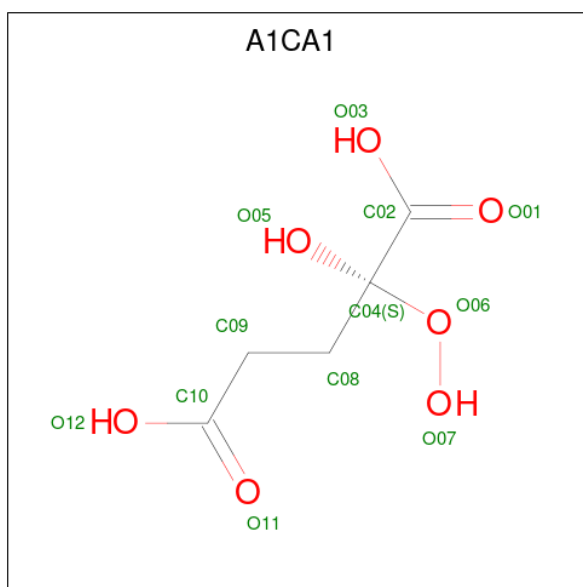
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 8 4 4	0	0
6	C	1	Total C O 8 4 4	0	0
6	F	1	Total C O 8 4 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total 8	C 4	O 4	0	0
6	H	1	Total 8	C 4	O 4	0	0

- 
- Chemical structure of YLO (2-chloro-4-aminopentan-3-one) is shown. The structure includes a carboxylic acid group (HO-C(=O)-) attached to a five-carbon chain. The chain is substituted with an amino group (NH<sub>2</sub>) at C4 and a chlorine atom (Cl) at C2. The atoms are labeled as follows: O11, O10, C09, C07(S), C06, C04(R), C03, C02, N08, N01, and Cl05.

- Molecule 8 is (2S)-2-hydroperoxy-2-hydroxypentanedioic acid (CCD ID: A1CA1) (formula:  $C_5H_8O_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			12	5	7		

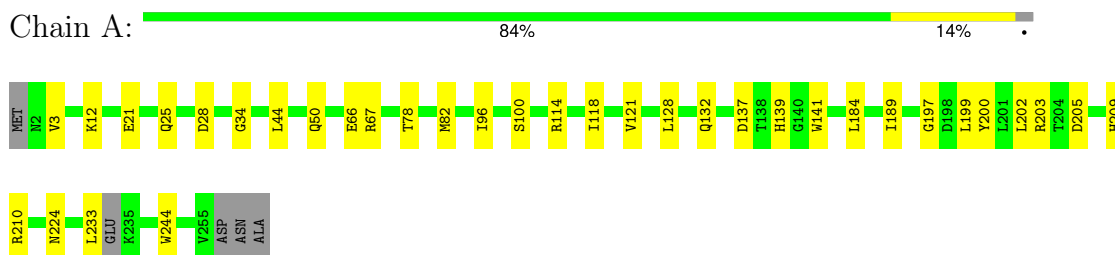
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	101	Total	O	0	0
			101	101		
9	B	103	Total	O	0	0
			103	103		
9	C	94	Total	O	0	0
			94	94		
9	D	96	Total	O	0	0
			96	96		
9	E	82	Total	O	0	0
			82	82		
9	F	78	Total	O	0	0
			78	78		
9	G	73	Total	O	0	0
			73	73		
9	H	70	Total	O	0	0
			70	70		

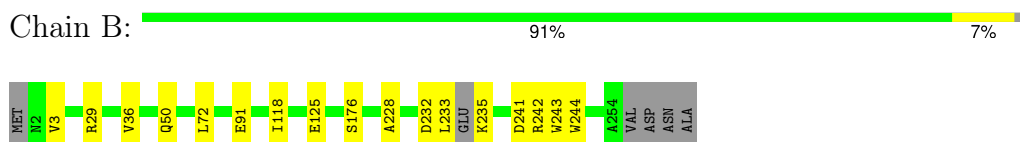
### 3 Residue-property plots

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.

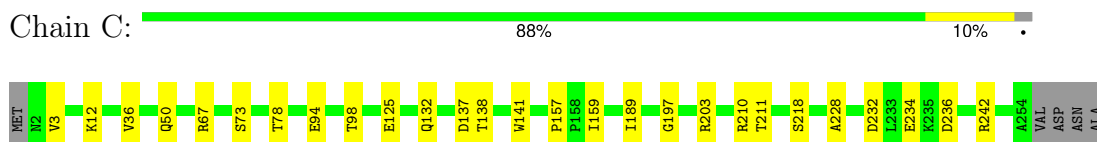
- Molecule 1: Lysine halogenase



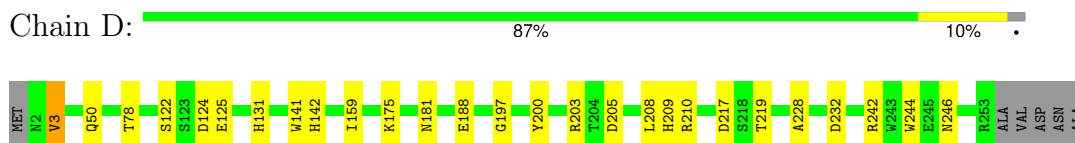
- Molecule 1: Lysine halogenase



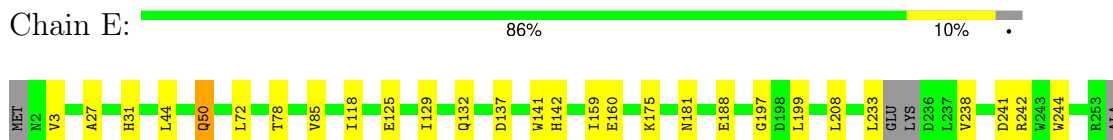
- Molecule 1: Lysine halogenase



- Molecule 1: Lysine halogenase

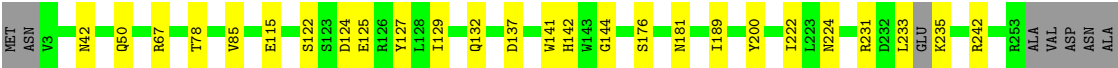
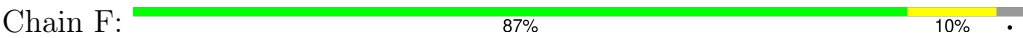


- Molecule 1: Lysine halogenase

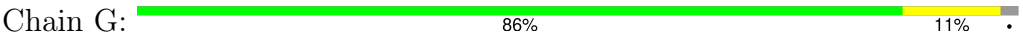


VAL  
ASP  
ASN  
ALA

• Molecule 1: Lysine halogenase

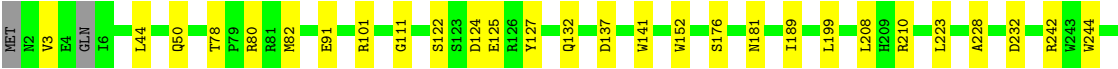
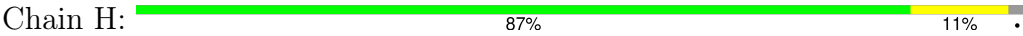


• Molecule 1: Lysine halogenase



A254  
VAL  
ASP  
ASN  
ALA

• Molecule 1: Lysine halogenase



A254  
VAL  
ASP  
ASN  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.30Å 147.30Å 287.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.96 – 1.72 95.96 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.96-1.72) 99.7 (95.96-1.72)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.168 , 0.201 0.171 , 0.203	Depositor DCC
$R_{free}$ test set	12536 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 24.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.446 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.460 for h,-h-k,-l	Depositor
Outliers	0 of 246749 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	16420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, A1CA1, FE2, YL0, AKG, SIN

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	0.19	0/1999	0.36	0/2724
1	B	0.22	0/2004	0.39	0/2730
1	C	0.20	0/1992	0.40	1/2719 (0.0%)
1	D	0.17	0/1977	0.33	0/2698
1	E	0.16	0/1988	0.32	0/2709
1	F	0.18	0/1979	0.37	0/2698
1	G	0.18	0/1990	0.35	0/2713
1	H	0.17	0/1975	0.33	0/2695
All	All	0.19	0/15904	0.36	1/21686 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	GLU	N-CA-C	-5.52	106.38	113.01

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1956	0	1850	23	0
1	B	1960	0	1855	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1947	0	1821	17	0
1	D	1933	0	1797	22	0
1	E	1944	0	1837	17	0
1	F	1935	0	1827	19	0
1	G	1946	0	1829	17	0
1	H	1931	0	1798	17	0
2	A	10	0	12	1	0
2	B	10	0	12	1	0
2	E	10	0	12	0	0
2	F	10	0	12	0	0
2	H	10	0	12	1	0
3	A	10	0	4	2	0
3	D	10	0	4	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	1	0
5	G	1	0	0	1	0
5	H	1	0	0	0	0
6	B	8	0	4	0	0
6	C	8	0	4	0	0
6	F	8	0	4	2	0
6	G	8	0	4	1	0
6	H	8	0	4	0	0
7	C	11	0	0	0	0
7	D	11	0	0	0	0
7	G	11	0	0	0	0
8	E	12	0	0	2	0
9	A	101	0	0	5	0
9	B	103	0	0	2	0
9	C	94	0	0	3	0
9	D	96	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	82	0	0	2	0
9	F	78	0	0	2	0
9	G	73	0	0	2	0
9	H	70	0	0	2	0
All	All	16420	0	14702	136	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 4.

The worst 5 of 136 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:F:233:LEU:C	1:F:235:LYS:N	2.29	0.90
1:B:233:LEU:C	1:B:235:LYS:N	2.30	0.90
1:A:96:ILE:O	9:A:401:HOH:O	2.01	0.77
5:G:304:CL:CL	9:G:448:HOH:O	2.44	0.73
1:A:28:ASP:OD1	1:A:114:ARG:NH2	2.21	0.71

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	249/258 (96%)	242 (97%)	6 (2%)	1 (0%)	30	17
1	B	248/258 (96%)	236 (95%)	11 (4%)	1 (0%)	30	17
1	C	251/258 (97%)	241 (96%)	9 (4%)	1 (0%)	30	17
1	D	250/258 (97%)	240 (96%)	8 (3%)	2 (1%)	16	5
1	E	246/258 (95%)	236 (96%)	9 (4%)	1 (0%)	30	17
1	F	246/258 (95%)	242 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	248/258 (96%)	240 (97%)	7 (3%)	1 (0%)	30	17
1	H	248/258 (96%)	237 (96%)	10 (4%)	1 (0%)	30	17
All	All	1986/2064 (96%)	1914 (96%)	64 (3%)	8 (0%)	30	17

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	B	3	VAL
1	H	3	VAL
1	C	3	VAL
1	D	3	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/229 (87%)	198 (100%)	1 (0%)	86	82
1	B	201/229 (88%)	199 (99%)	2 (1%)	73	63
1	C	196/229 (86%)	194 (99%)	2 (1%)	73	63
1	D	194/229 (85%)	194 (100%)	0	100	100
1	E	200/229 (87%)	199 (100%)	1 (0%)	86	82
1	F	197/229 (86%)	196 (100%)	1 (0%)	86	82
1	G	197/229 (86%)	197 (100%)	0	100	100
1	H	194/229 (85%)	192 (99%)	2 (1%)	73	63
All	All	1578/1832 (86%)	1569 (99%)	9 (1%)	84	78

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	50	GLN
1	H	176	SER

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Mol	Chain	Res	Type
1	C	36	VAL
1	C	236	ASP
1	E	50	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	132	GLN
1	F	63	GLN
1	H	161	HIS
1	H	50	GLN
1	D	9	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	LYS	A	301	-	8,9,9	0.86	1 (12%)	7,10,10	1.01	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	YL0	C	301	-	7,10,10	0.86	0	5,12,12	1.02	0
2	LYS	E	301	-	8,9,9	0.87	1 (12%)	7,10,10	1.11	1 (14%)
6	SIN	F	302	4	7,7,7	1.13	0	8,8,8	1.69	4 (50%)
7	YL0	D	301	-	7,10,10	0.99	0	5,12,12	1.09	0
2	LYS	H	301	-	8,9,9	0.86	1 (12%)	7,10,10	1.09	1 (14%)
3	AKG	A	302	4	9,9,9	1.42	2 (22%)	11,11,11	2.05	3 (27%)
7	YL0	G	301	-	7,10,10	0.92	0	5,12,12	0.94	0
6	SIN	B	302	4	7,7,7	1.06	0	8,8,8	1.66	2 (25%)
8	A1CA1	E	302	4	9,11,11	1.12	0	8,15,15	1.22	1 (12%)
6	SIN	G	302	4	7,7,7	1.14	0	8,8,8	1.47	2 (25%)
2	LYS	B	301	-	8,9,9	0.84	1 (12%)	7,10,10	1.04	1 (14%)
6	SIN	H	302	4	7,7,7	1.08	0	8,8,8	1.59	1 (12%)
6	SIN	C	302	4	7,7,7	1.06	0	8,8,8	1.59	1 (12%)
3	AKG	D	302	4	9,9,9	1.34	1 (11%)	11,11,11	2.26	3 (27%)
2	LYS	F	301	-	8,9,9	0.88	1 (12%)	7,10,10	0.95	1 (14%)

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	LYS	A	301	-	-	1/9/9/9	-
7	YL0	C	301	-	-	2/11/11/11	-
2	LYS	E	301	-	-	0/9/9/9	-
6	SIN	F	302	4	-	2/5/5/5	-
7	YL0	D	301	-	-	3/11/11/11	-
2	LYS	H	301	-	-	3/9/9/9	-
3	AKG	A	302	4	-	0/9/9/9	-
7	YL0	G	301	-	-	3/11/11/11	-
6	SIN	B	302	4	-	0/5/5/5	-
8	A1CA1	E	302	4	-	9/11/15/15	-
6	SIN	G	302	4	-	2/5/5/5	-
2	LYS	B	301	-	-	2/9/9/9	-
6	SIN	H	302	4	-	2/5/5/5	-
6	SIN	C	302	4	-	3/5/5/5	-
3	AKG	D	302	4	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	F	301	-	-	2/9/9/9	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	AKG	O2-C1	-2.36	1.24	1.30
2	E	301	LYS	OXT-C	-2.33	1.23	1.30
2	A	301	LYS	OXT-C	-2.31	1.23	1.30
2	F	301	LYS	OXT-C	-2.30	1.23	1.30
3	D	302	AKG	O2-C1	-2.28	1.24	1.30

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	AKG	O1-C1-C2	-5.84	114.55	121.81
3	A	302	AKG	O1-C1-C2	-5.27	115.26	121.81
3	A	302	AKG	C4-C3-C2	2.88	118.32	112.91
2	H	301	LYS	OXT-C-O	-2.74	117.87	124.08
2	E	301	LYS	OXT-C-O	-2.70	117.96	124.08

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	302	AKG	O2-C1-C2-C3
7	D	301	YL0	C04-C06-C07-N08
7	G	301	YL0	N01-C02-C03-C04
7	G	301	YL0	C04-C06-C07-N08
8	E	302	A1CA1	O01-C02-C04-C08

There are no ring outliers.

8 monomers are involved in 13 short contacts:

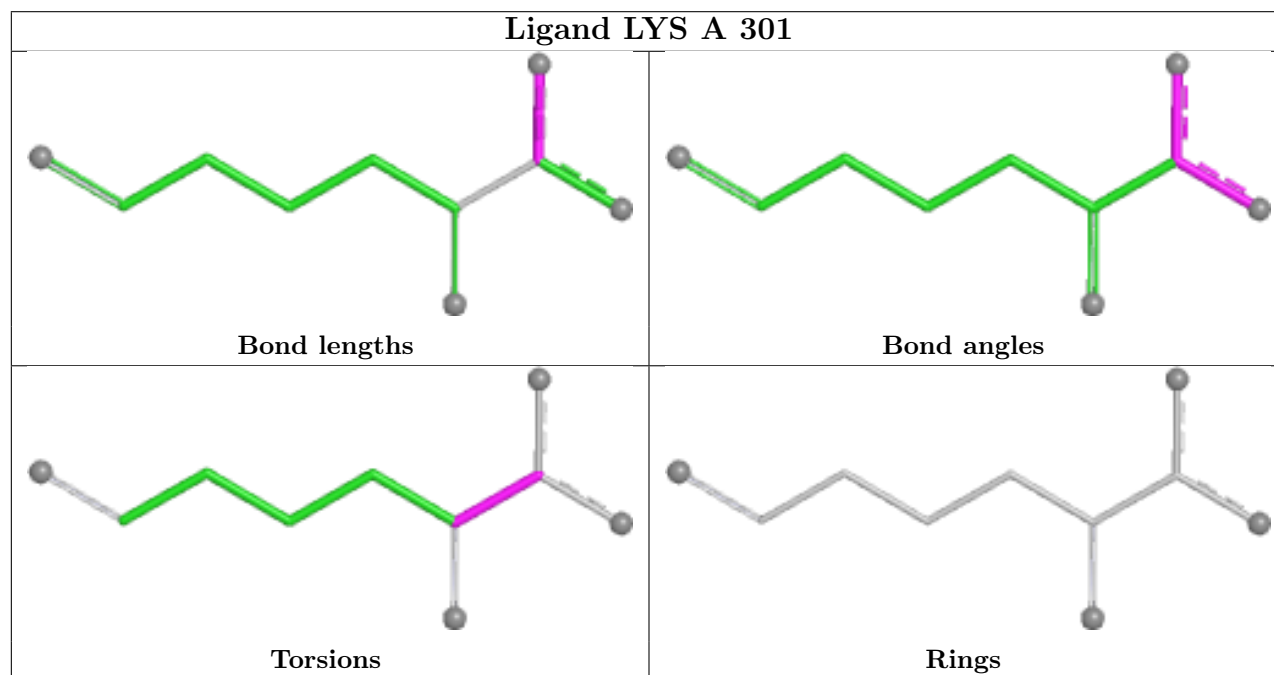
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	LYS	1	0
6	F	302	SIN	2	0
2	H	301	LYS	1	0
3	A	302	AKG	2	0
8	E	302	A1CA1	2	0
6	G	302	SIN	1	0
2	B	301	LYS	1	0

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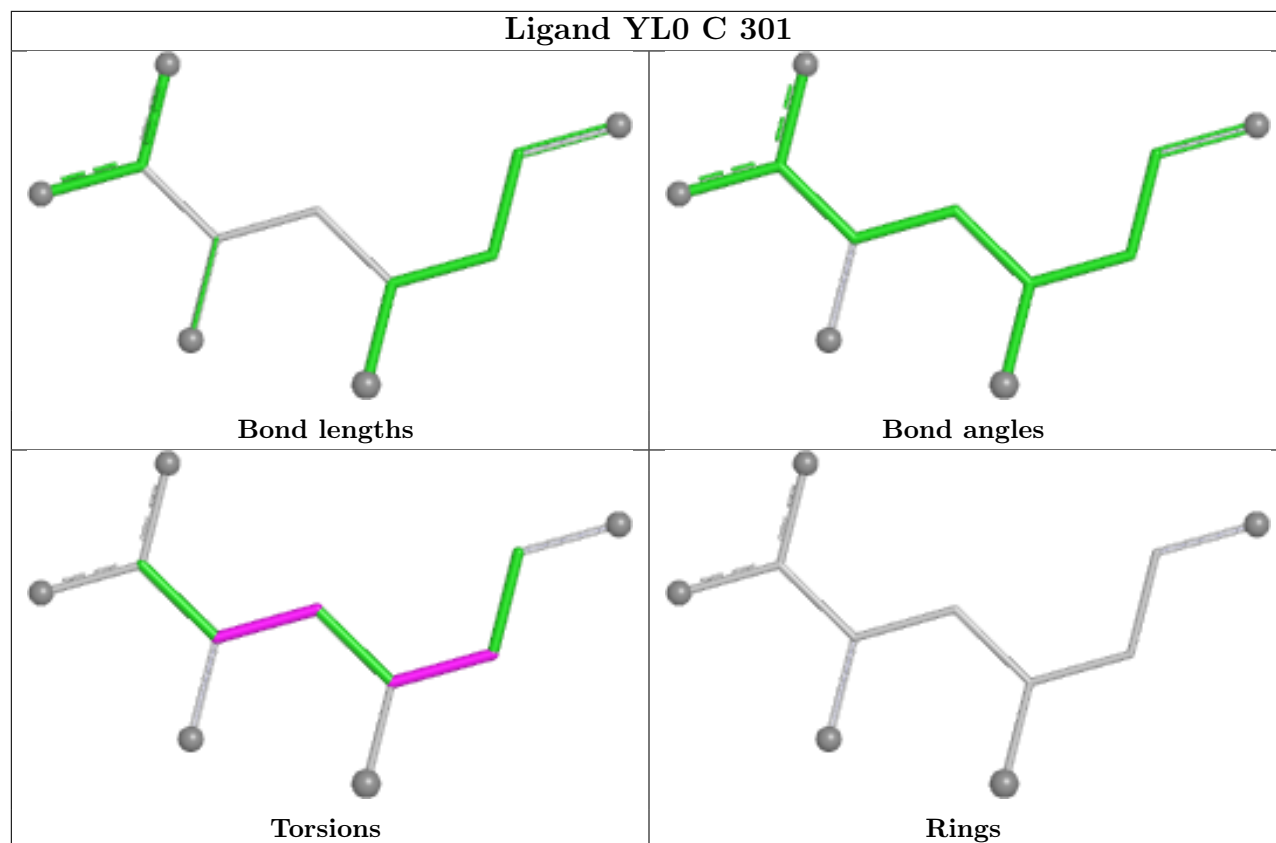
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	AKG	3	0

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.

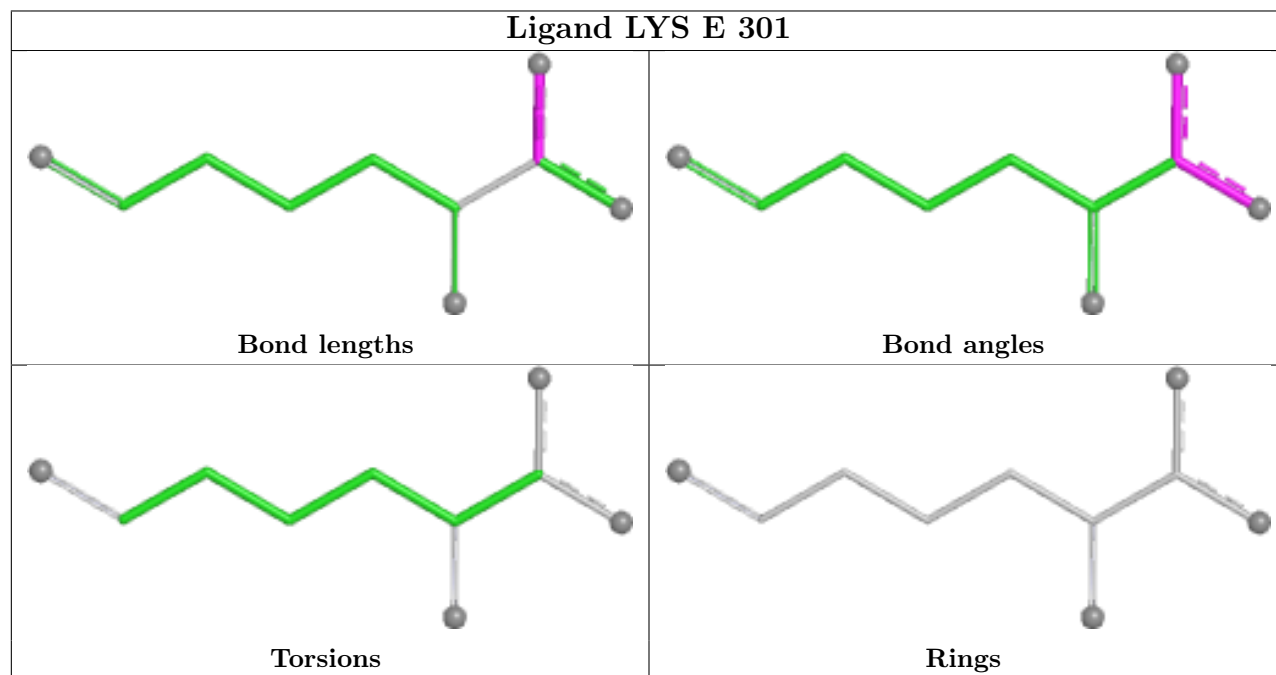


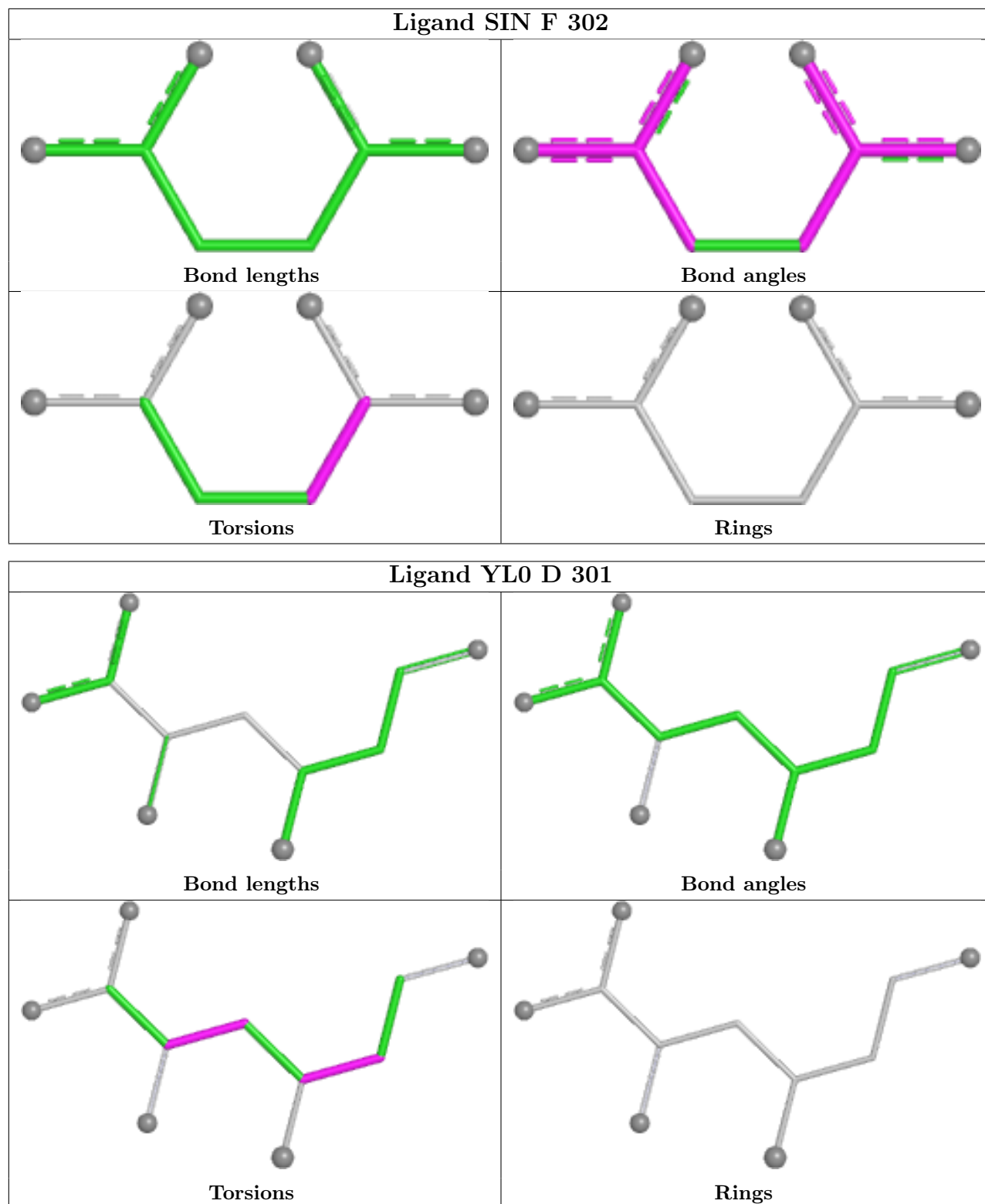


## Ligand YL0 C 301

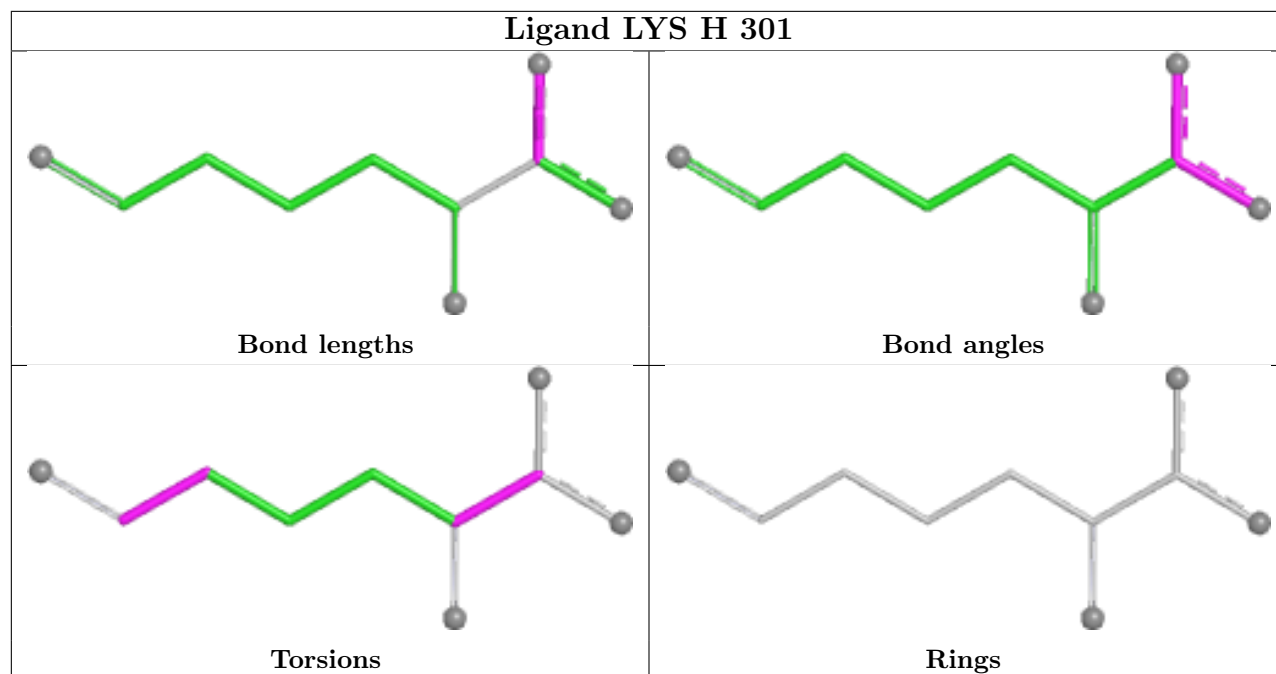


## Ligand LYS E 301

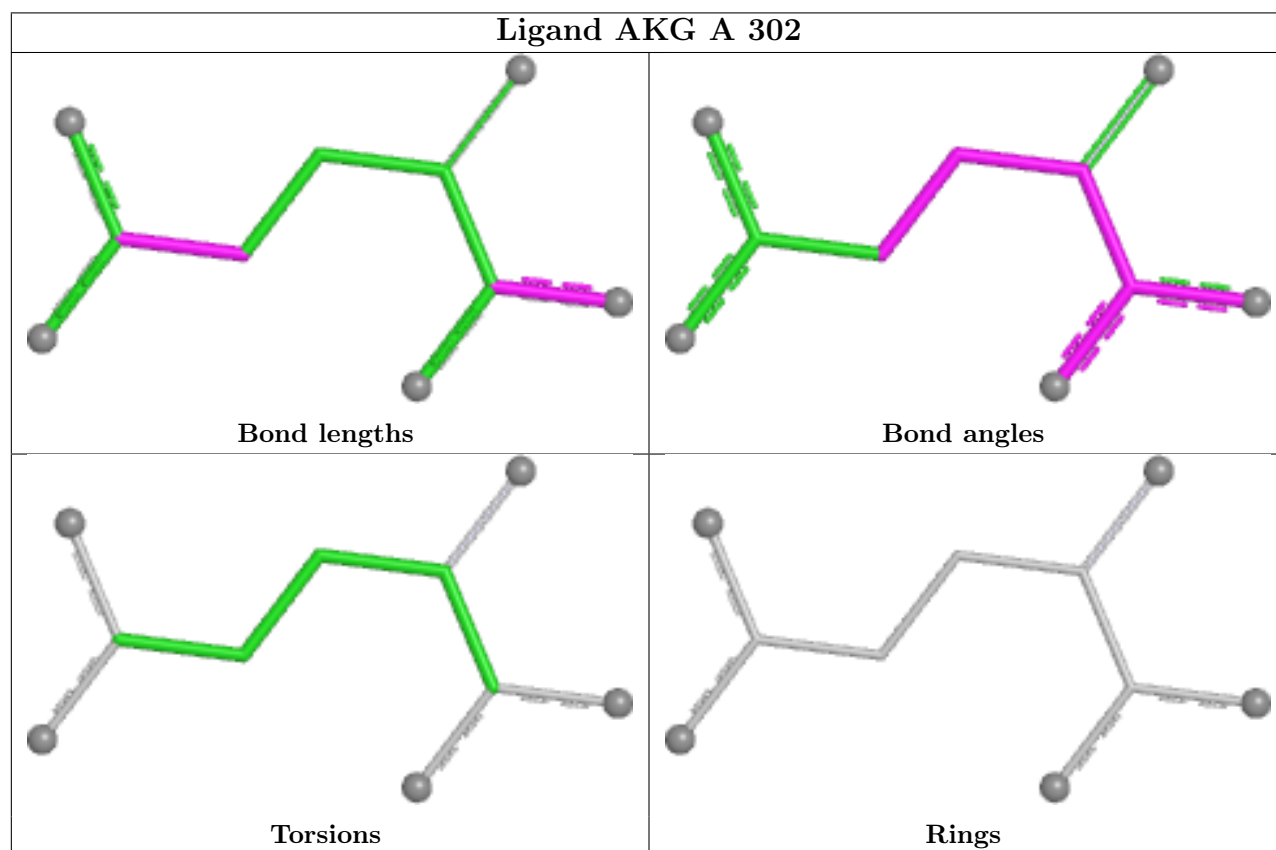


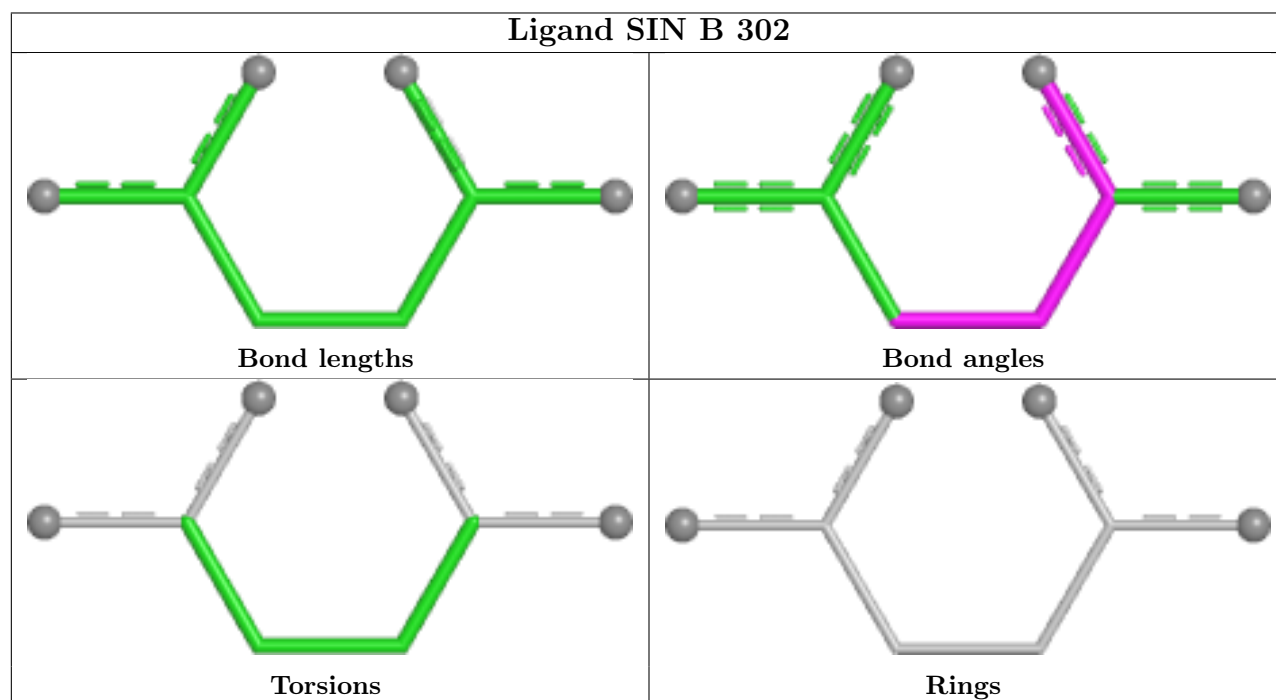
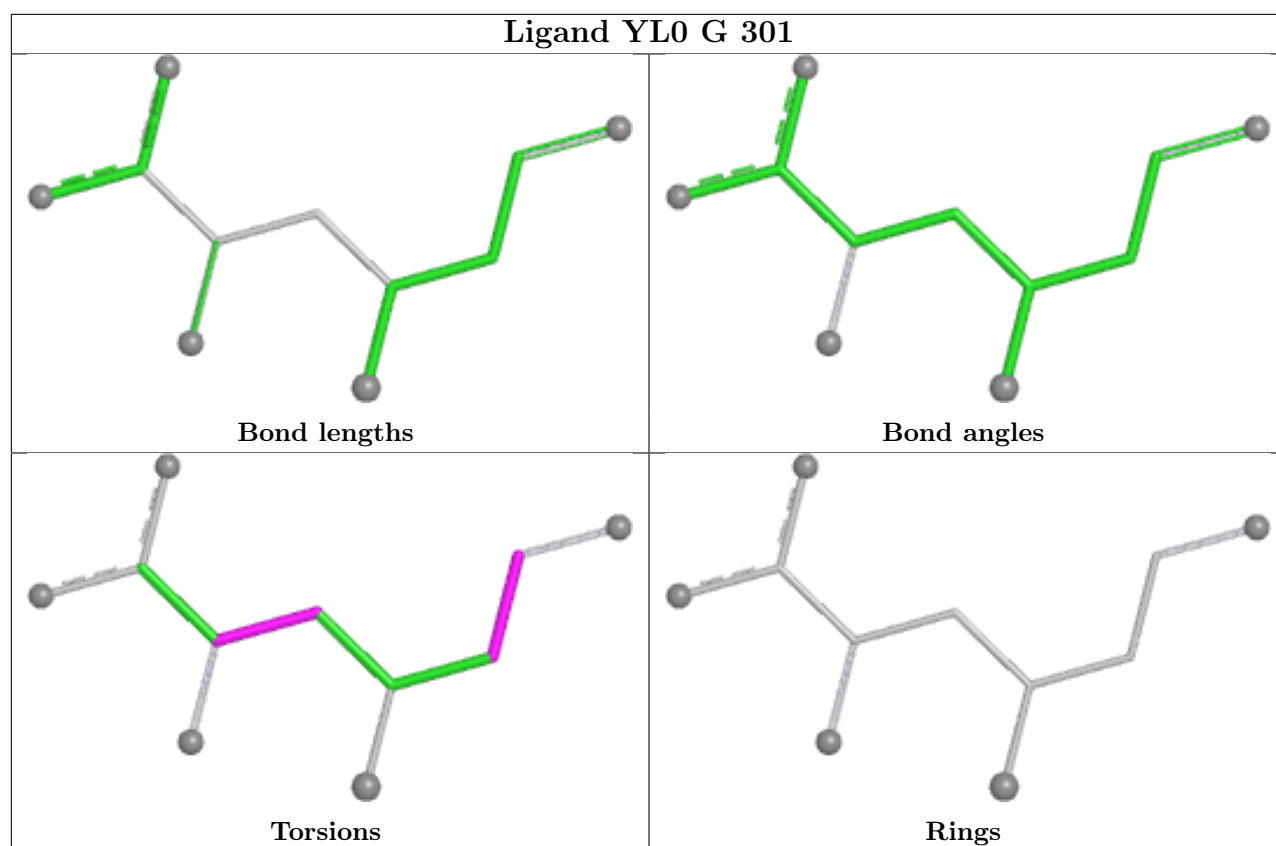


## Ligand LYS H 301

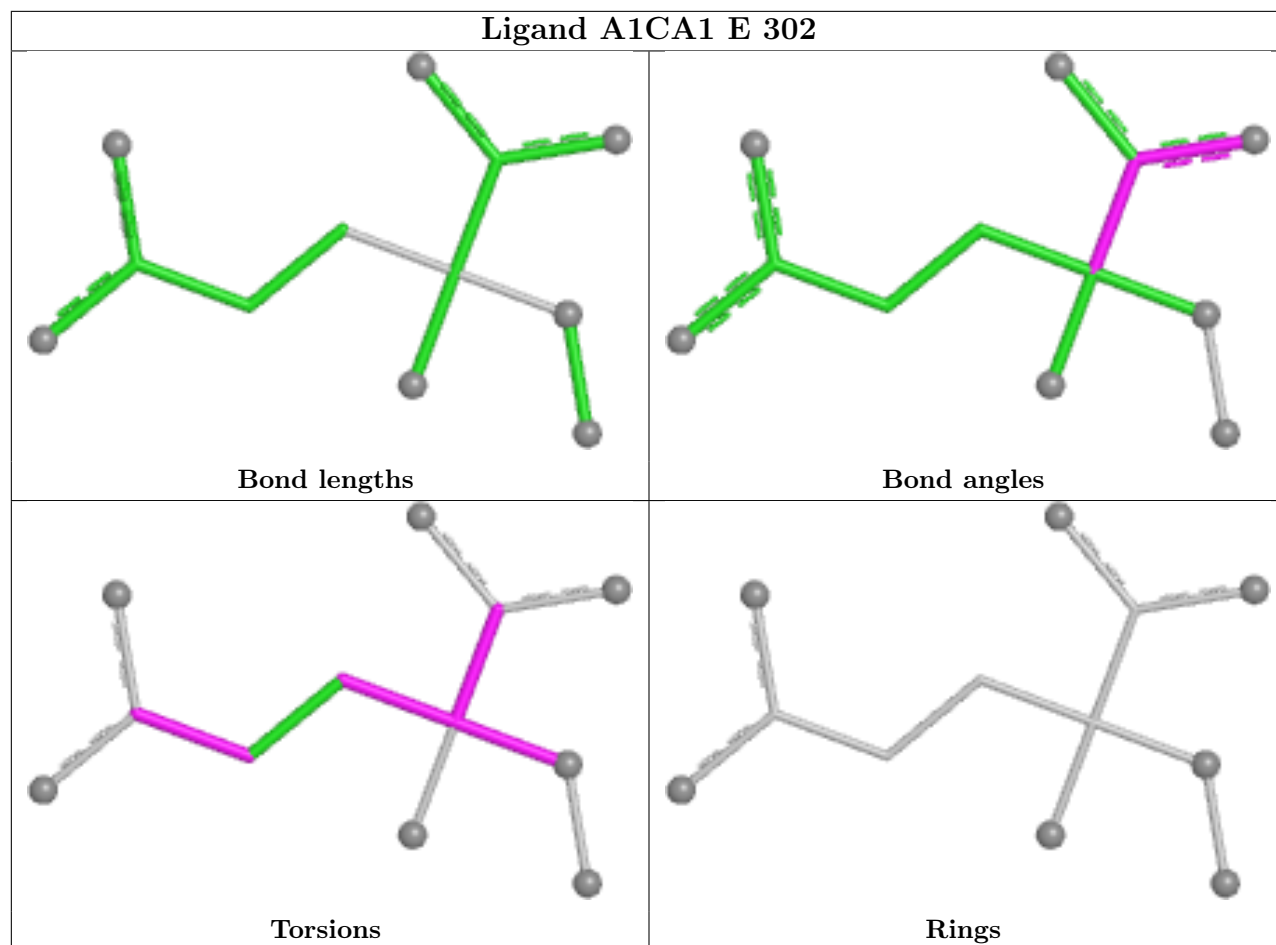


## Ligand AKG A 302

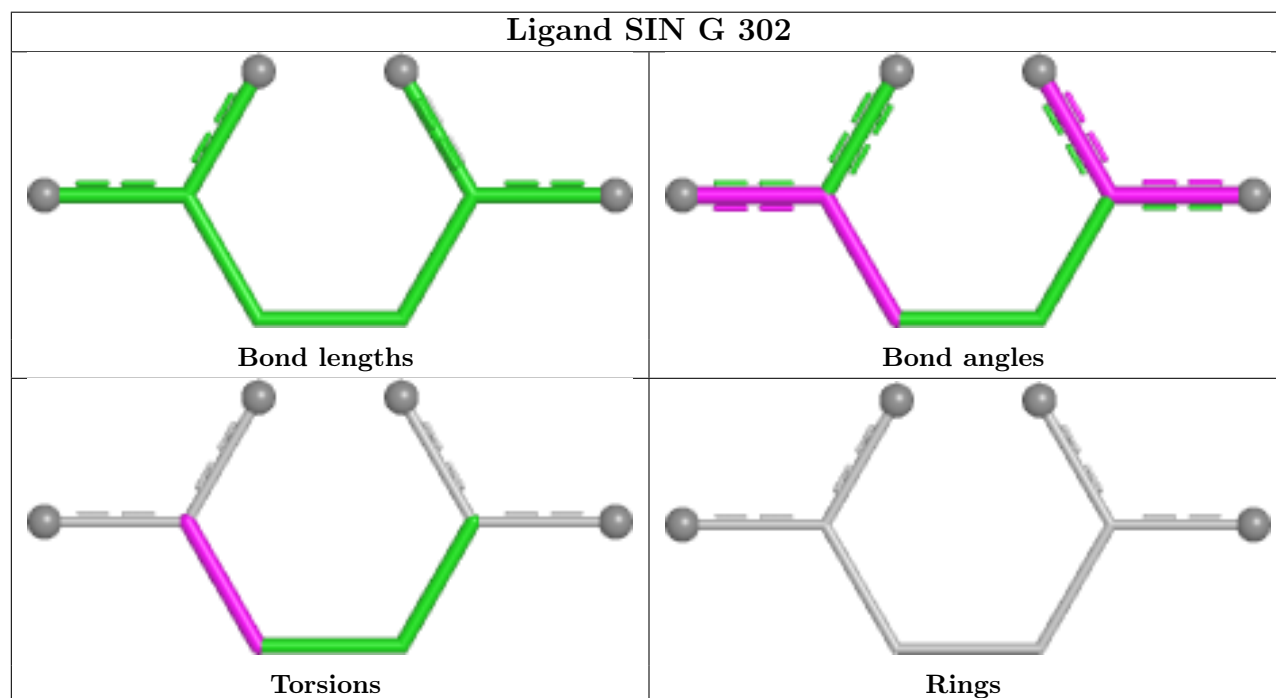




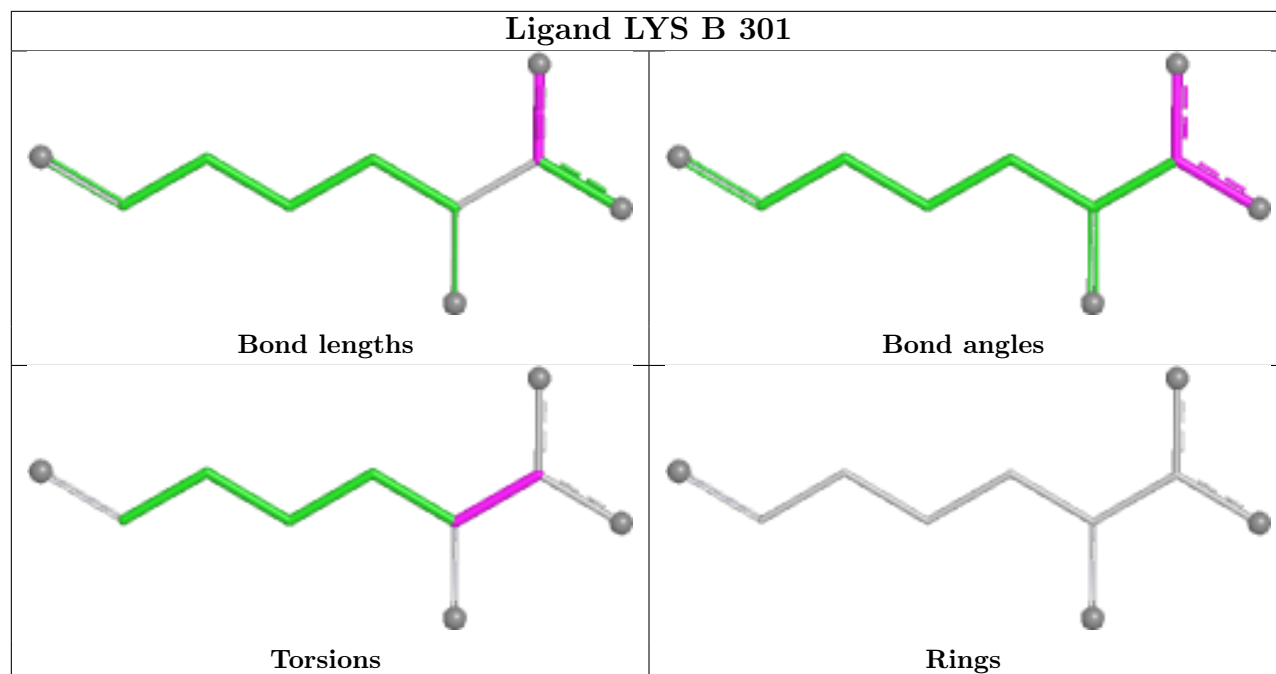
## Ligand A1CA1 E 302



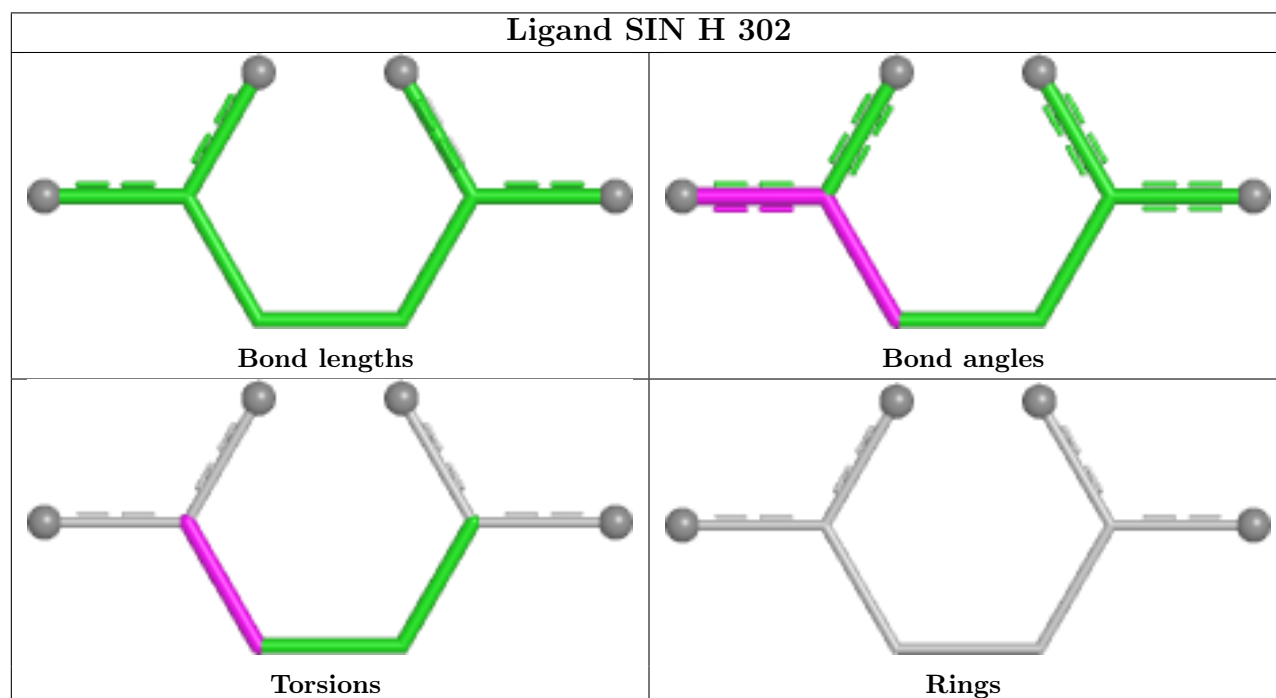
## Ligand SIN G 302

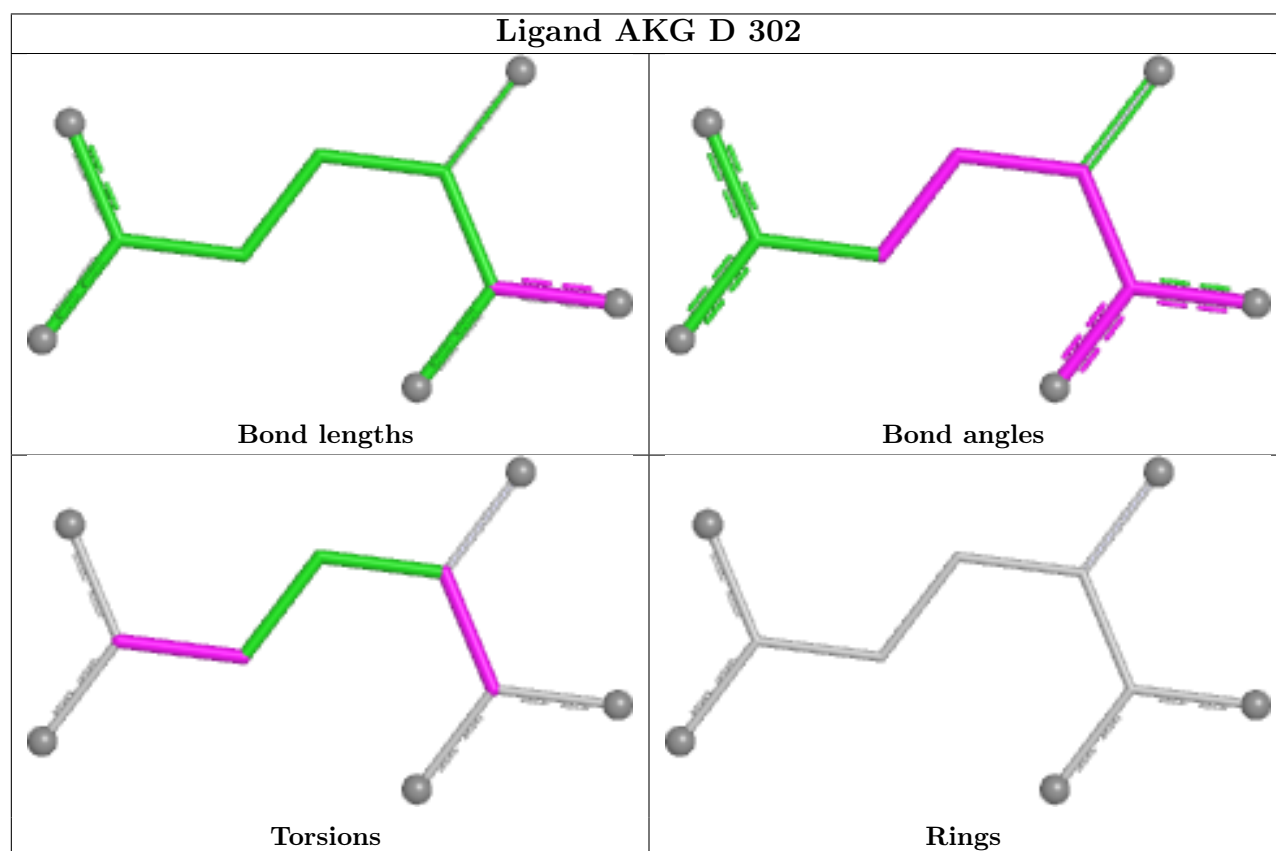
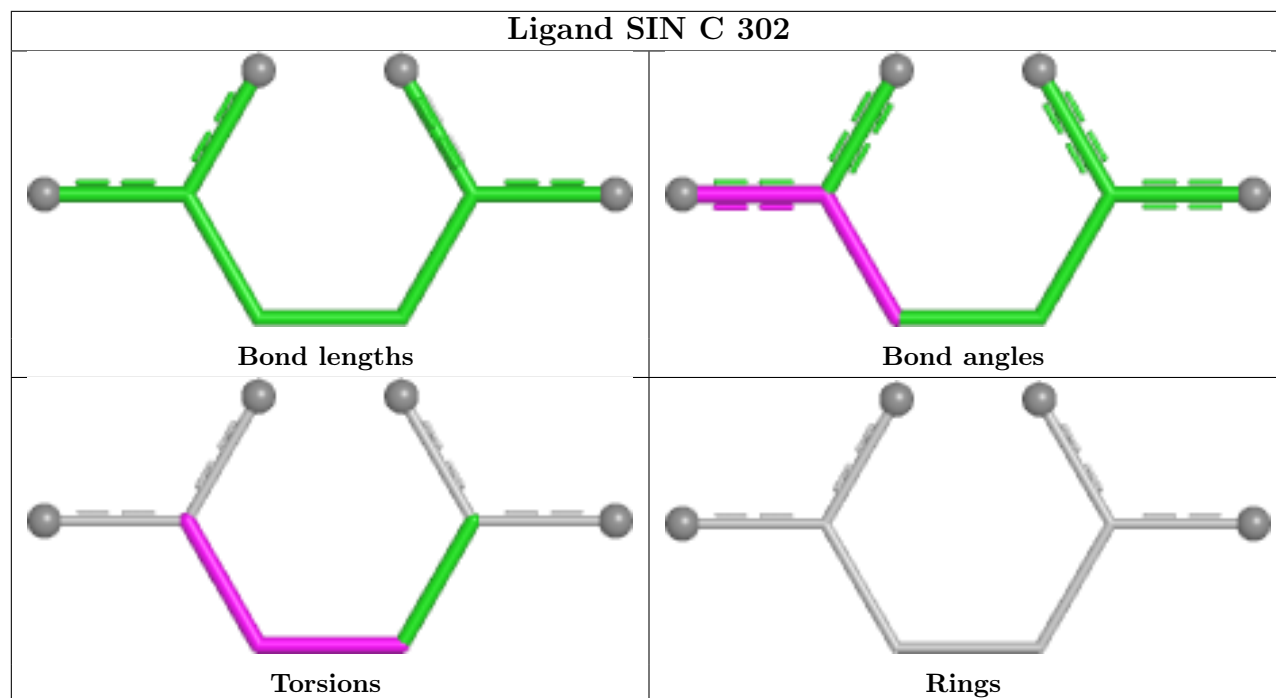


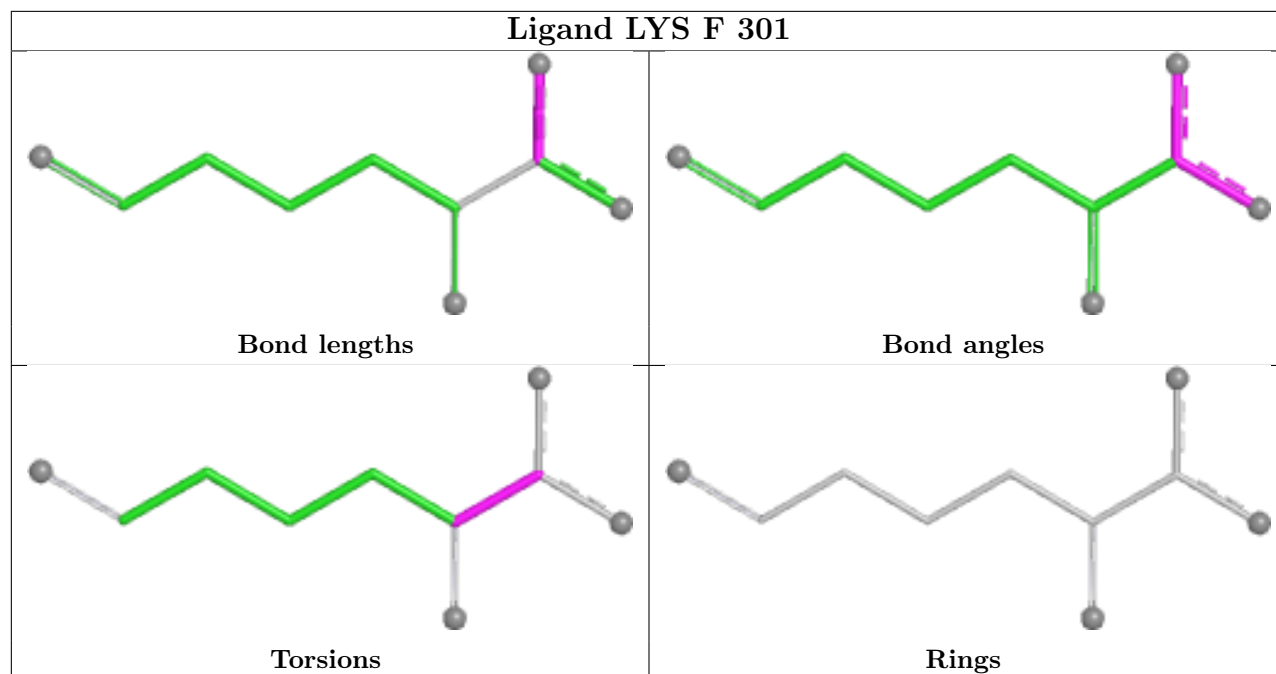
## Ligand LYS B 301



## Ligand SIN H 302







## 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	253/258 (98%)	-1.23	0 100 100	17, 23, 33, 54	0
1	B	252/258 (97%)	-1.19	0 100 100	17, 24, 35, 50	0
1	C	253/258 (98%)	-1.17	0 100 100	18, 25, 36, 54	0
1	D	252/258 (97%)	-1.15	0 100 100	18, 25, 38, 53	0
1	E	250/258 (96%)	-1.16	0 100 100	18, 25, 35, 50	0
1	F	250/258 (96%)	-1.15	0 100 100	18, 26, 38, 52	0
1	G	252/258 (97%)	-1.09	0 100 100	19, 29, 40, 62	0
1	H	252/258 (97%)	-1.05	0 100 100	20, 29, 41, 62	0
All	All	2014/2064 (97%)	-1.15	0 100 100	17, 25, 38, 62	0

There are no RSRZ outliers to report.

### 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](#)

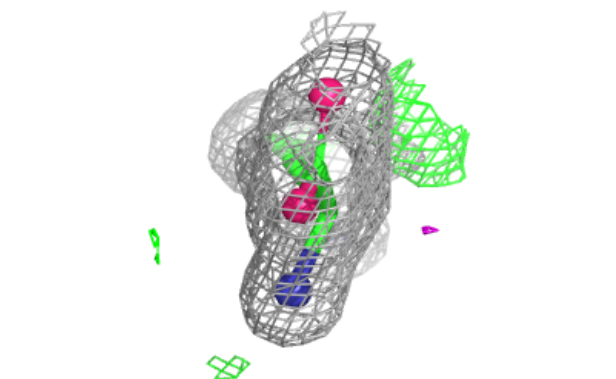
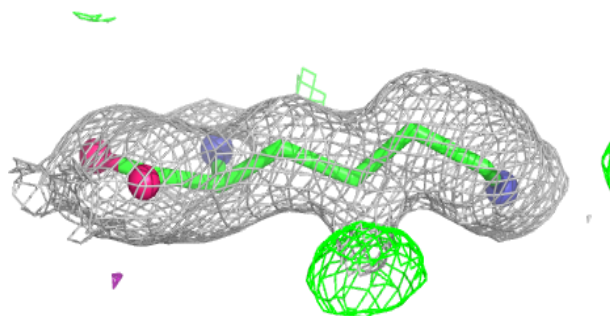
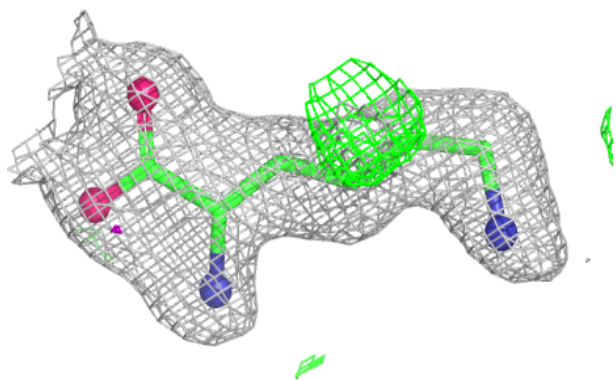
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
2	LYS	H	301	10/10	0.98	0.04	23,27,30,31	0
3	AKG	D	302	10/10	0.98	0.04	24,27,29,34	0
6	SIN	F	302	8/8	0.98	0.05	25,28,31,33	0
7	YL0	C	301	11/11	0.98	0.04	22,23,26,37	0
8	A1CA1	E	302	12/12	0.98	0.05	24,29,32,33	0
3	AKG	A	302	10/10	0.99	0.04	19,23,29,30	0
2	LYS	B	301	10/10	0.99	0.03	19,23,26,28	0
5	CL	A	304	1/1	0.99	0.06	29,29,29,29	0
5	CL	C	304	1/1	0.99	0.04	28,28,28,28	0
5	CL	D	304	1/1	0.99	0.05	29,29,29,29	0
5	CL	E	304	1/1	0.99	0.08	32,32,32,32	0
5	CL	H	304	1/1	0.99	0.05	30,30,30,30	0
6	SIN	B	302	8/8	0.99	0.03	21,24,28,29	0
6	SIN	C	302	8/8	0.99	0.03	23,26,31,35	0
2	LYS	E	301	10/10	0.99	0.04	20,23,29,30	0
6	SIN	G	302	8/8	0.99	0.04	24,31,35,39	0
6	SIN	H	302	8/8	0.99	0.03	26,30,33,34	0
2	LYS	F	301	10/10	0.99	0.04	22,24,27,28	0
7	YL0	D	301	11/11	0.99	0.04	23,25,27,39	0
7	YL0	G	301	11/11	0.99	0.04	26,28,31,47	0
2	LYS	A	301	10/10	0.99	0.04	19,22,23,23	0
5	CL	G	304	1/1	1.00	0.04	31,31,31,31	0
4	FE2	E	303	1/1	1.00	0.02	28,28,28,28	0
4	FE2	F	303	1/1	1.00	0.01	29,29,29,29	0
4	FE2	G	303	1/1	1.00	0.01	30,30,30,30	0
4	FE2	H	303	1/1	1.00	0.02	29,29,29,29	0
4	FE2	A	303	1/1	1.00	0.01	25,25,25,25	0
5	CL	B	304	1/1	1.00	0.03	34,34,34,34	0
4	FE2	B	303	1/1	1.00	0.01	25,25,25,25	0
4	FE2	C	303	1/1	1.00	0.01	24,24,24,24	0
4	FE2	D	303	1/1	1.00	0.02	26,26,26,26	0
5	CL	F	304	1/1	1.00	0.09	41,41,41,41	0

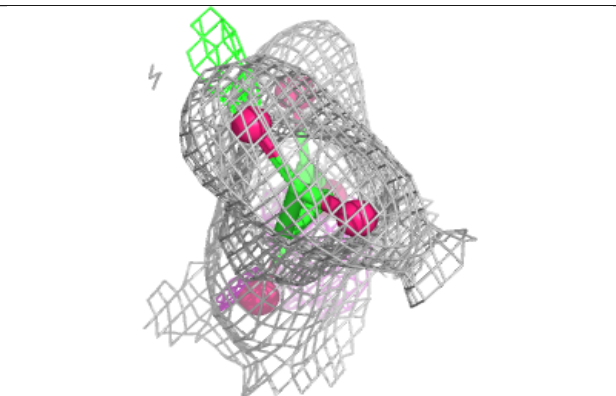
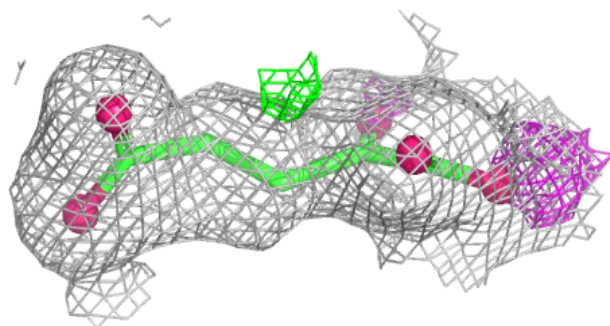
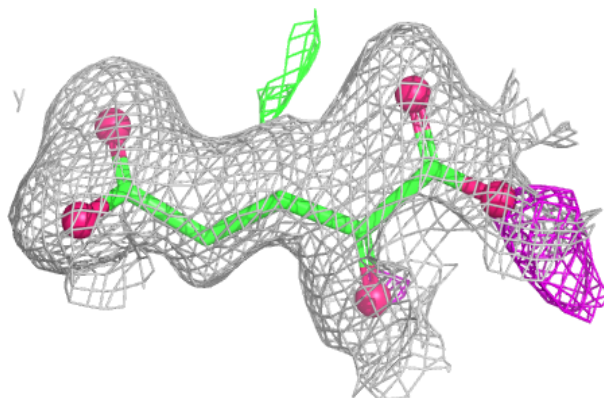
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around LYS H 301:**

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

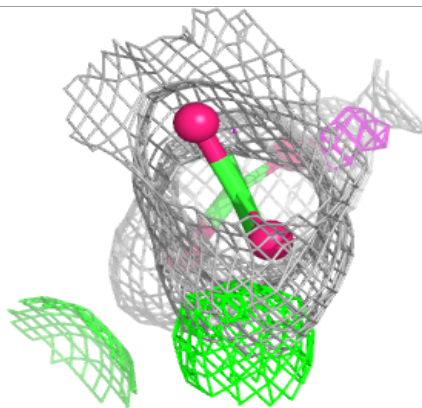
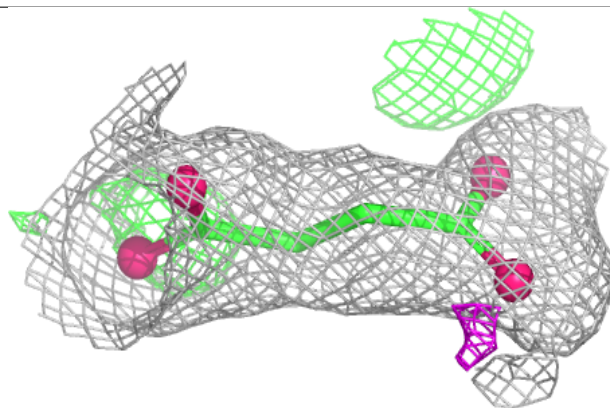
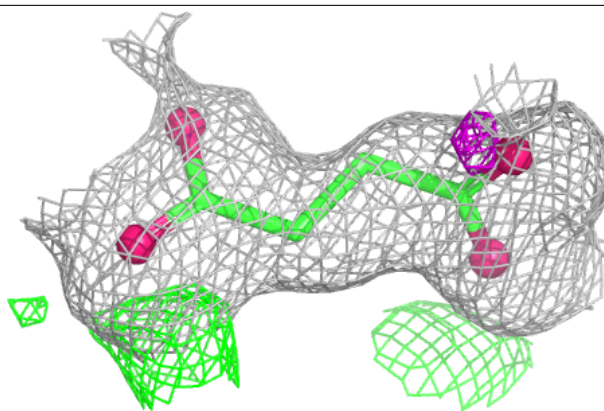
**Electron density around AKG D 302:**

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and green (positive)

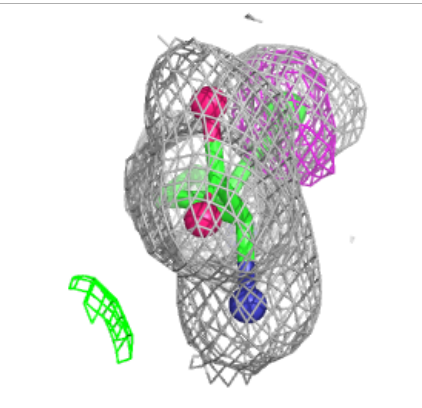
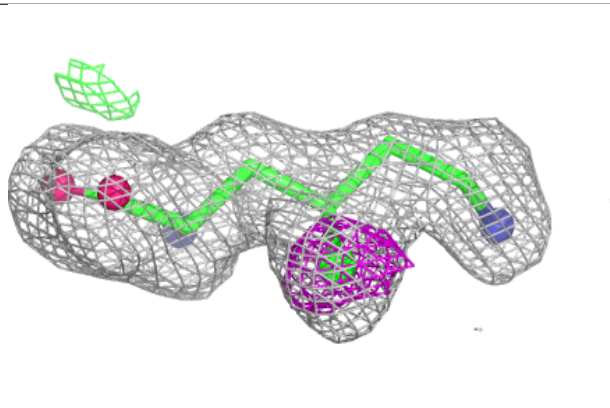
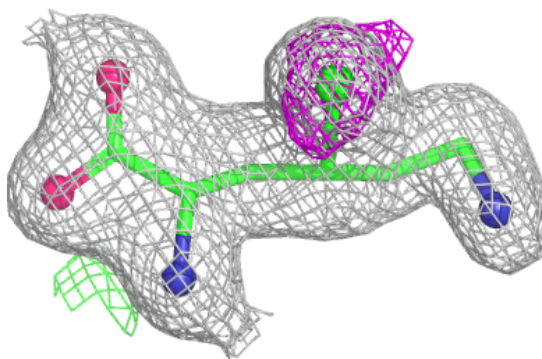


**Electron density around SIN F 302:**

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

**Electron density around YL0 C 301:**

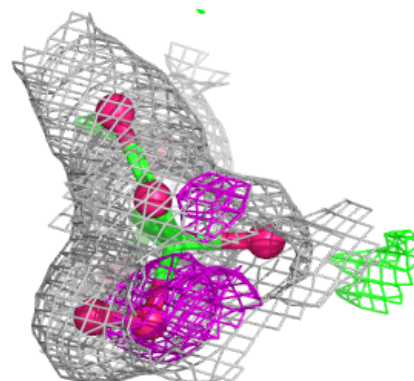
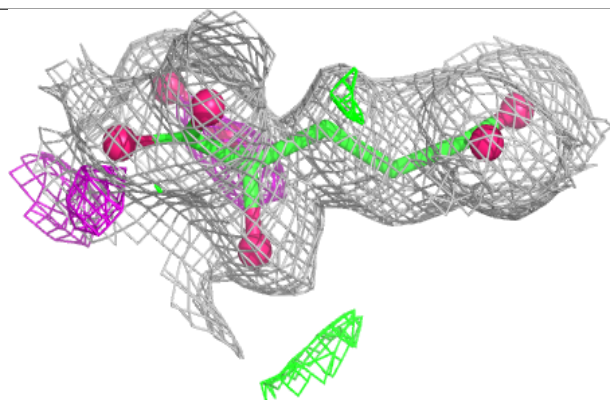
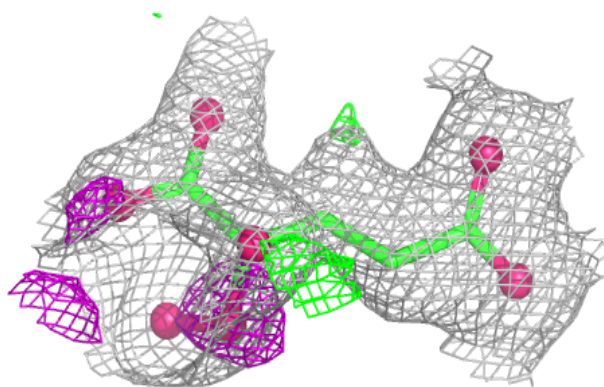
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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



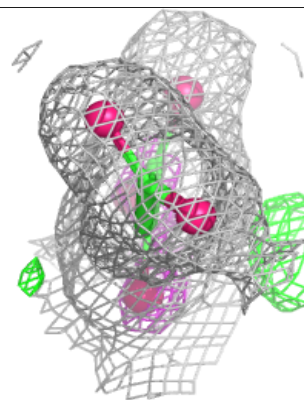
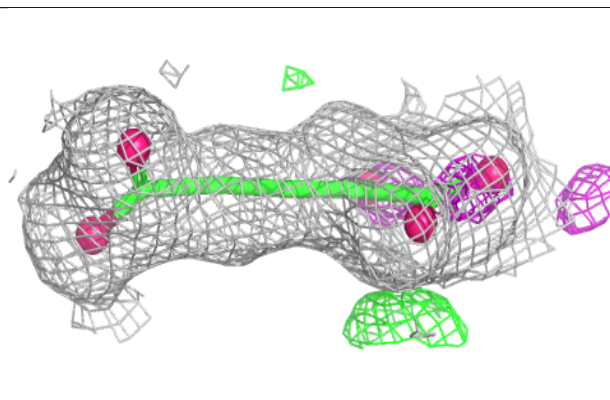
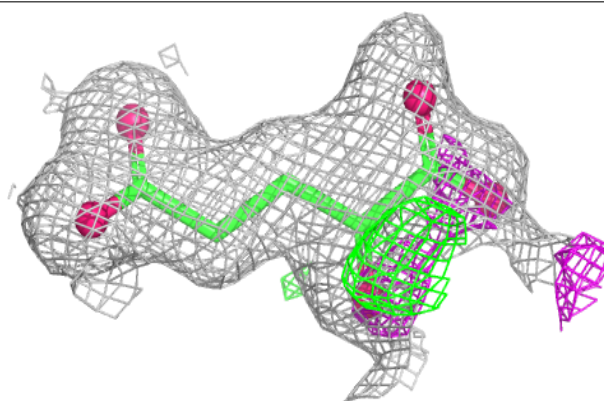


**Electron density around A1CA1 E 302:**

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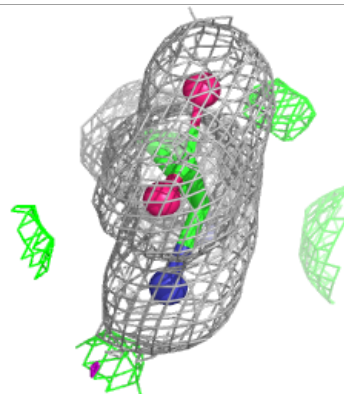
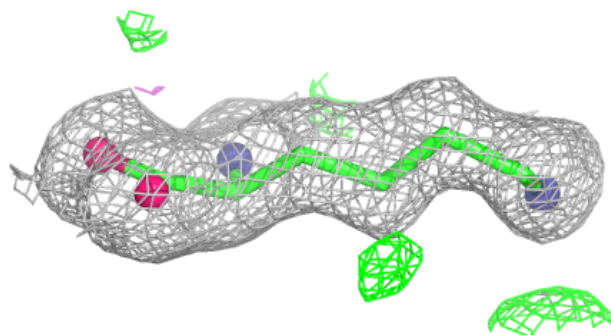
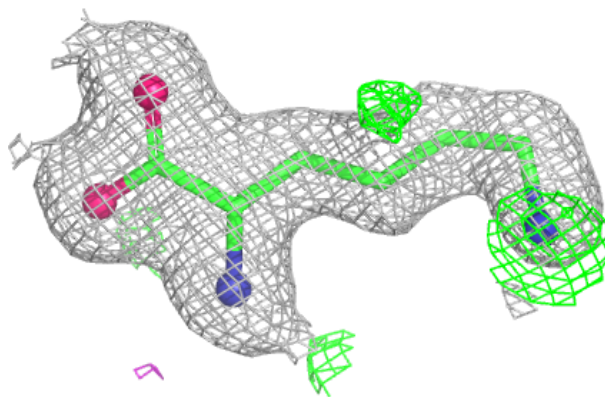
**Electron density around AKG A 302:**

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and green (positive)



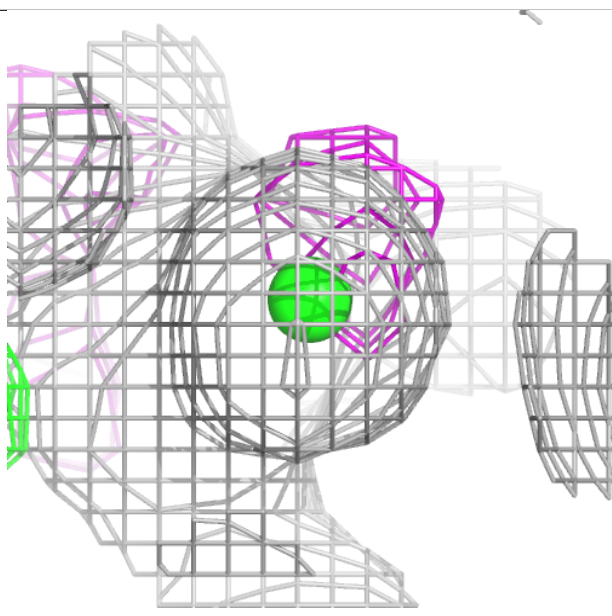
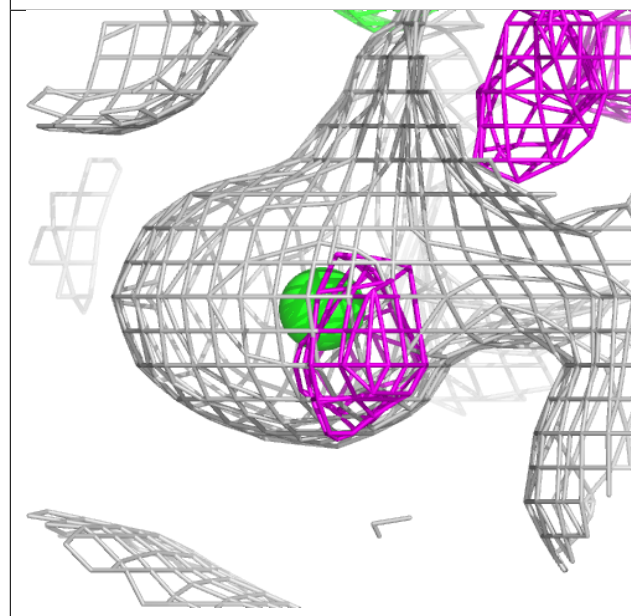
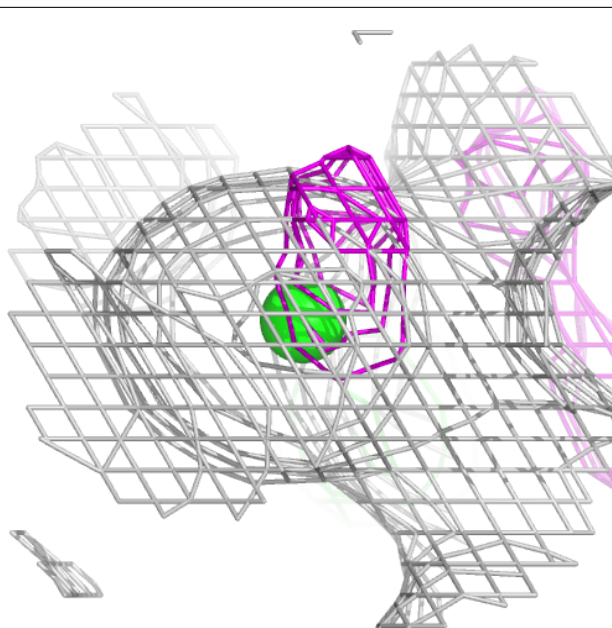
**Electron density around LYS B 301:**

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and green (positive)



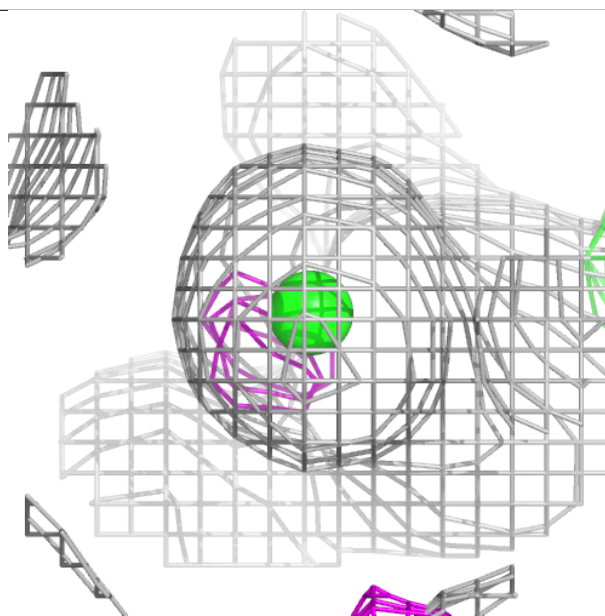
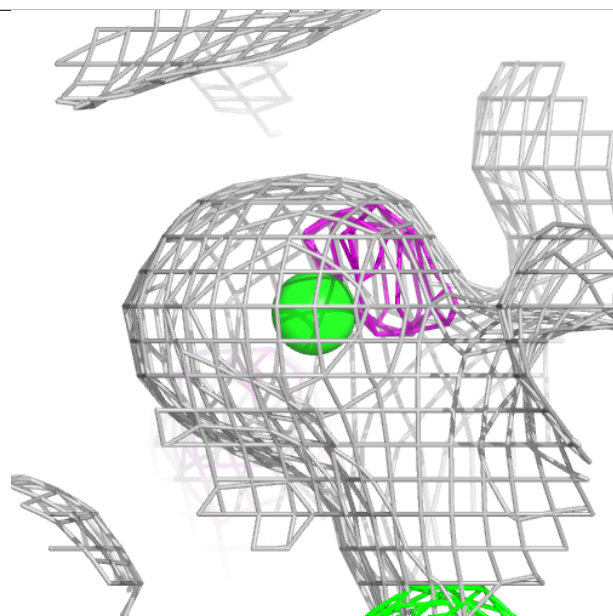
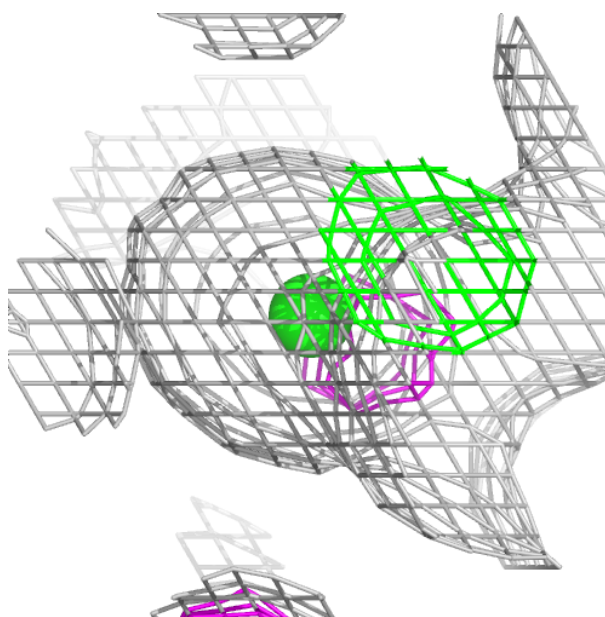
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and green (positive)



**Electron density around CL C 304:**

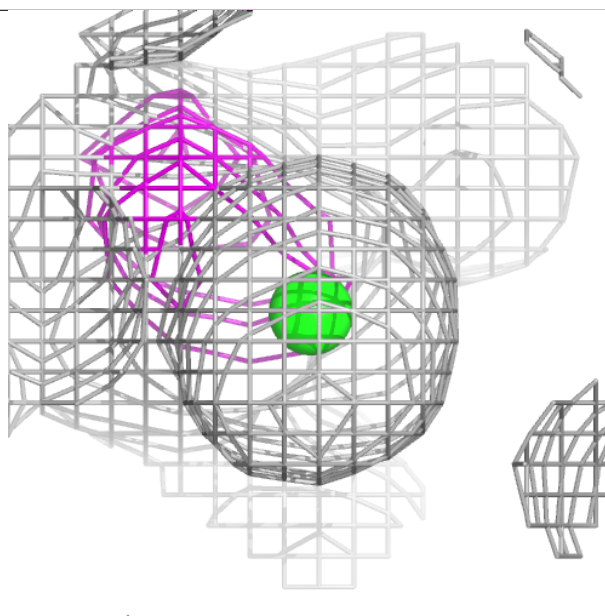
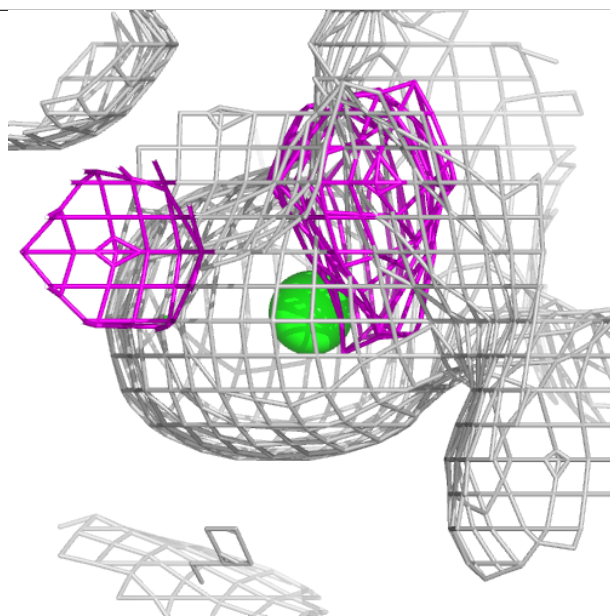
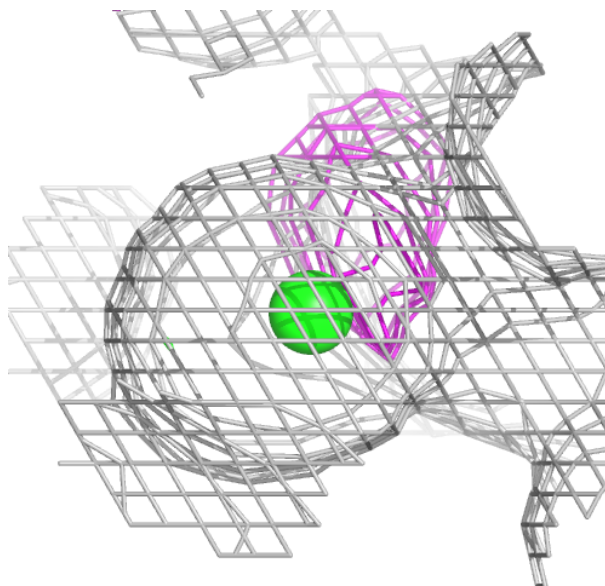
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





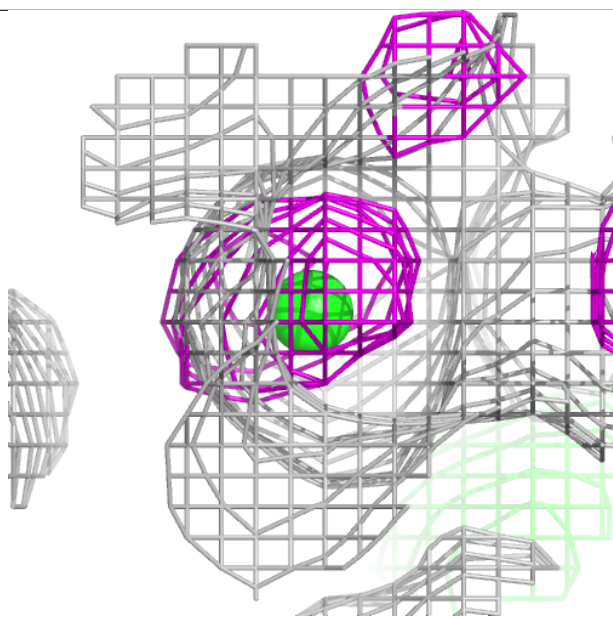
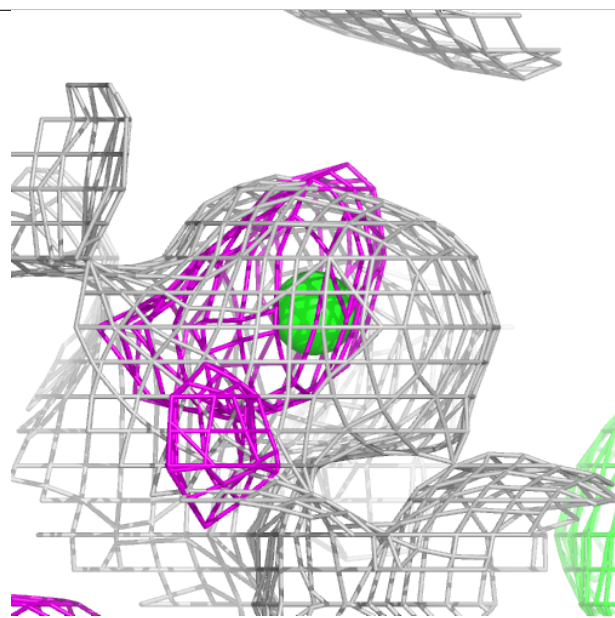
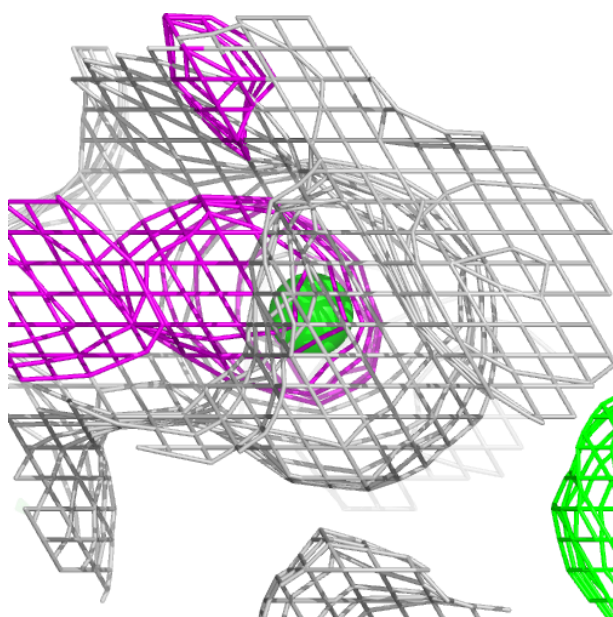
**Electron density around CL D 304:**

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



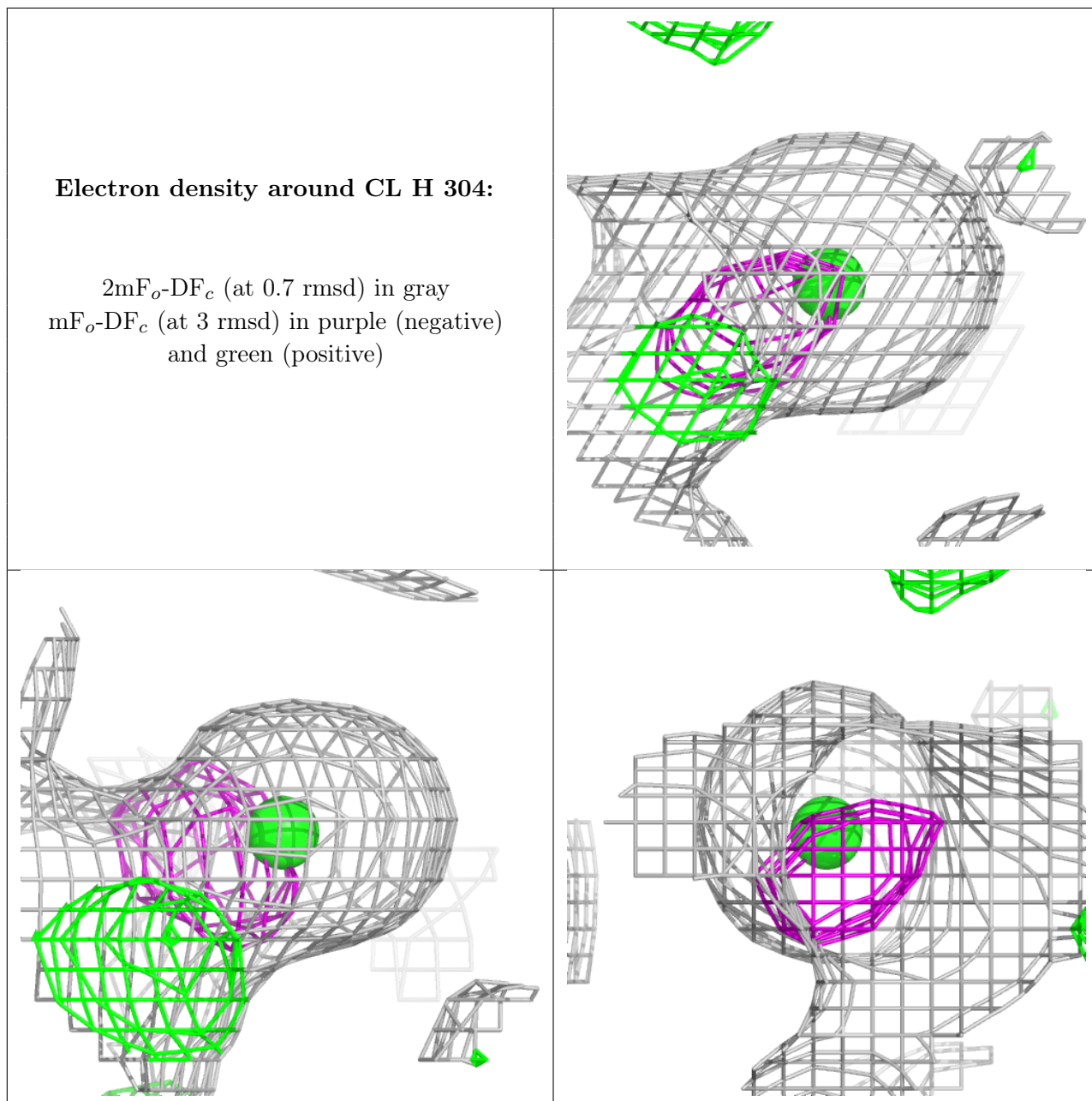
**Electron density around CL E 304:**

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



**Electron density around CL H 304:**

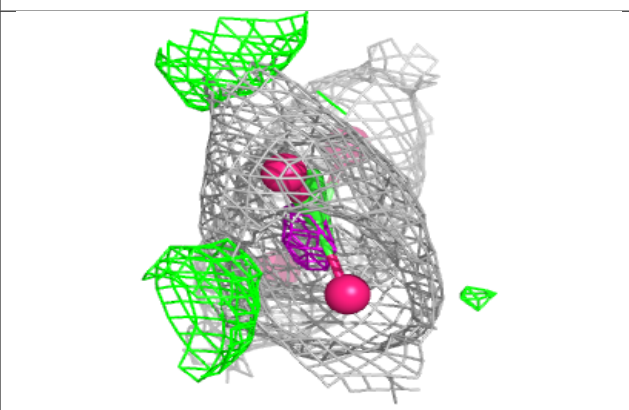
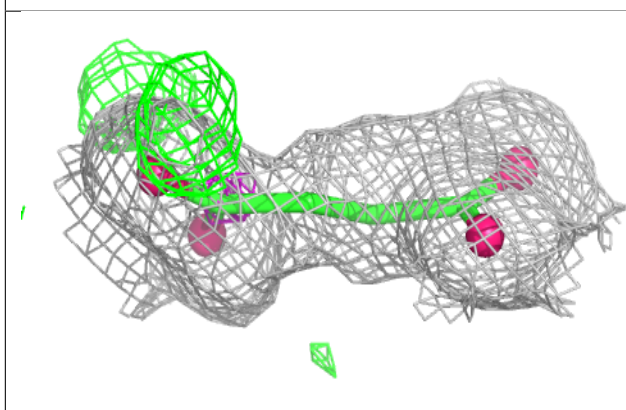
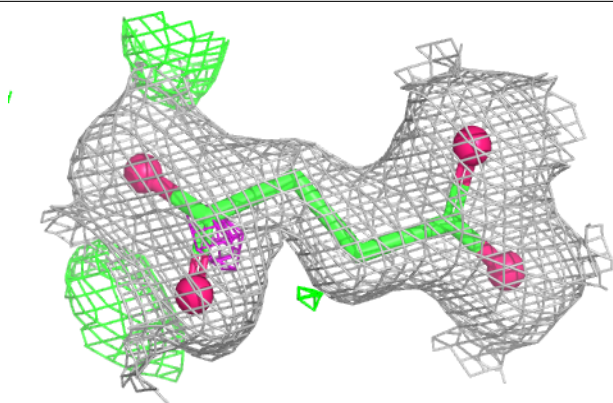
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



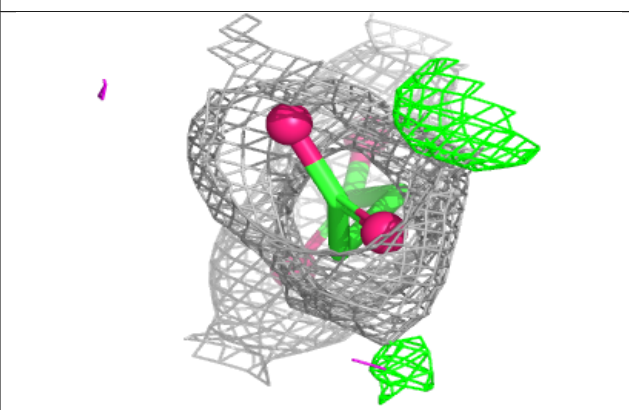
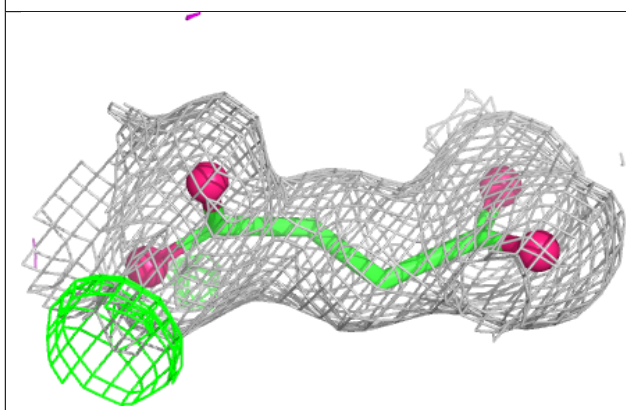
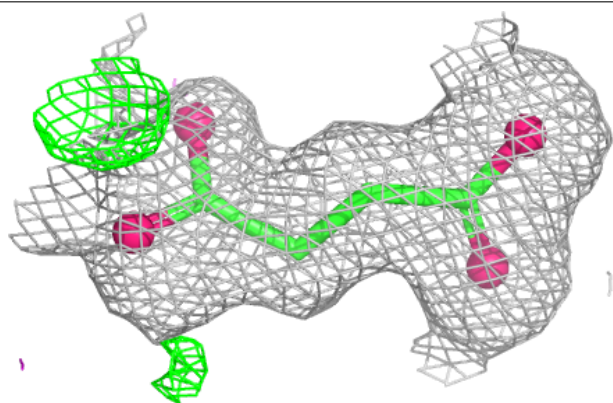


**Electron density around SIN B 302:**

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

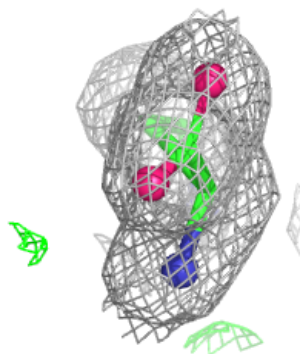
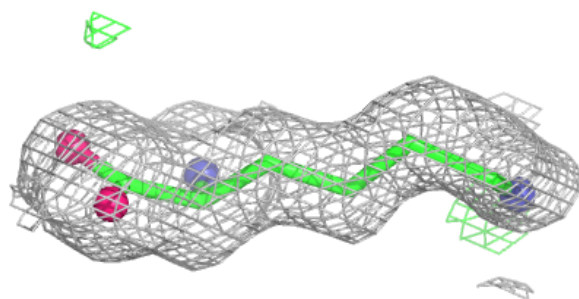
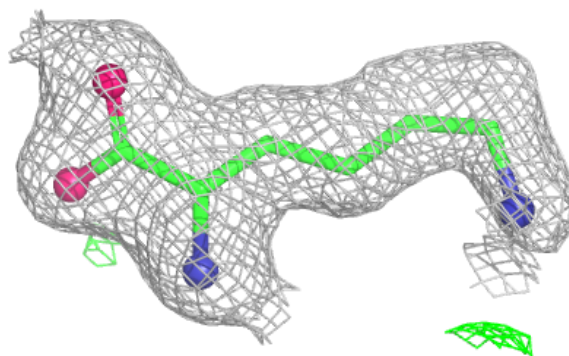
**Electron density around SIN C 302:**

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

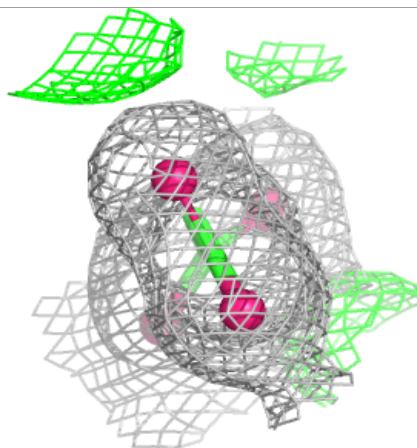
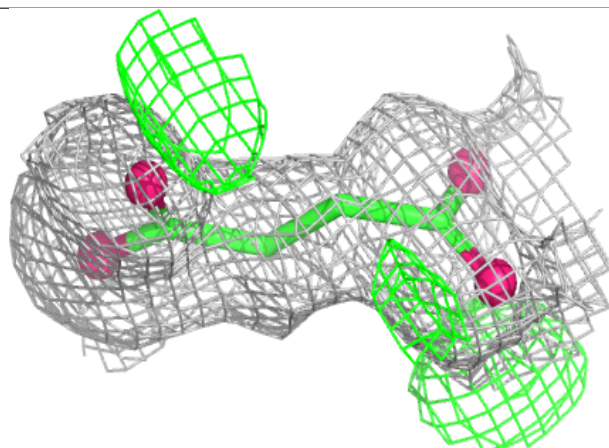
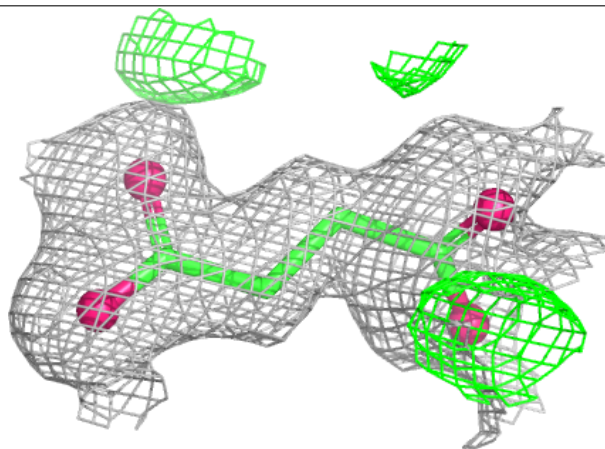


**Electron density around LYS E 301:**

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

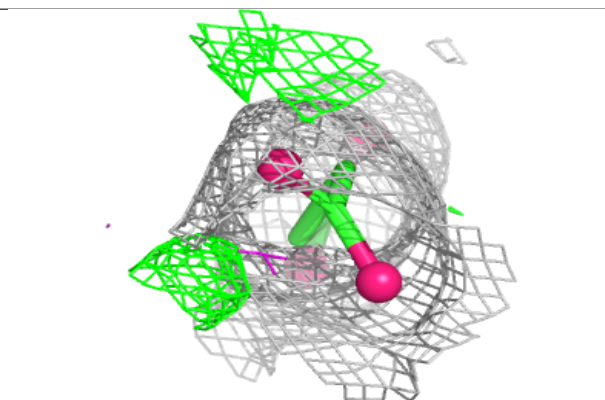
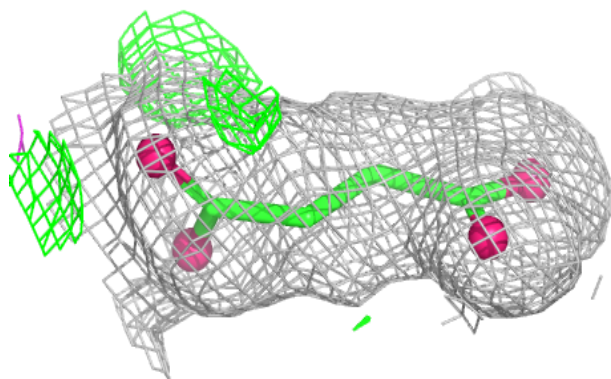
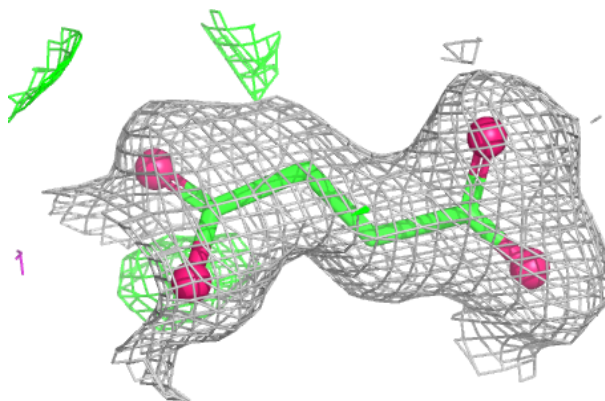
**Electron density around SIN G 302:**

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

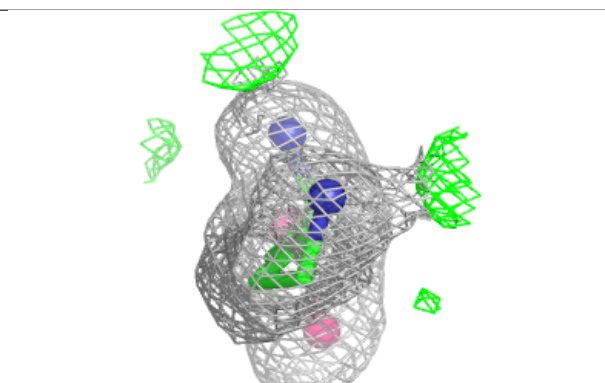
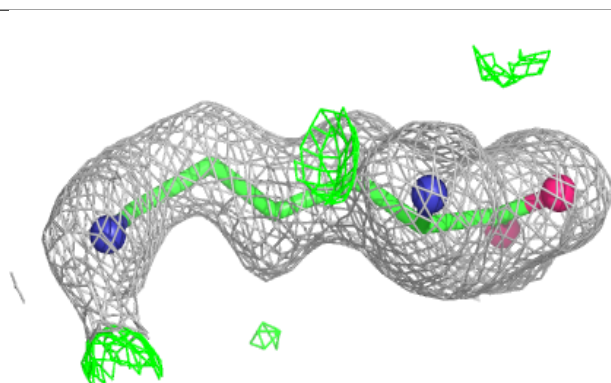
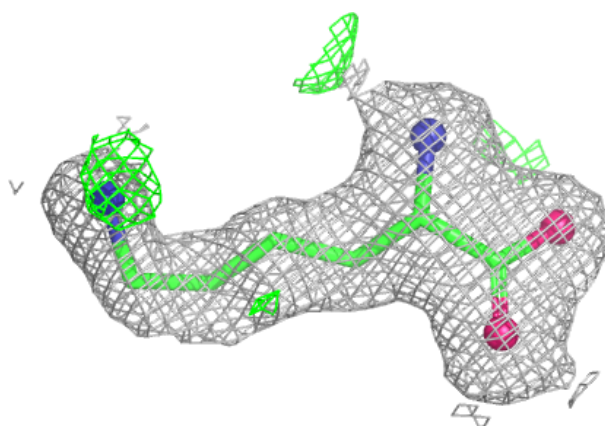


**Electron density around SIN H 302:**

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

**Electron density around LYS F 301:**

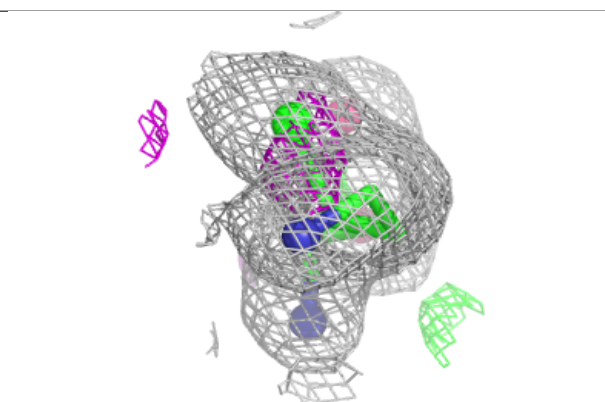
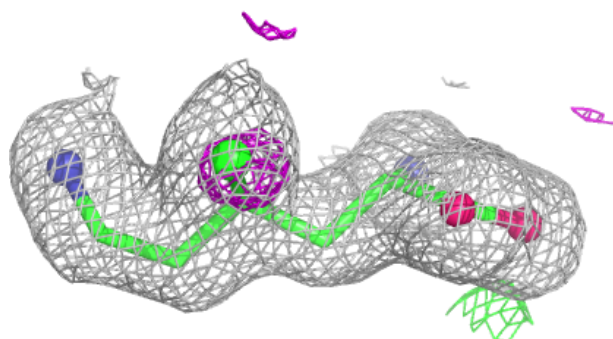
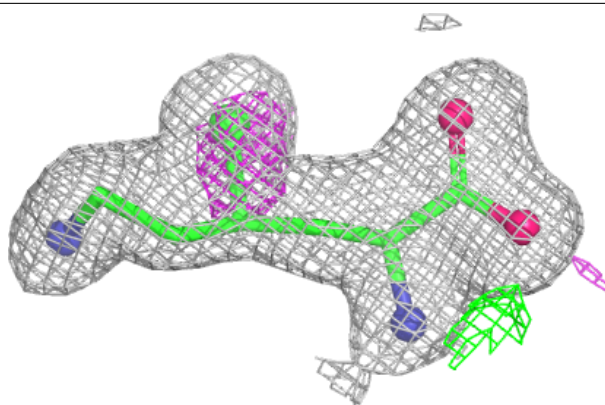
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



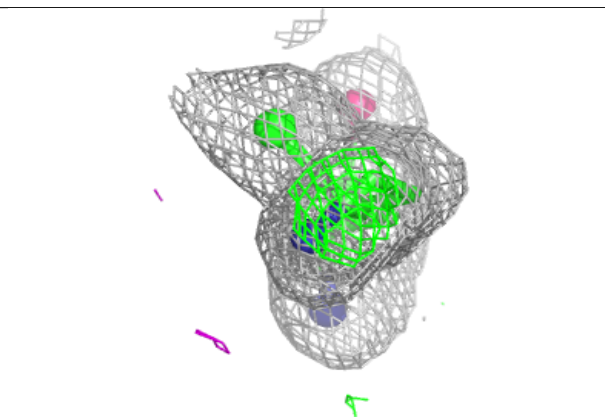
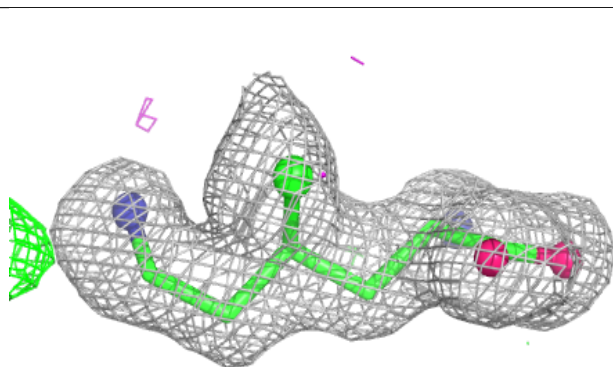
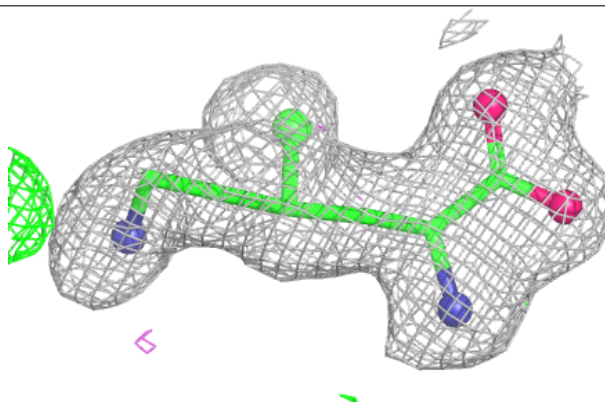


**Electron density around YL0 D 301:**

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

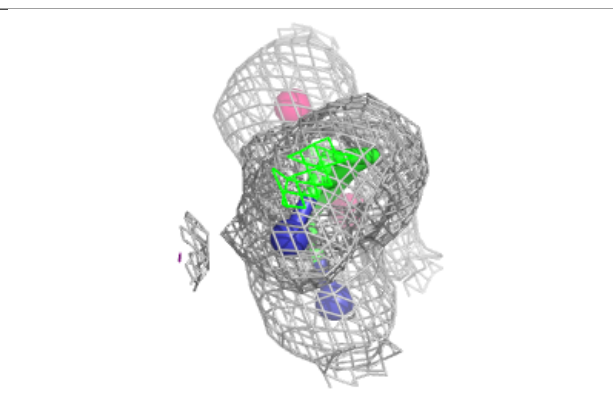
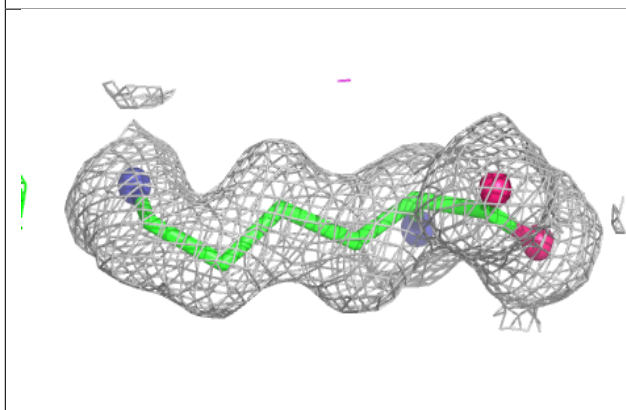
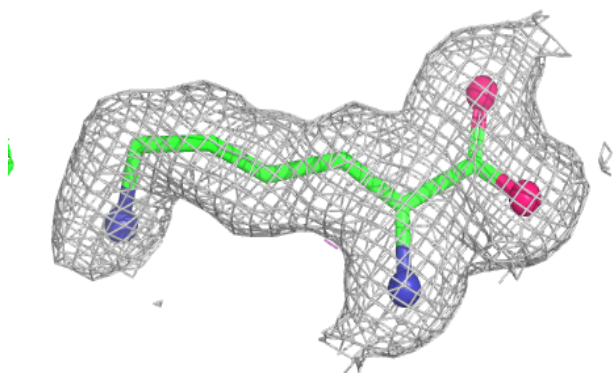
**Electron density around YL0 G 301:**

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



**Electron density around LYS A 301:**

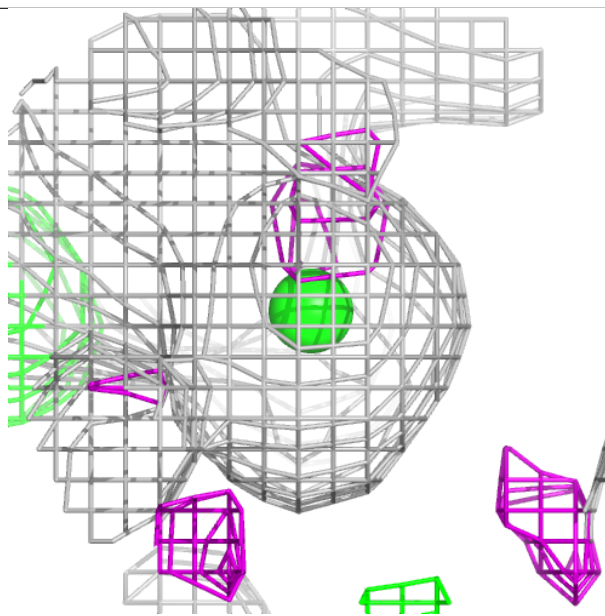
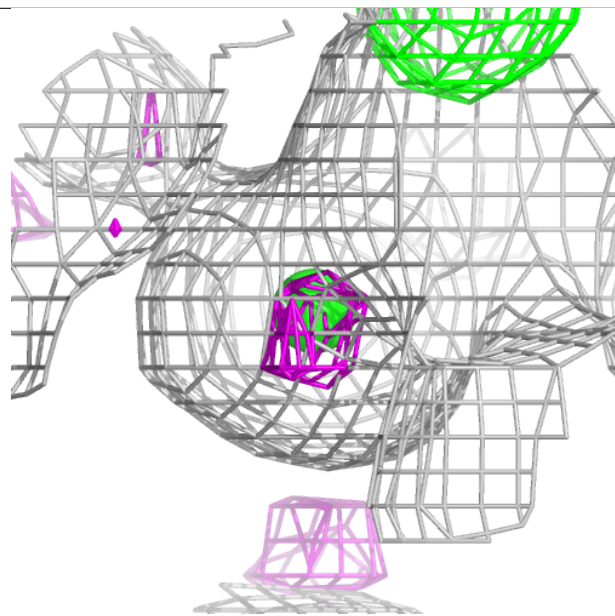
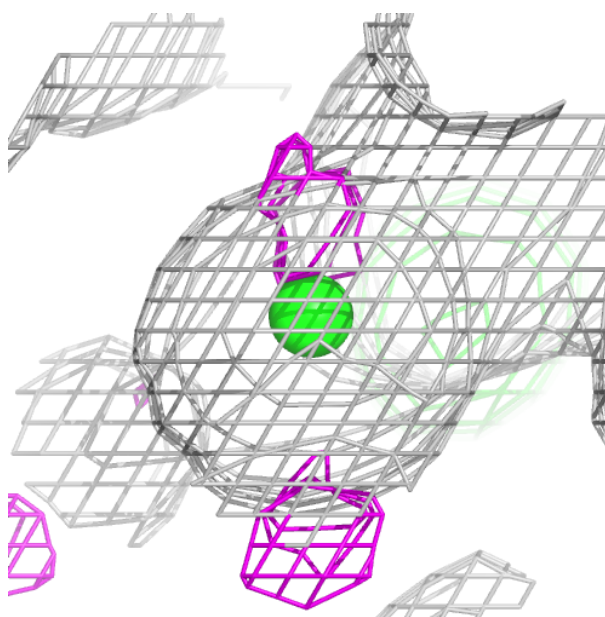
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





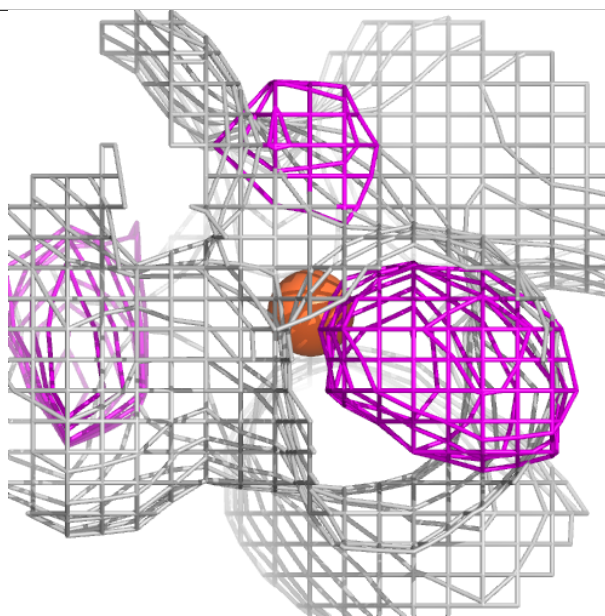
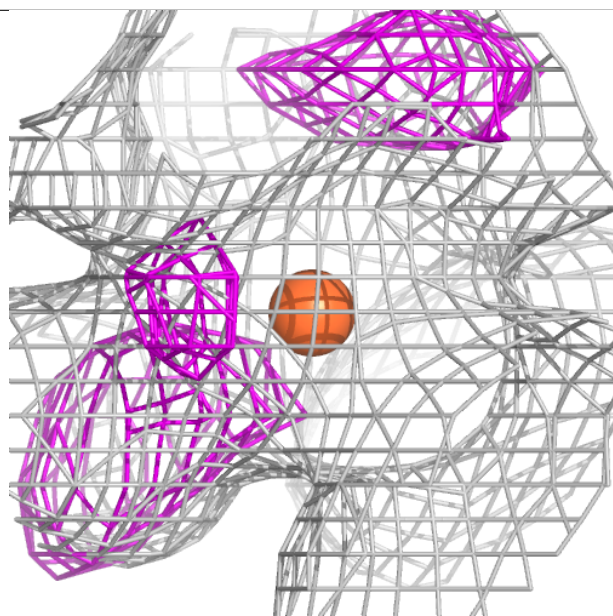
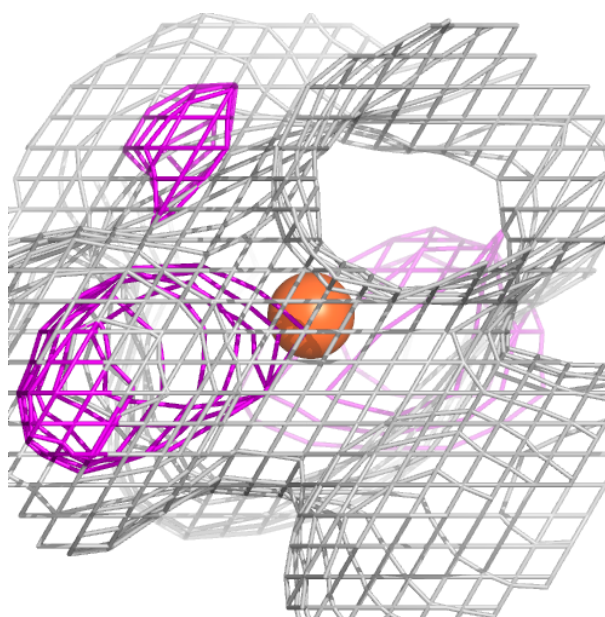
**Electron density around CL G 304:**

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



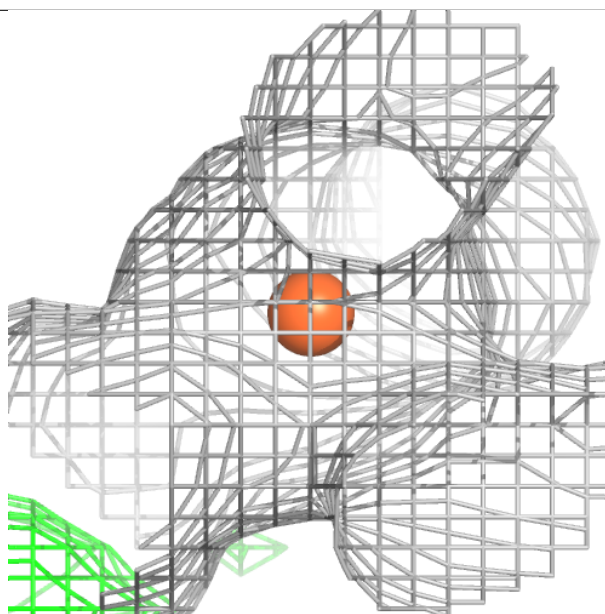
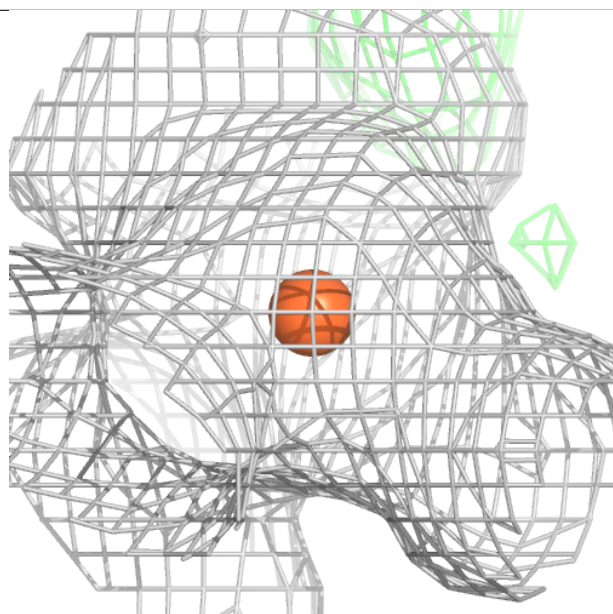
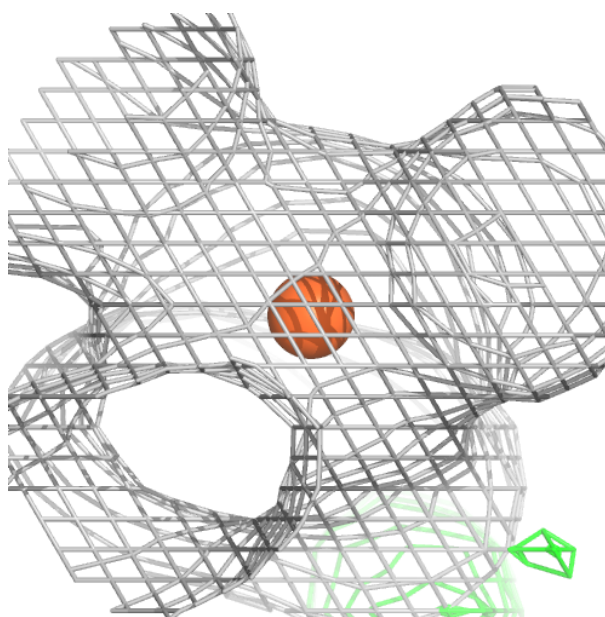
**Electron density around FE2 E 303:**

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



**Electron density around FE2 F 303:**

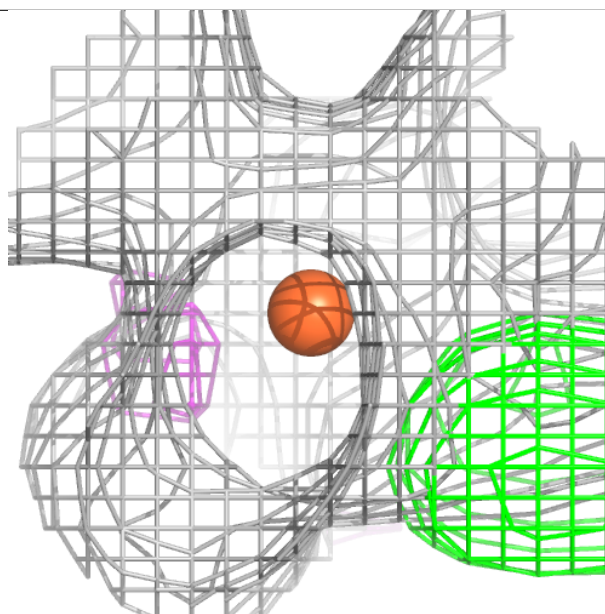
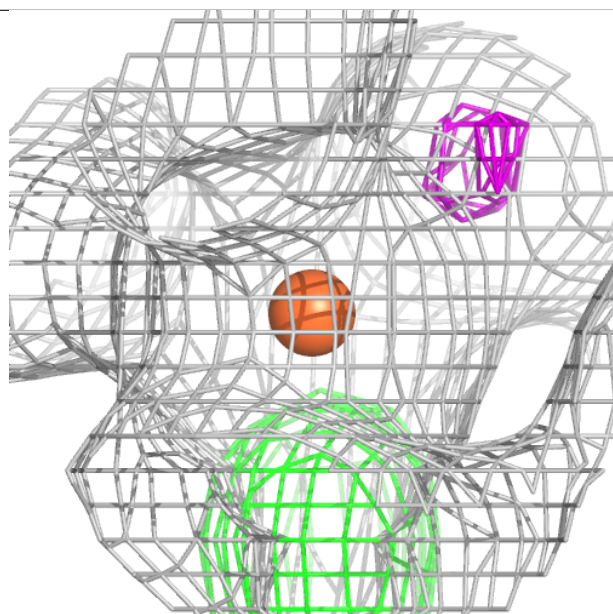
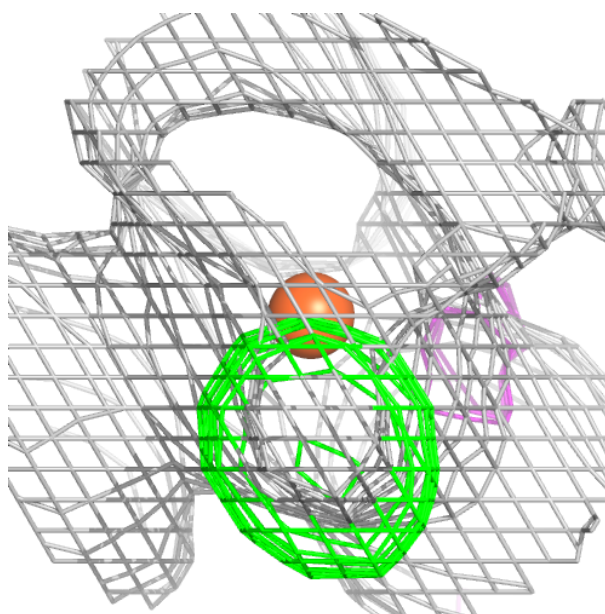
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





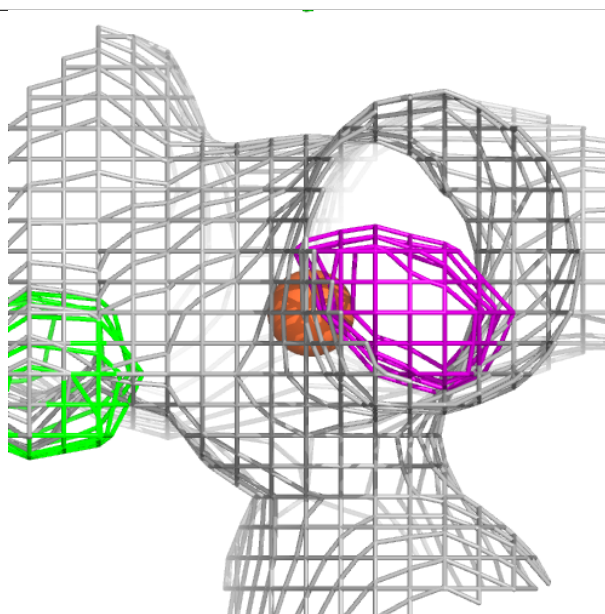
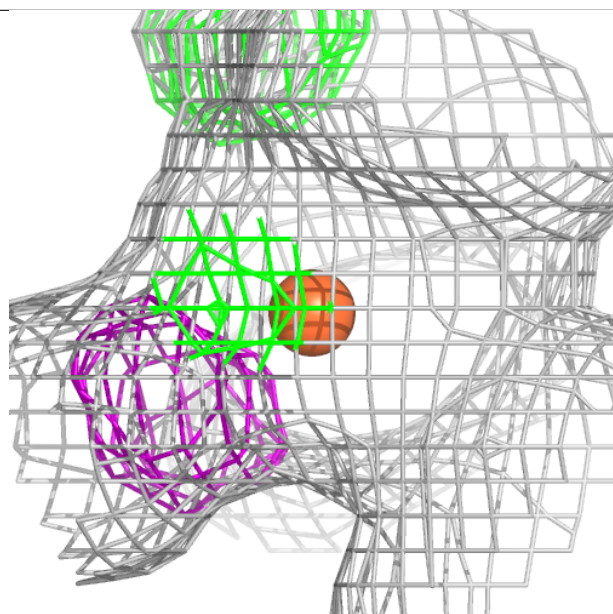
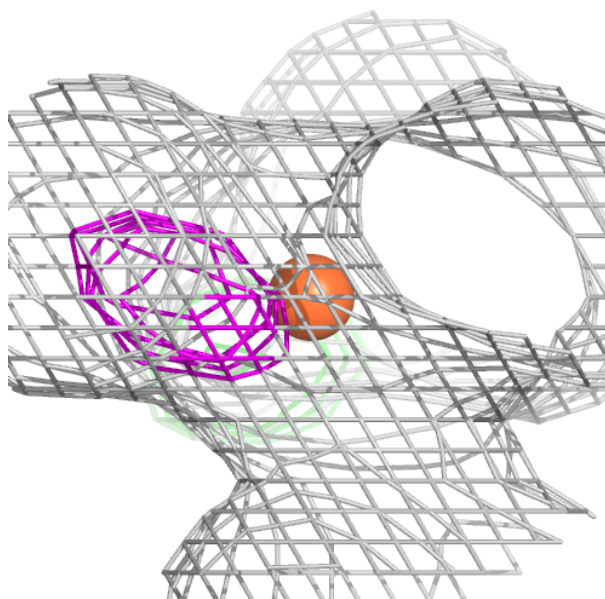
**Electron density around FE2 G 303:**

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



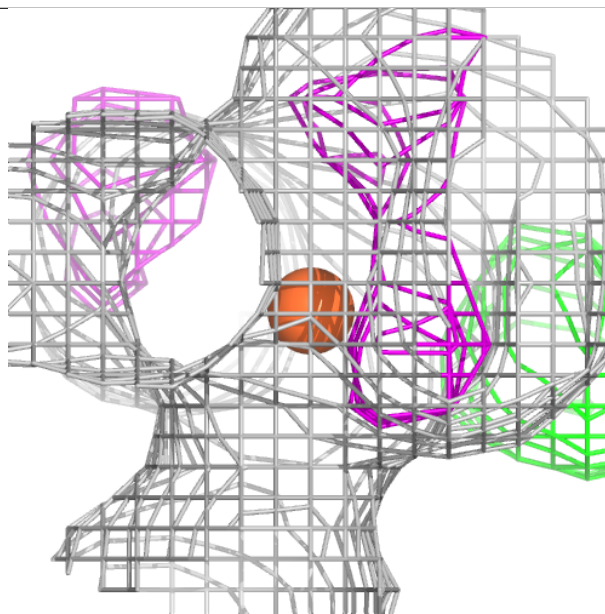
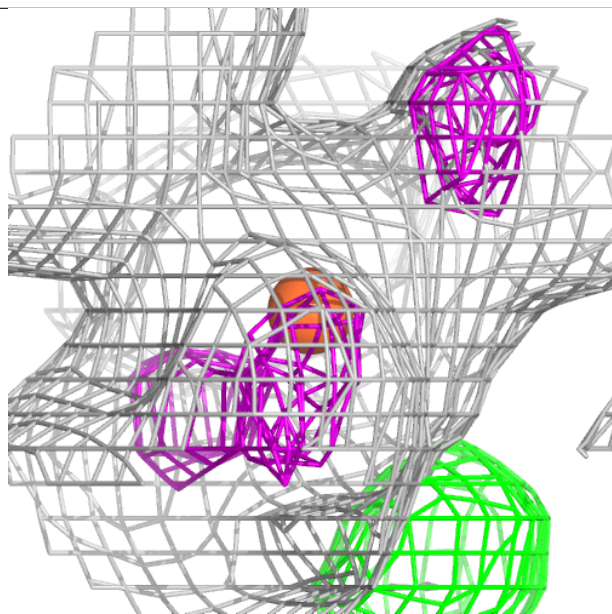
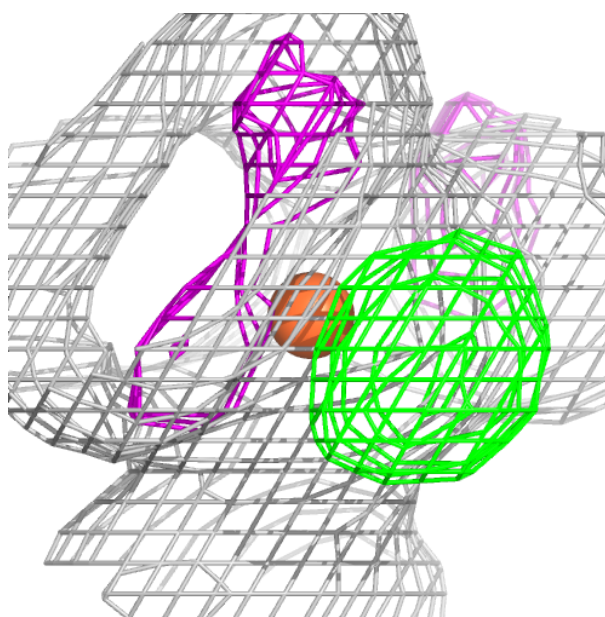
**Electron density around FE2 H 303:**

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



**Electron density around FE2 A 303:**

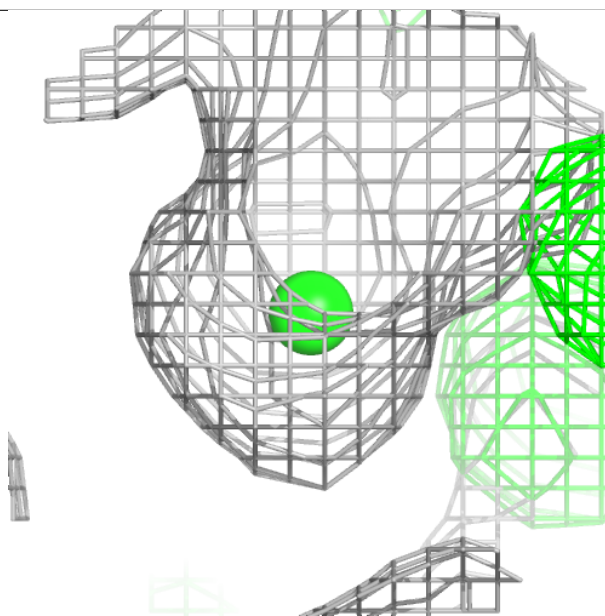
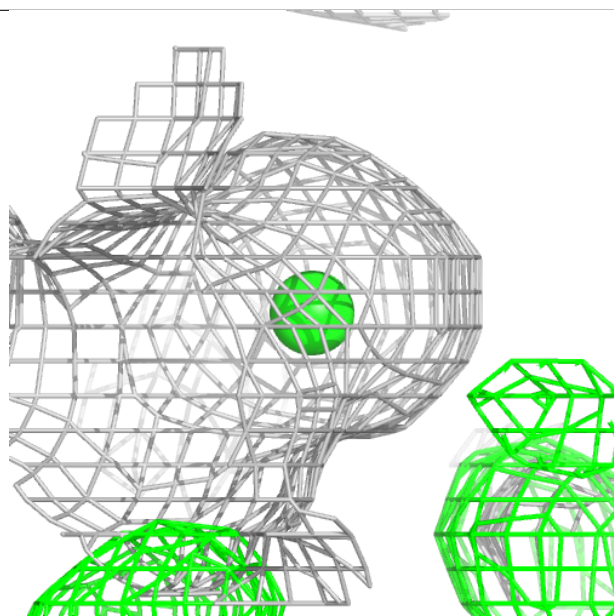
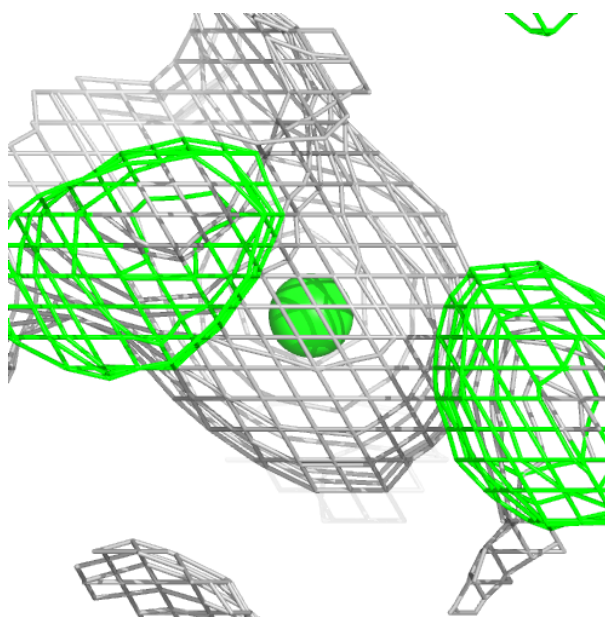
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





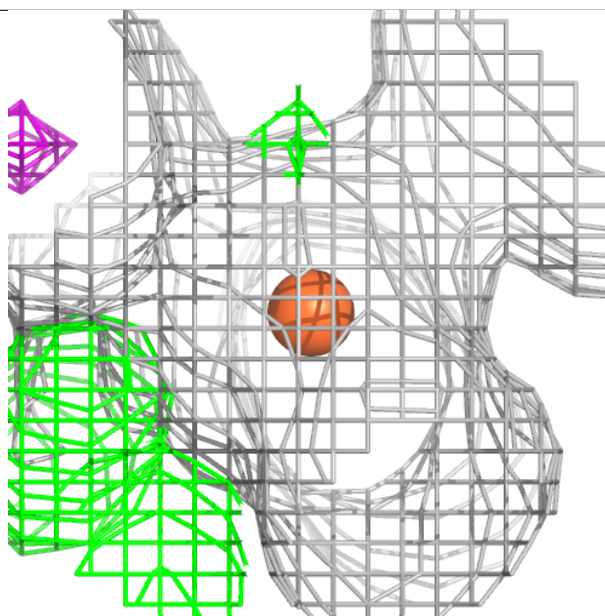
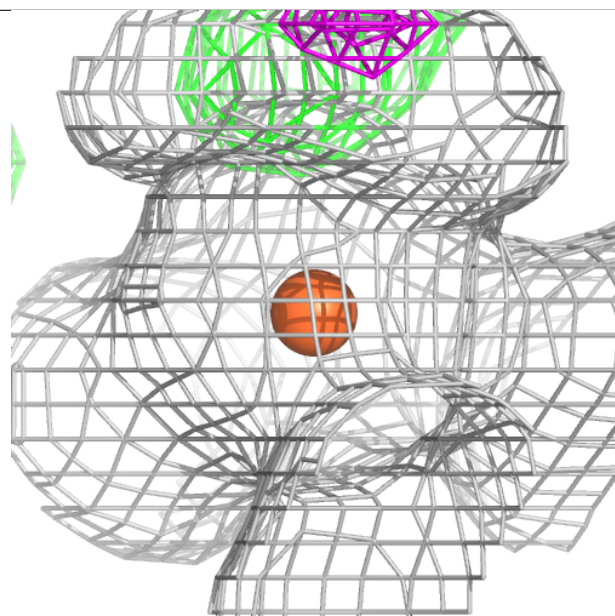
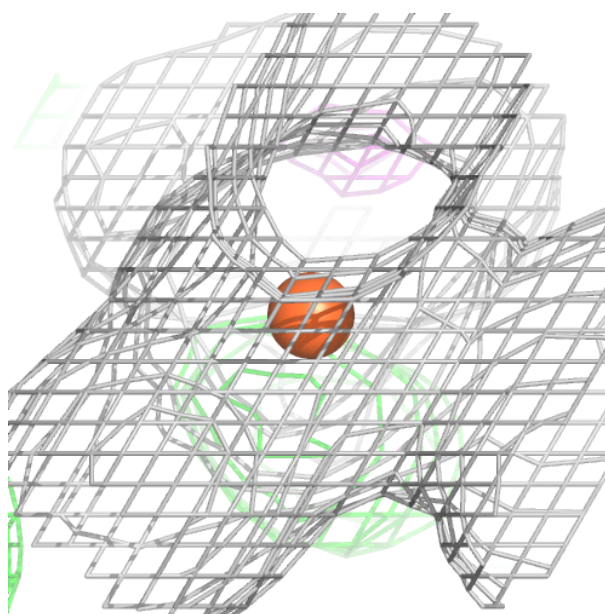
**Electron density around CL B 304:**

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



**Electron density around FE2 B 303:**

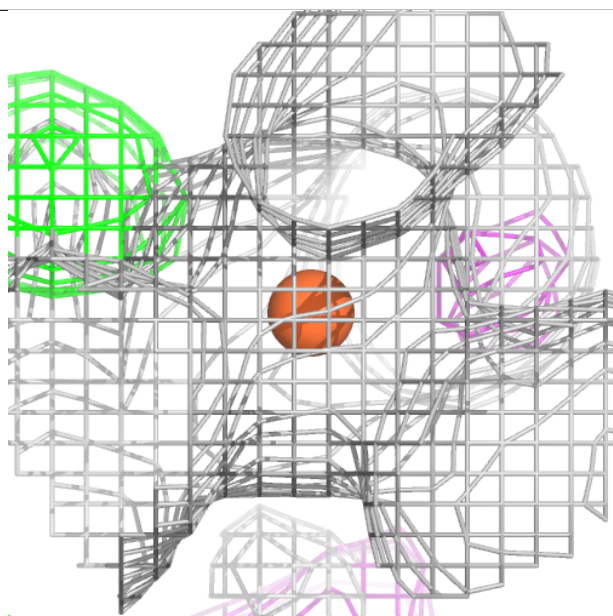
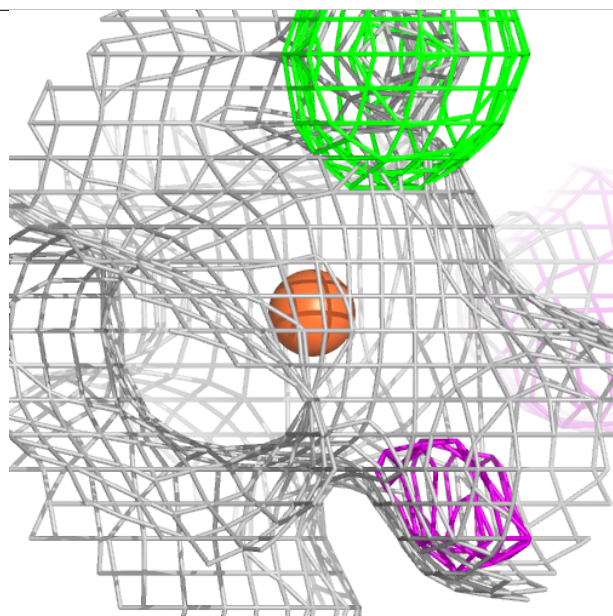
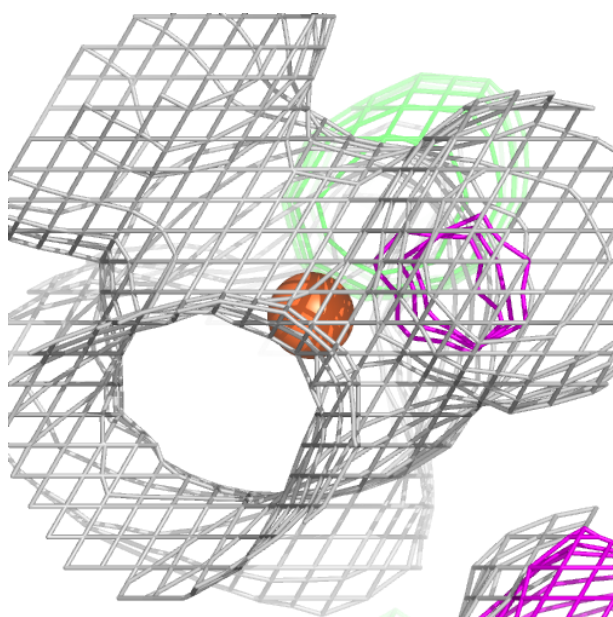
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





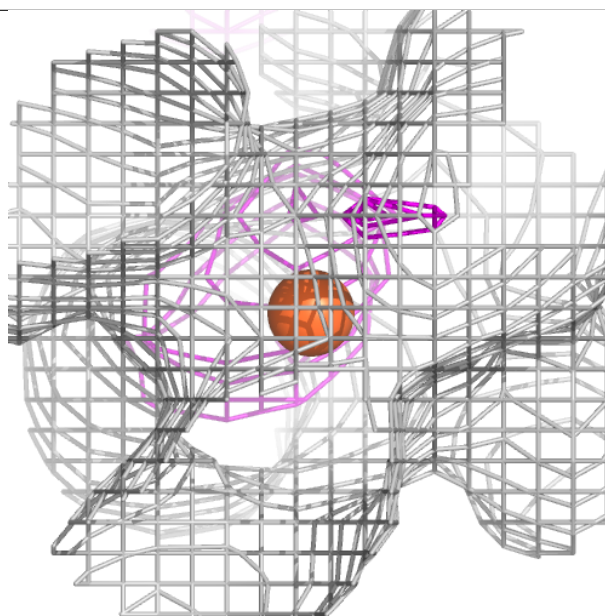
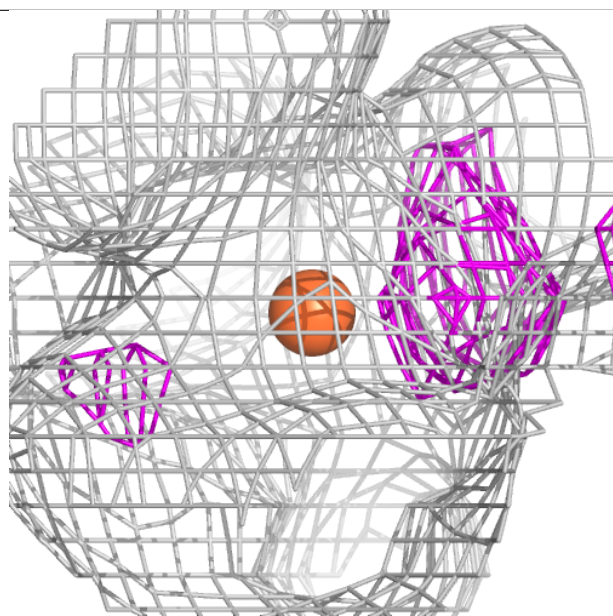
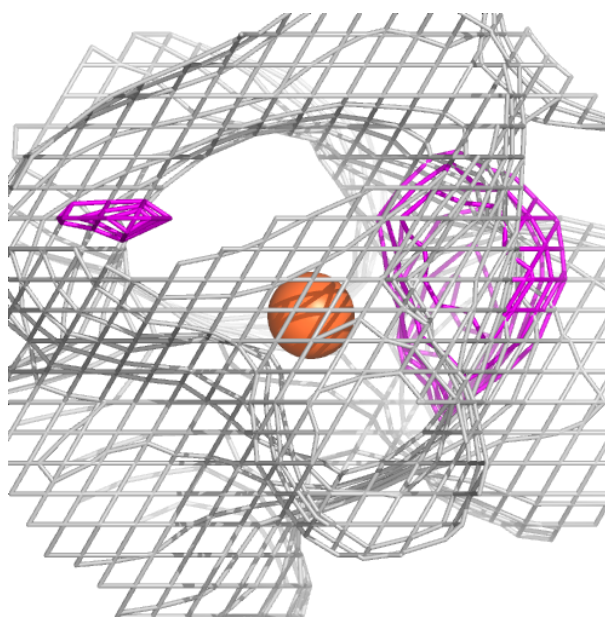
**Electron density around FE2 C 303:**

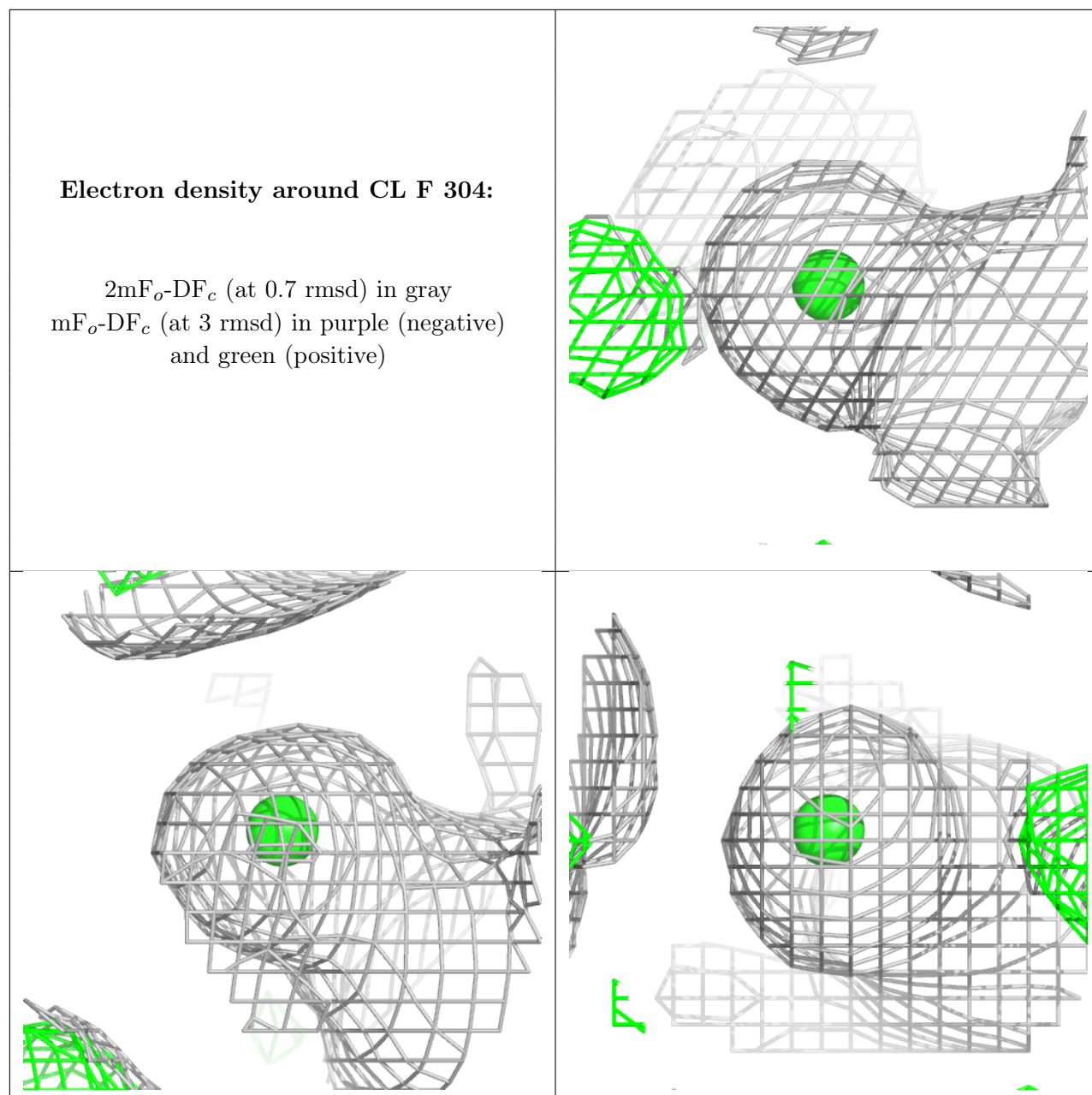
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FE2 D 303:**

$2mF_o-DF_c$  (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.