



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2021 – 12:13 PM EST

PDB ID : 7L2C  
Title : Crystallographic structure of neutralizing antibody 2-51 in complex with SARS-CoV-2 spike N-terminal domain (NTD)  
Authors : Cerutti, G.; Reddem, E.R.; Shapiro, L.  
Deposited on : 2020-12-16  
Resolution : 3.65 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.16

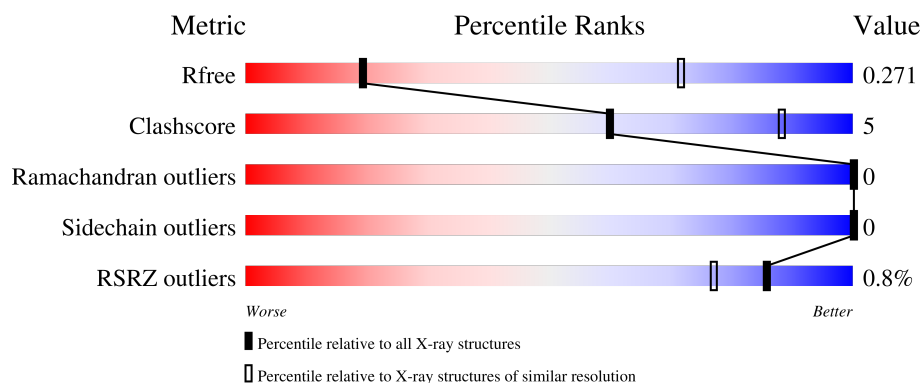
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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.




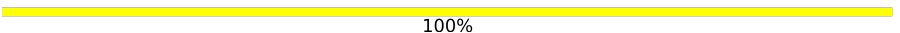
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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	342	<div> <div></div> <div>71% 11% 16%</div> </div>
1	B	342	<div> <div></div> <div>68% 11% 20%</div> </div>
2	C	227	<div> <div></div> <div>85% 13%</div> </div>
2	H	227	<div> <div></div> <div>86% 11%</div> </div>
3	D	215	<div> <div></div> <div>85% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	215	 90% 9%
4	E	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	405	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11381 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2301	1487	380	426	8			
1	B	273	Total	C	N	O	S	0	1	0
			2210	1433	363	406	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	GLY	-	expression tag	UNP P0DTC2
A	336	SER	-	expression tag	UNP P0DTC2
A	337	LEU	-	expression tag	UNP P0DTC2
A	338	GLU	-	expression tag	UNP P0DTC2
A	339	VAL	-	expression tag	UNP P0DTC2
A	340	LEU	-	expression tag	UNP P0DTC2
A	341	PHE	-	expression tag	UNP P0DTC2
A	342	GLN	-	expression tag	UNP P0DTC2
B	335	GLY	-	expression tag	UNP P0DTC2
B	336	SER	-	expression tag	UNP P0DTC2
B	337	LEU	-	expression tag	UNP P0DTC2
B	338	GLU	-	expression tag	UNP P0DTC2
B	339	VAL	-	expression tag	UNP P0DTC2
B	340	LEU	-	expression tag	UNP P0DTC2
B	341	PHE	-	expression tag	UNP P0DTC2
B	342	GLN	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called 2-51 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	2	0
			1687	1071	272	336	8			
2	C	222	Total	C	N	O	S	0	2	0
			1696	1078	274	336	8			

- Molecule 3 is a protein called 2-51 light chain.

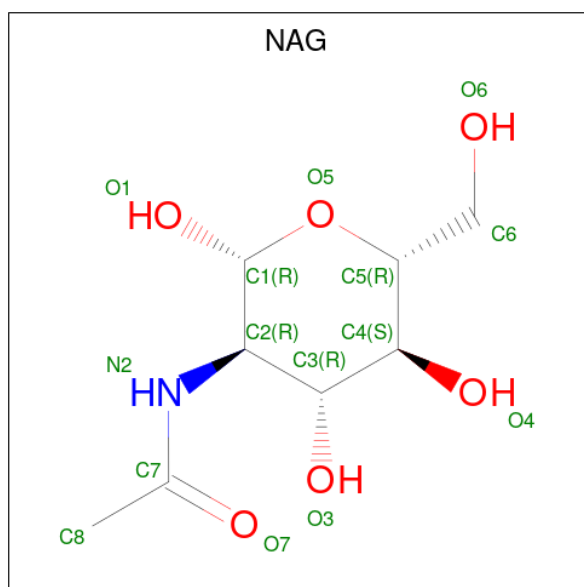
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1573	979	263	325	6			
3	D	213	Total	C	N	O	S	0	0	0
			1573	979	263	325	6			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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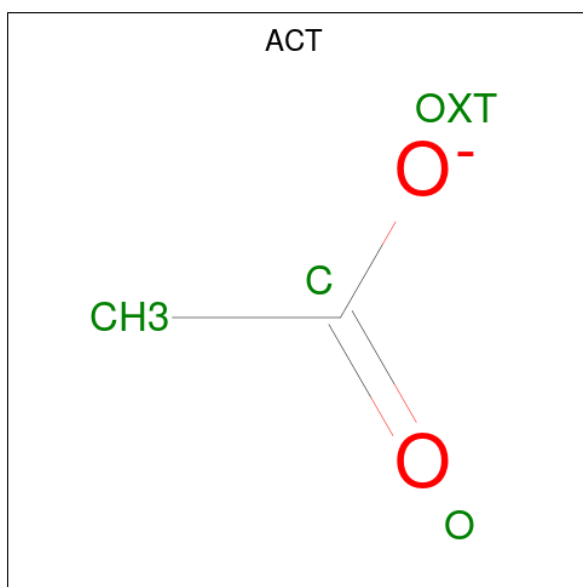
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
	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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

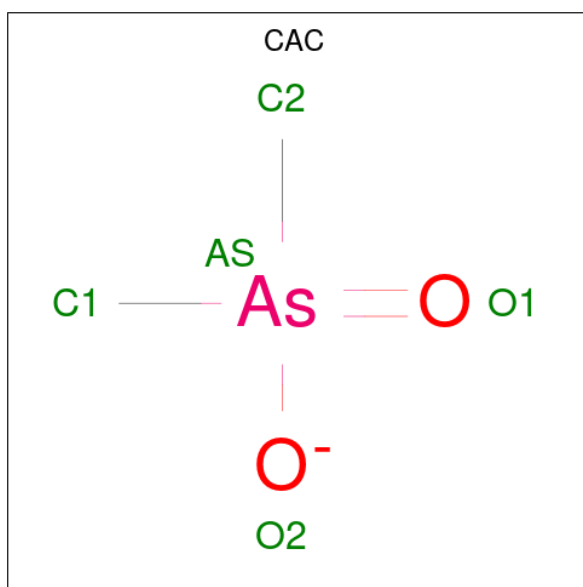
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	6	Total	Ca	0	0
			6	6		
6	H	7	Total	Ca	0	0
			7	7		
6	B	6	Total	Ca	0	0
			6	6		
6	C	11	Total	Ca	0	0
			11	11		
6	A	6	Total	Ca	0	0
			6	6		
6	L	3	Total	Ca	0	0
			3	3		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



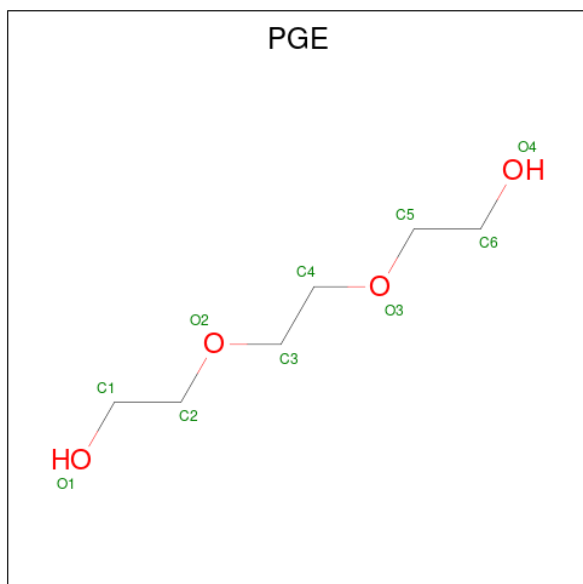
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	L	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

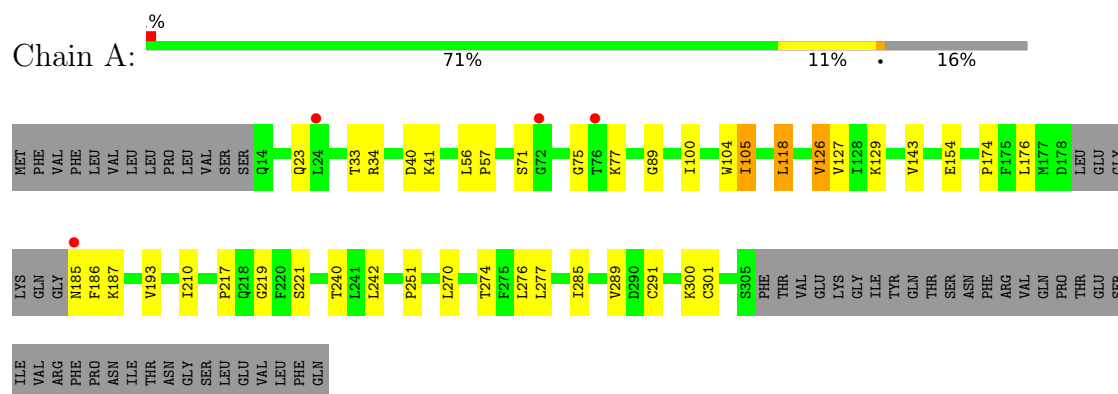


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	8	Total 8	O 8	0	0
10	B	9	Total 9	O 9	0	0
10	H	5	Total 5	O 5	0	0
10	L	4	Total 4	O 4	0	0
10	C	7	Total 7	O 7	0	0
10	D	8	Total 8	O 8	0	0

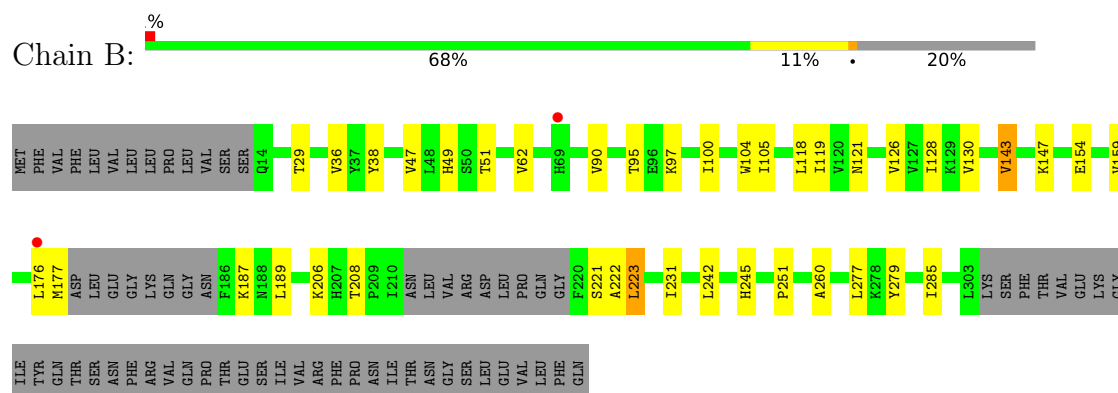
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

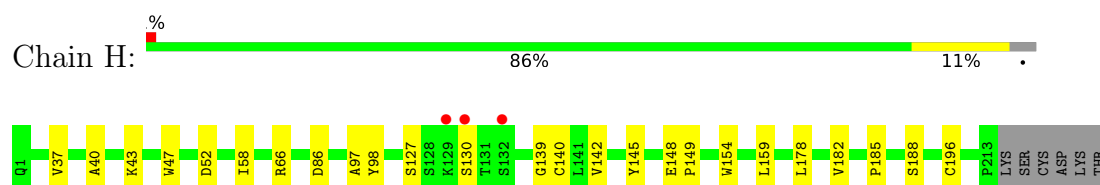
#### • Molecule 1: Spike glycoprotein



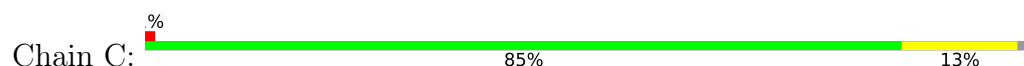
#### • Molecule 1: Spike glycoprotein

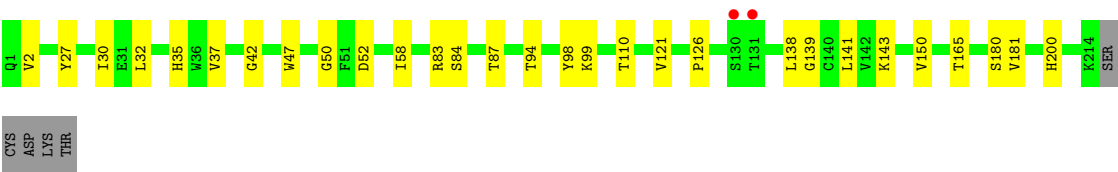


#### • Molecule 2: 2-51 heavy chain

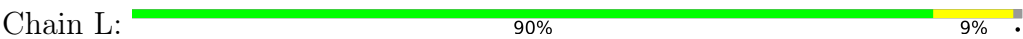


#### • Molecule 2: 2-51 heavy chain

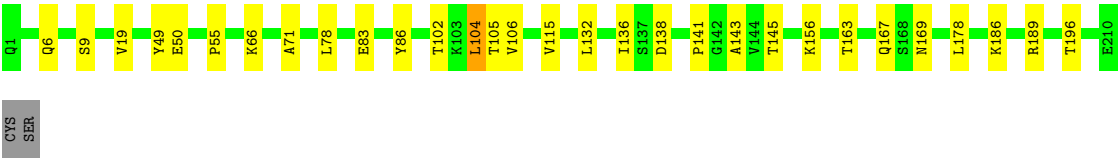
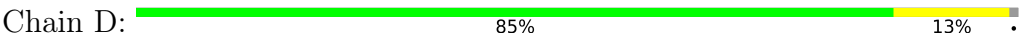




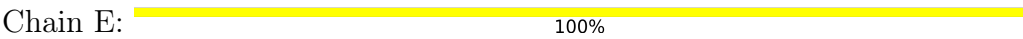
• Molecule 3: 2-51 light chain



• Molecule 3: 2-51 light chain



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.79Å 115.78Å 137.61Å 90.00° 99.97° 90.00°	Depositor
Resolution (Å)	88.03 – 3.65 88.03 – 3.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (88.03-3.65) 98.3 (88.03-3.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.67Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.216 , 0.272 0.216 , 0.271	Depositor DCC
$R_{free}$ test set	1128 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.4	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 79.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11381	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: CAC, CA, PGE, NAG, ACT

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	0.37	0/2366	0.77	6/3222 (0.2%)
1	B	0.52	4/2274 (0.2%)	0.78	6/3096 (0.2%)
2	C	0.35	0/1740	0.66	0/2372
2	H	0.45	2/1731 (0.1%)	0.74	2/2362 (0.1%)
3	D	0.40	1/1612 (0.1%)	0.65	1/2197 (0.0%)
3	L	0.39	0/1612	0.63	0/2197
All	All	0.42	7/11335 (0.1%)	0.71	15/15446 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	VAL	CB-CG2	-9.35	1.33	1.52
1	B	143	VAL	CB-CG2	-8.51	1.34	1.52
2	H	196	CYS	CB-SG	-6.37	1.71	1.82
1	B	143	VAL	CB-CG1	-6.35	1.39	1.52
1	B	159	VAL	CB-CG1	-6.32	1.39	1.52
2	H	140	CYS	CB-SG	-6.24	1.71	1.82
3	D	104	LEU	CG-CD2	-5.84	1.30	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ILE	CG1-CB-CG2	-8.40	92.92	111.40
1	B	223	LEU	CB-CG-CD2	-8.07	97.28	111.00
1	B	176	LEU	CB-CG-CD1	-8.02	97.36	111.00
1	B	97	LYS	CB-CG-CD	7.74	131.72	111.60
1	A	126	VAL	CG1-CB-CG2	7.11	122.27	110.90
1	B	90	VAL	CG1-CB-CG2	-6.82	99.98	110.90
1	A	118	LEU	CB-CG-CD1	6.80	122.56	111.00
3	D	104	LEU	CB-CG-CD2	6.43	121.94	111.00
1	B	97	LYS	CD-CE-NZ	6.28	126.14	111.70
2	H	149	PRO	N-CA-C	6.08	127.91	112.10
1	A	118	LEU	CB-CG-CD2	5.93	121.08	111.00
1	A	176	LEU	CA-CB-CG	5.69	128.38	115.30
1	B	159	VAL	CA-CB-CG2	5.43	119.05	110.90
1	A	23	GLN	CA-CB-CG	5.13	124.69	113.40
2	H	149	PRO	N-CA-CB	-5.09	97.00	102.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	97	ALA	Mainchain
2	H	98[A]	TYR	Mainchain

## 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	2301	0	2221	27	0
1	B	2210	0	2126	24	0
2	C	1696	0	1652	17	0
2	H	1687	0	1635	10	0
3	D	1573	0	1516	18	0
3	L	1573	0	1516	11	0
4	E	28	0	25	0	0
5	A	98	0	91	0	0
5	B	84	0	78	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	11	0	0	0	0
6	D	6	0	0	0	0
6	H	7	0	0	0	0
6	L	3	0	0	0	0
7	A	12	0	9	0	0
7	B	8	0	6	0	0
7	D	4	0	3	0	0
7	H	8	0	6	0	0
7	L	4	0	3	0	0
8	A	5	0	0	0	0
9	C	10	0	14	1	0
10	A	8	0	0	0	0
10	B	9	0	0	0	0
10	C	7	0	0	0	0
10	D	8	0	0	0	0
10	H	5	0	0	0	0
10	L	4	0	0	0	0
All	All	11381	0	10901	103	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 5.

All (103) 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:121:ASN:OD1	1:B:126:VAL:HG22	1.90	0.71
1:A:33:THR:HB	1:A:219:GLY:HA3	1.73	0.70
1:A:126:VAL:HG22	1:A:174:PRO:HA	1.75	0.69
1:B:245[B]:HIS:H	1:B:260:ALA:HB2	1.57	0.68
3:L:33:VAL:HG22	3:L:90:SER:HB3	1.77	0.65
3:D:49:TYR:CD2	3:D:50:GLU:HG3	2.32	0.64
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.80	0.63
3:D:6:GLN:NE2	3:D:86:TYR:O	2.32	0.62
3:D:186:LYS:O	3:D:189:ARG:NH2	2.33	0.62
1:B:245[A]:HIS:H	1:B:260:ALA:HB2	1.63	0.62
1:B:38:TYR:CE1	1:B:222:ALA:HB1	2.34	0.62
1:A:34:ARG:HE	1:A:217:PRO:HD2	1.66	0.61
2:C:37:VAL:HG12	2:C:47:TRP:HA	1.83	0.60
2:H:37:VAL:HG12	2:H:47:TRP:HA	1.83	0.60
1:B:38:TYR:HE1	1:B:222:ALA:HB1	1.66	0.59
1:B:277:LEU:HD23	1:B:285:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:138:ASP:OD1	3:D:167:GLN:NE2	2.37	0.57
2:H:52:ASP:HB2	2:H:58:ILE:HD11	1.85	0.57
3:D:86:TYR:CE1	3:D:104:LEU:HD12	2.40	0.57
1:B:206:LYS:HE3	1:B:221:SER:HB3	1.86	0.56
1:B:121:ASN:ND2	1:B:177:MET:H	2.03	0.56
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.87	0.56
1:A:34:ARG:HH12	1:A:221:SER:HB2	1.71	0.55
1:B:100:ILE:HG22	1:B:242:LEU:HD12	1.87	0.55
1:B:104:TRP:H	1:B:119:ILE:HG23	1.71	0.54
1:A:251:PRO:HD2	3:L:55:PRO:HB3	1.90	0.54
1:B:121:ASN:HD21	1:B:177:MET:H	1.56	0.54
3:D:9:SER:HB2	3:D:143:ALA:HB3	1.90	0.53
1:B:147:LYS:HE2	2:C:30:ILE:HA	1.89	0.53
1:A:40:ASP:OD1	1:A:41:LYS:N	2.42	0.53
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.90	0.53
3:L:111:ALA:HB3	3:L:140:TYR:H	1.75	0.52
1:B:143:VAL:HG22	1:B:154:GLU:HG2	1.90	0.52
1:A:276:LEU:HD22	1:A:301:CYS:HA	1.92	0.52
1:A:34:ARG:NE	1:A:217:PRO:HD2	2.24	0.51
1:B:29:THR:HG23	1:B:62:VAL:HG23	1.93	0.51
3:L:34:SER:OG	3:L:89:SER:OG	2.29	0.51
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.45	0.50
1:B:119:ILE:HD12	1:B:128:ILE:HG12	1.92	0.50
3:L:145:THR:HB	3:L:196:THR:HB	1.94	0.50
3:L:132:LEU:HD12	3:L:178:LEU:HD23	1.94	0.50
2:C:150:VAL:HG12	2:C:200:HIS:HB2	1.95	0.48
3:D:156:LYS:HG2	3:D:156:LYS:H	1.45	0.48
3:D:66:LYS:HA	3:D:71:ALA:HA	1.96	0.47
2:C:87:THR:HG23	2:C:110:THR:HA	1.97	0.47
1:B:105:ILE:HG22	1:B:118:LEU:HD12	1.95	0.47
1:A:71:SER:HB2	1:A:75:GLY:HA3	1.97	0.47
2:C:2:VAL:HG12	2:C:27:TYR:HB2	1.97	0.47
2:C:83:ARG:HG2	2:C:84:SER:H	1.80	0.46
3:L:194:GLN:HG2	3:L:203:GLU:HG3	1.97	0.46
1:A:143:VAL:HG12	1:A:154:GLU:HG2	1.97	0.46
3:D:105:THR:HG21	3:D:141:PRO:HB3	1.98	0.46
1:A:105:ILE:HG22	1:A:118:LEU:HD12	1.98	0.46
1:A:105:ILE:HD13	1:A:105:ILE:HG21	1.79	0.46
1:B:251:PRO:HD2	3:D:55:PRO:HB3	1.98	0.45
1:A:289:VAL:HG21	1:A:300:LYS:HD2	1.96	0.45
1:B:47:VAL:HG12	1:B:279:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:PRO:HB2	2:H:188:SER:HB3	1.98	0.45
1:B:36:VAL:O	1:B:223:LEU:HB2	2.17	0.45
2:C:42:GLY:HA3	3:D:163:THR:HG21	1.98	0.45
2:H:127:SER:H	2:H:130:SER:HB2	1.80	0.45
2:C:2:VAL:HG11	2:C:32:LEU:HD13	1.98	0.45
1:B:206:LYS:NZ	1:B:208:THR:OG1	2.47	0.45
1:B:130:VAL:HG21	1:B:231:ILE:HB	1.98	0.45
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.99	0.45
1:A:185:ASN:O	1:A:186:PHE:C	2.56	0.44
2:C:141:LEU:CD2	2:C:143:LYS:HB2	2.47	0.44
3:D:83:GLU:HB2	3:D:106:VAL:HG23	1.98	0.44
1:A:185:ASN:HB3	1:A:187:LYS:HG3	2.00	0.43
2:C:32:LEU:HD12	2:C:94:THR:OG1	2.19	0.43
1:A:127:VAL:HG11	1:A:129:LYS:HE3	2.00	0.43
3:D:132:LEU:HD12	3:D:178:LEU:HD23	1.99	0.43
1:A:77:LYS:HB3	1:A:77:LYS:HE2	1.78	0.43
2:C:126:PRO:HG3	2:C:138:LEU:HD12	2.00	0.43
2:C:139:GLY:HA3	2:C:181:VAL:HG12	2.01	0.43
2:C:35:HIS:ND1	2:C:50:GLY:HA3	2.34	0.43
3:D:145:THR:HB	3:D:196:THR:HG23	2.01	0.43
1:B:95:THR:HG22	1:B:187:LYS:HB3	2.00	0.43
3:D:167:GLN:HG3	3:D:169:ASN:H	1.84	0.43
2:C:121:VAL:H	9:C:312:PGE:H5	1.83	0.42
2:H:139:GLY:HA2	2:H:154:TRP:CZ2	2.55	0.42
2:C:98[B]:TYR:CE1	2:C:99:LYS:HG2	2.54	0.42
3:L:85:ASP:OD1	3:L:103:LYS:HD3	2.19	0.42
2:H:142:VAL:HB	2:H:178:LEU:HG	2.02	0.42
3:L:33:VAL:HG22	3:L:90:SER:CB	2.46	0.42
1:A:187:LYS:HB2	1:A:210:ILE:HG13	2.02	0.42
1:A:104:TRP:CD1	1:A:240:THR:HG22	2.55	0.42
1:A:34:ARG:HD2	1:A:219:GLY:HA2	2.02	0.42
1:A:100:ILE:HG22	1:A:242:LEU:HD12	2.02	0.41
1:A:89:GLY:HA3	1:A:270:LEU:HD12	2.02	0.41
2:C:52:ASP:HB2	2:C:58:ILE:HD11	2.01	0.41
2:H:145:TYR:HE1	2:H:148:GLU:HG2	1.85	0.41
3:L:165:SER:O	3:L:172:TYR:HA	2.20	0.41
1:A:34:ARG:HH22	1:A:221:SER:HB2	1.85	0.41
1:B:95:THR:HA	1:B:189:LEU:HA	2.03	0.41
3:D:115:VAL:HG22	3:D:136:ILE:HG23	2.03	0.41
3:D:19:VAL:HG23	3:D:78:LEU:HD11	2.03	0.41
1:B:49:HIS:NE2	1:B:51:THR:OG1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:GLN:HG2	3:D:102:THR:OG1	2.21	0.41
1:A:193:VAL:HG13	1:A:270:LEU:HD11	2.04	0.40
1:A:277:LEU:HD23	1:A:285:ILE:HD13	2.03	0.40
1:A:274:THR:HG23	1:A:291:CYS:HB2	2.03	0.40
2:C:165:THR:HG23	2:C:180:SER:HB2	2.03	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	282/342 (82%)	256 (91%)	26 (9%)	0	100	100
1	B	268/342 (78%)	254 (95%)	14 (5%)	0	100	100
2	C	222/227 (98%)	210 (95%)	12 (5%)	0	100	100
2	H	221/227 (97%)	210 (95%)	11 (5%)	0	100	100
3	D	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
3	L	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
All	All	1415/1568 (90%)	1332 (94%)	83 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/310 (83%)	258 (100%)	0	100	100
1	B	247/310 (80%)	247 (100%)	0	100	100
2	C	190/193 (98%)	190 (100%)	0	100	100
2	H	189/193 (98%)	189 (100%)	0	100	100
3	D	176/178 (99%)	176 (100%)	0	100	100
3	L	176/178 (99%)	176 (100%)	0	100	100
All	All	1236/1362 (91%)	1236 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	69	HIS
1	A	99	ASN
1	A	121	ASN
1	A	239	GLN
1	B	30	ASN
1	B	66	HIS
1	B	115	GLN
2	H	1	GLN
2	C	1	GLN
2	C	164	HIS

### 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 ⓘ

2 monosaccharides are modelled in this entry.

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
4	NAG	E	1	1,4	14,14,15	0.69	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	E	2	4	14,14,15	1.62	2 (14%)	17,19,21	0.93	1 (5%)

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
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	C1-C2	5.55	1.60	1.52
4	E	2	NAG	O5-C1	2.17	1.47	1.43
4	E	1	NAG	O5-C1	2.10	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C4-C3-C2	2.33	114.44	111.02
4	E	1	NAG	C4-C3-C2	-2.11	107.93	111.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 63 ligands modelled in this entry, 39 are monoatomic - leaving 24 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
7	ACT	H	308	-	1,3,3	6.40	1 (100%)	0,3,3	0.00	-
7	ACT	A	416	-	1,3,3	6.16	1 (100%)	0,3,3	0.00	-
7	ACT	A	414	-	1,3,3	6.44	1 (100%)	0,3,3	0.00	-
5	NAG	B	403	1	14,14,15	0.25	0	17,19,21	0.56	0
5	NAG	B	402	1,6	14,14,15	0.53	0	17,19,21	0.46	0
7	ACT	A	415	-	1,3,3	6.43	1 (100%)	0,3,3	0.00	-
7	ACT	B	413	-	1,3,3	7.29	1 (100%)	0,3,3	0.00	-
9	PGE	C	312	-	9,9,9	0.29	0	8,8,8	0.46	0
5	NAG	A	403	1	14,14,15	0.91	1 (7%)	17,19,21	2.36	2 (11%)
8	CAC	A	417	-	0,4,4	0.00	-	0,6,6	0.00	-
5	NAG	A	406	1	14,14,15	0.43	0	17,19,21	1.24	2 (11%)
7	ACT	D	307	-	1,3,3	6.69	1 (100%)	0,3,3	0.00	-
5	NAG	B	404	1	14,14,15	0.45	0	17,19,21	1.55	2 (11%)
5	NAG	A	405	1	14,14,15	0.99	1 (7%)	17,19,21	1.34	3 (17%)
7	ACT	L	304	-	1,3,3	6.22	1 (100%)	0,3,3	0.00	-
5	NAG	A	404	1	14,14,15	0.19	0	17,19,21	0.57	0
5	NAG	A	401	1	14,14,15	0.43	0	17,19,21	0.56	0
5	NAG	A	402	1	14,14,15	0.36	0	17,19,21	0.60	1 (5%)
7	ACT	B	414	-	1,3,3	6.34	1 (100%)	0,3,3	0.00	-
7	ACT	H	309	-	1,3,3	6.47	1 (100%)	0,3,3	0.00	-
5	NAG	A	407	1	14,14,15	1.16	1 (7%)	17,19,21	1.64	3 (17%)
5	NAG	B	405	1	14,14,15	0.56	0	17,19,21	1.30	2 (11%)
5	NAG	B	401	1	14,14,15	0.28	0	17,19,21	0.38	0
5	NAG	B	406	1	14,14,15	0.55	0	17,19,21	1.27	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	404	1	-	5/6/23/26	0/1/1/1
5	NAG	A	402	1	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1	-	3/6/23/26	0/1/1/1
5	NAG	A	407	1	-	4/6/23/26	0/1/1/1
9	PGE	C	312	-	-	1/7/7/7	-
5	NAG	B	403	1	-	1/6/23/26	0/1/1/1
5	NAG	A	403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	402	1,6	-	1/6/23/26	0/1/1/1
5	NAG	A	404	1	-	0/6/23/26	0/1/1/1
5	NAG	B	405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	401	1	-	3/6/23/26	0/1/1/1
5	NAG	B	401	1	-	0/6/23/26	0/1/1/1
5	NAG	B	406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	406	1	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	413	ACT	CH3-C	7.29	1.58	1.48
7	D	307	ACT	CH3-C	6.69	1.57	1.48
7	H	309	ACT	CH3-C	6.47	1.57	1.48
7	A	414	ACT	CH3-C	6.44	1.56	1.48
7	A	415	ACT	CH3-C	6.43	1.56	1.48
7	H	308	ACT	CH3-C	6.40	1.56	1.48
7	B	414	ACT	CH3-C	6.34	1.56	1.48
7	L	304	ACT	CH3-C	6.22	1.56	1.48
7	A	416	ACT	CH3-C	6.16	1.56	1.48
5	A	407	NAG	O5-C1	-4.10	1.37	1.43
5	A	405	NAG	C1-C2	3.33	1.57	1.52
5	A	403	NAG	O5-C1	3.15	1.48	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	NAG	C2-N2-C7	6.62	132.33	122.90
5	A	403	NAG	C1-C2-N2	6.20	121.08	110.49
5	B	404	NAG	C1-O5-C5	4.09	117.73	112.19
5	A	407	NAG	C2-N2-C7	4.06	128.69	122.90
5	B	406	NAG	C2-N2-C7	4.01	128.62	122.90
5	A	407	NAG	C1-C2-N2	-3.69	104.19	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	404	NAG	O5-C5-C6	-3.29	102.04	107.20
5	B	405	NAG	C1-O5-C5	-3.25	107.79	112.19
5	A	406	NAG	C1-O5-C5	3.24	116.58	112.19
5	A	405	NAG	C4-C3-C2	3.13	115.61	111.02
5	A	406	NAG	C1-C2-N2	-2.76	105.77	110.49
5	B	405	NAG	O5-C5-C4	-2.44	104.90	110.83
5	A	405	NAG	C1-C2-N2	-2.26	106.63	110.49
5	A	405	NAG	C2-N2-C7	2.17	126.00	122.90
5	A	407	NAG	C4-C3-C2	-2.12	107.92	111.02
5	A	402	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	NAG	C3-C2-N2-C7
5	A	406	NAG	C8-C7-N2-C2
5	A	406	NAG	O7-C7-N2-C2
5	B	404	NAG	C1-C2-N2-C7
5	B	404	NAG	C8-C7-N2-C2
5	B	404	NAG	O7-C7-N2-C2
5	A	407	NAG	C8-C7-N2-C2
5	B	406	NAG	C8-C7-N2-C2
5	A	407	NAG	O7-C7-N2-C2
5	A	407	NAG	C4-C5-C6-O6
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2
5	B	406	NAG	O7-C7-N2-C2
5	B	404	NAG	O5-C5-C6-O6
5	B	404	NAG	C4-C5-C6-O6
5	A	403	NAG	O7-C7-N2-C2
5	A	405	NAG	C1-C2-N2-C7
5	B	403	NAG	O5-C5-C6-O6
5	A	407	NAG	O5-C5-C6-O6
5	A	405	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	B	402	NAG	O5-C5-C6-O6
9	C	312	PGE	O2-C3-C4-O3
5	A	405	NAG	C3-C2-N2-C7

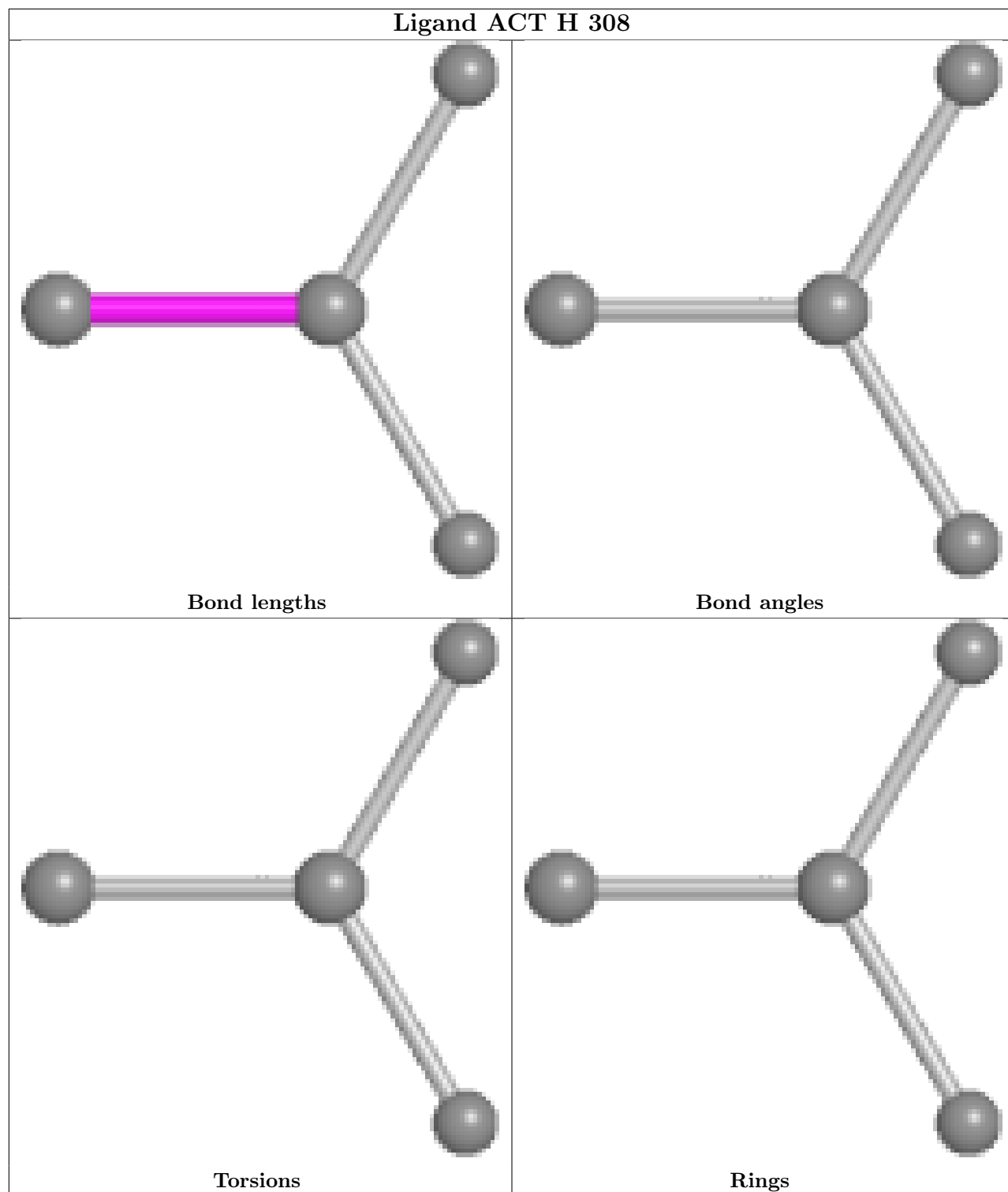
There are no ring outliers.

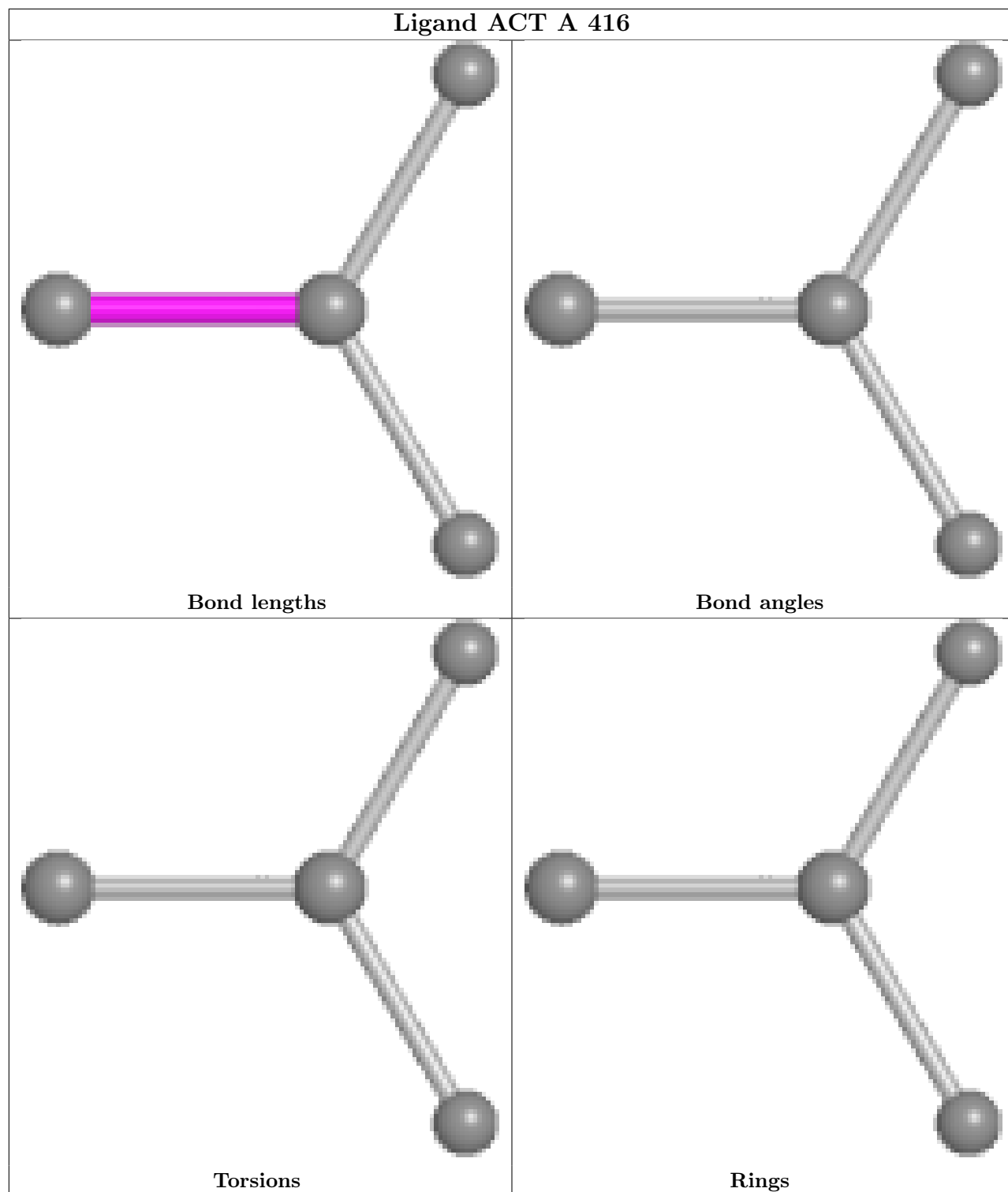
1 monomer is involved in 1 short contact:

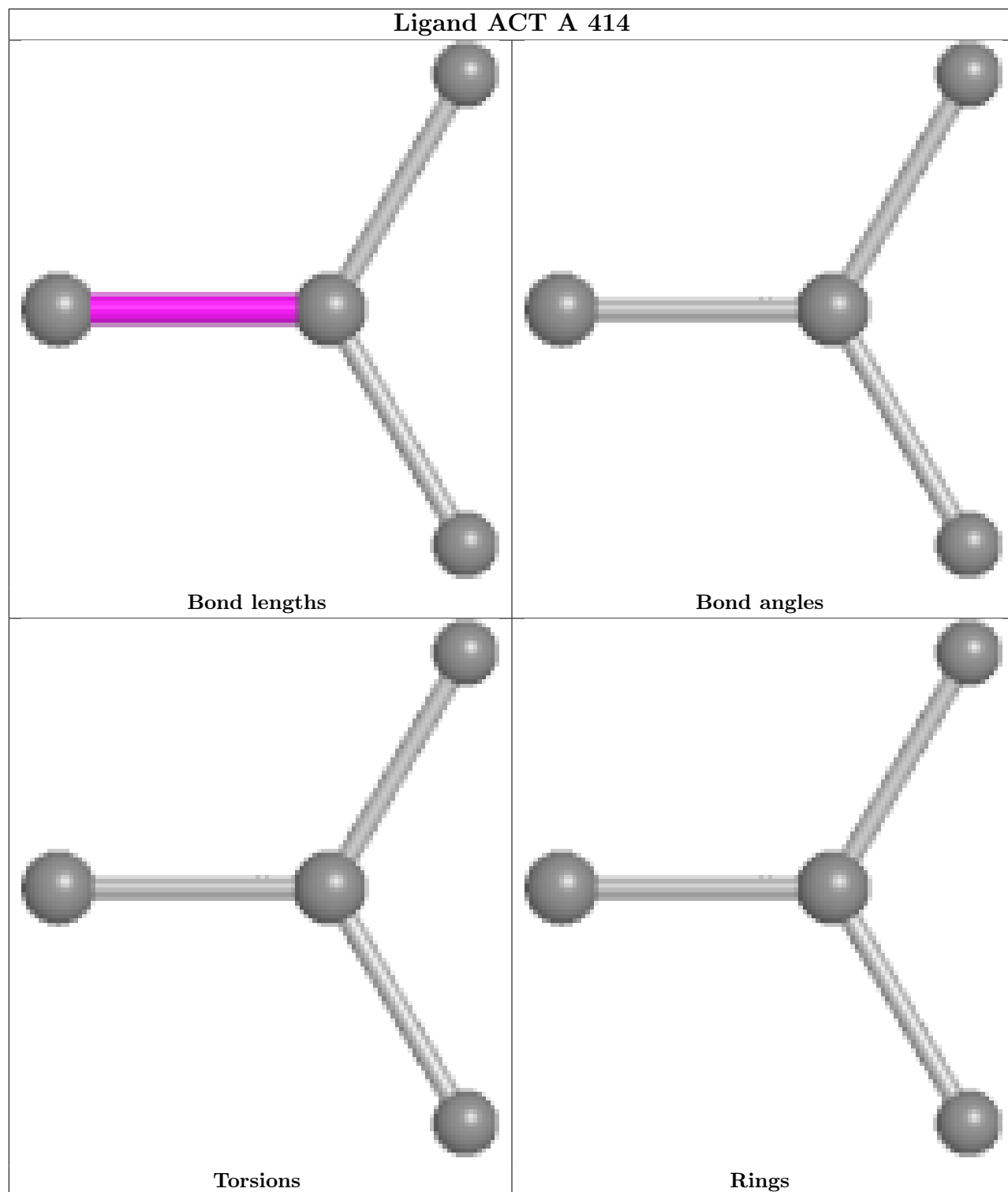
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9	C	312	PGE	1	0

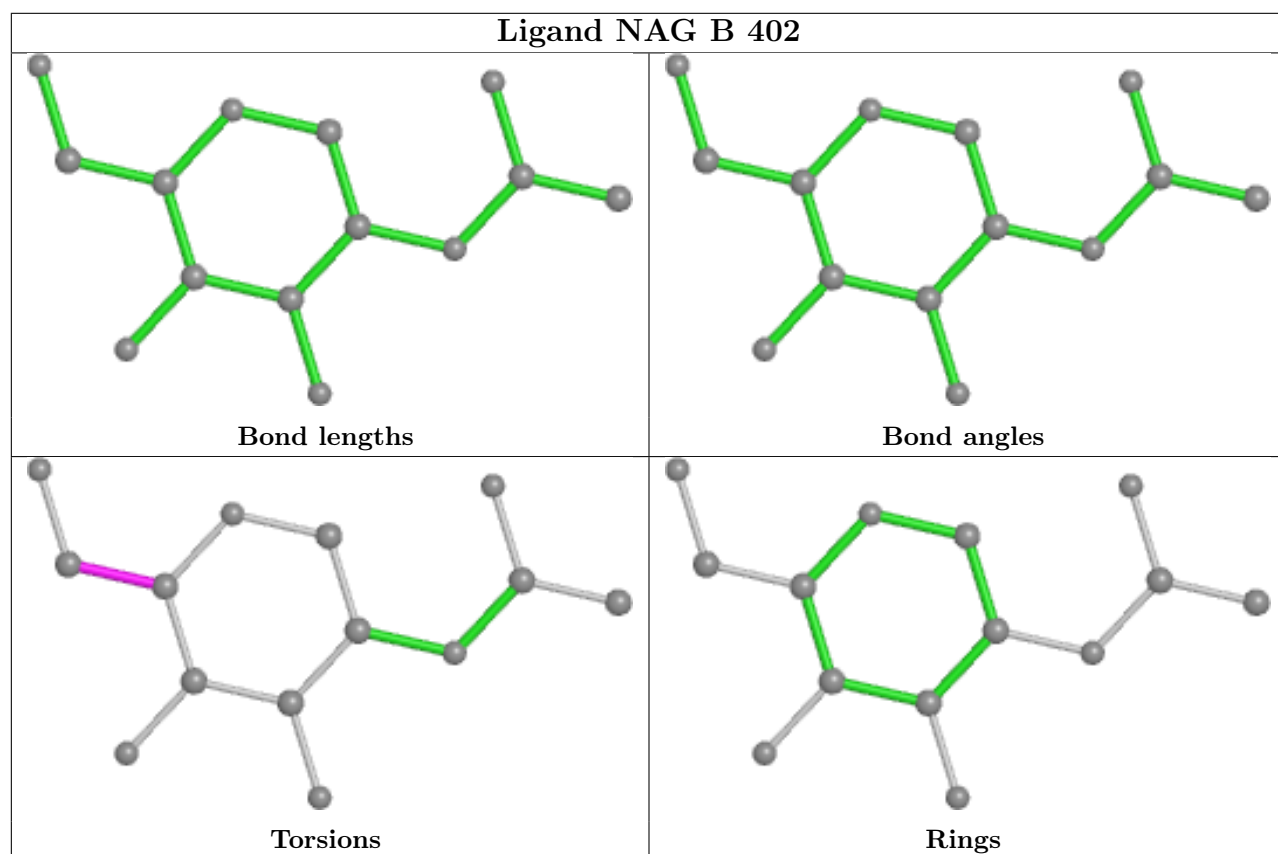
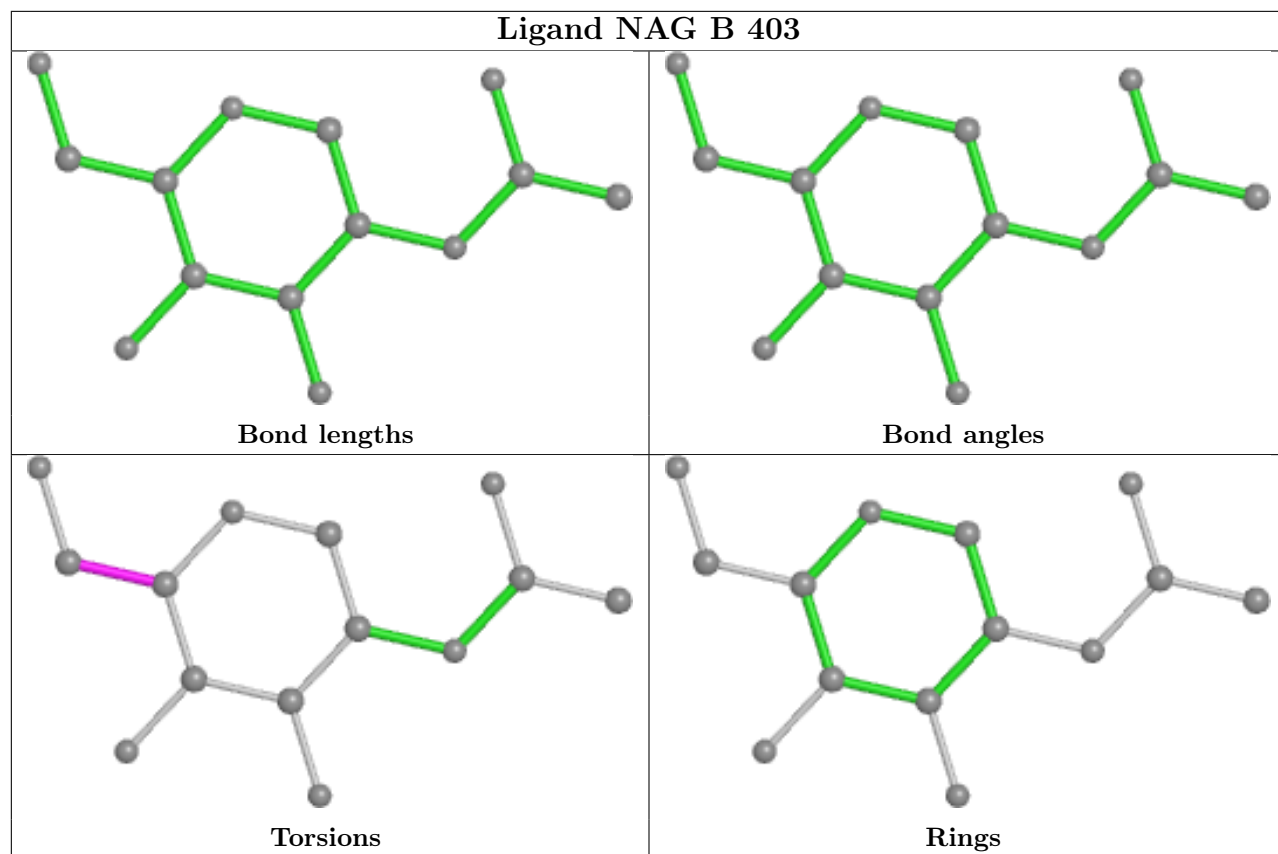
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

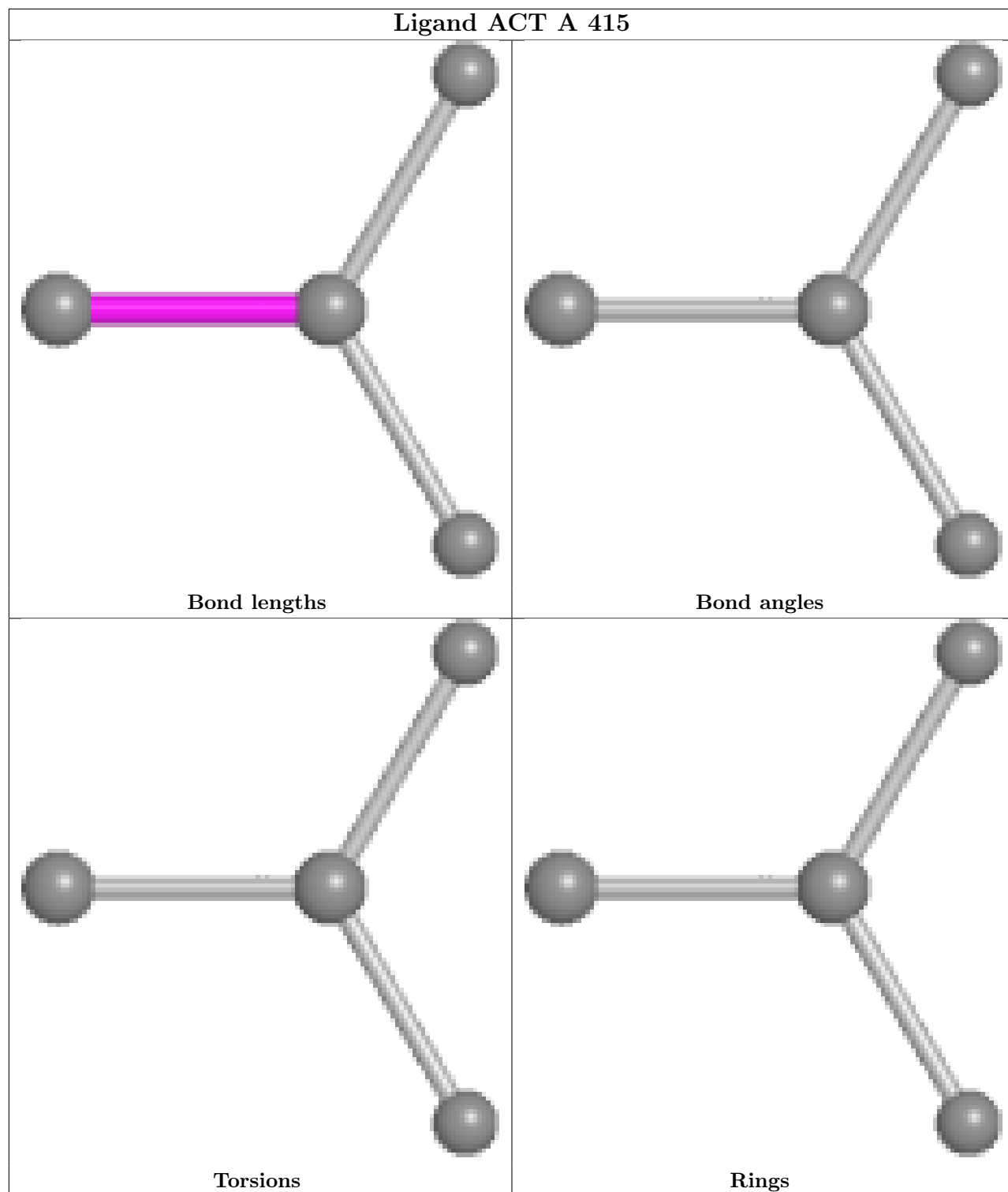


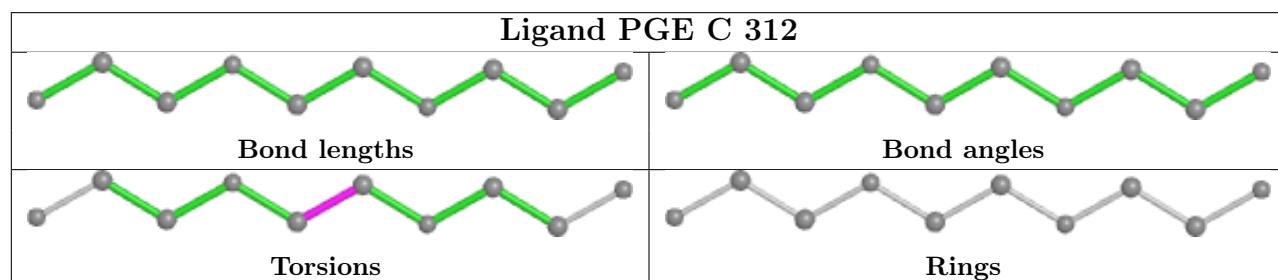
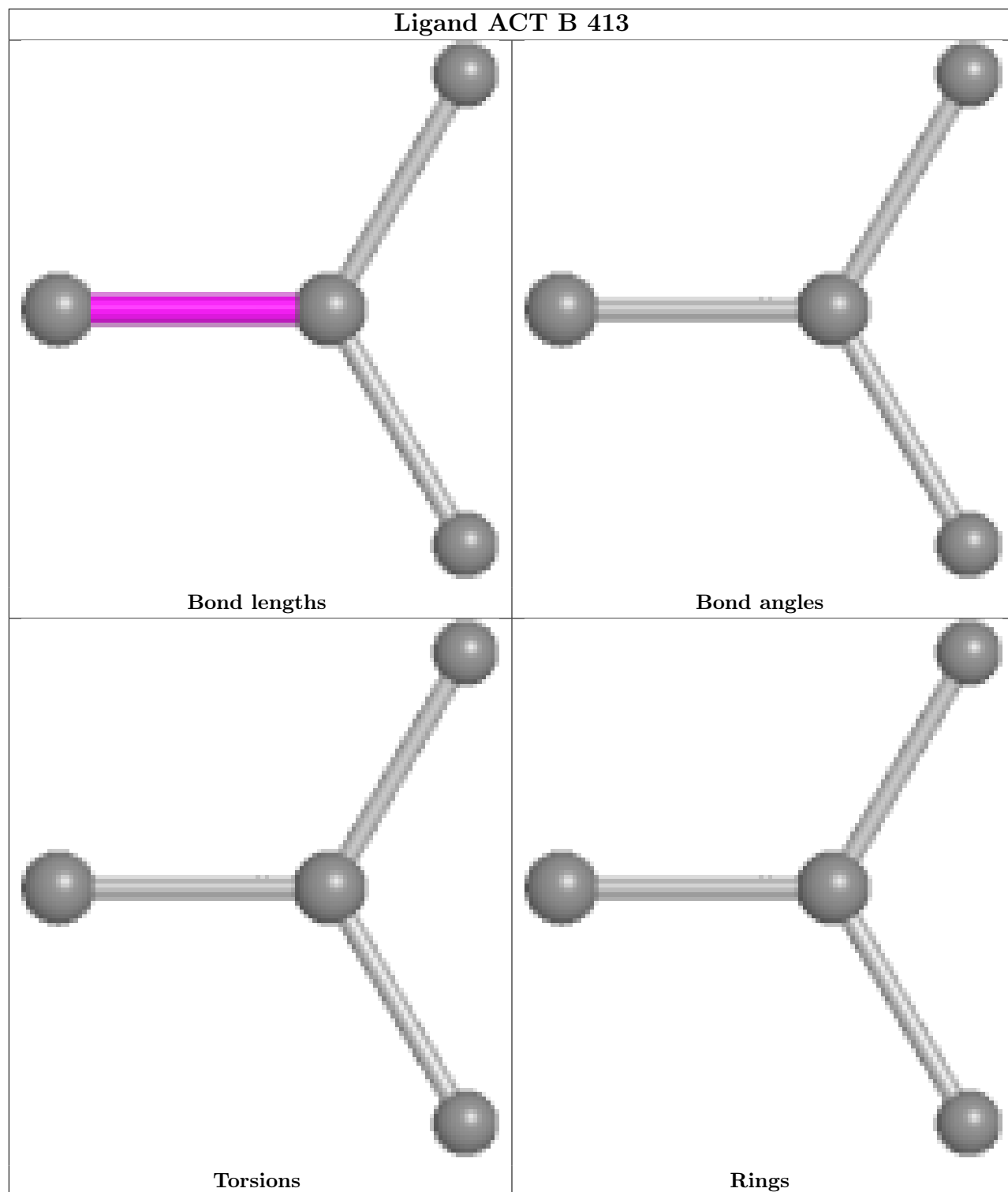


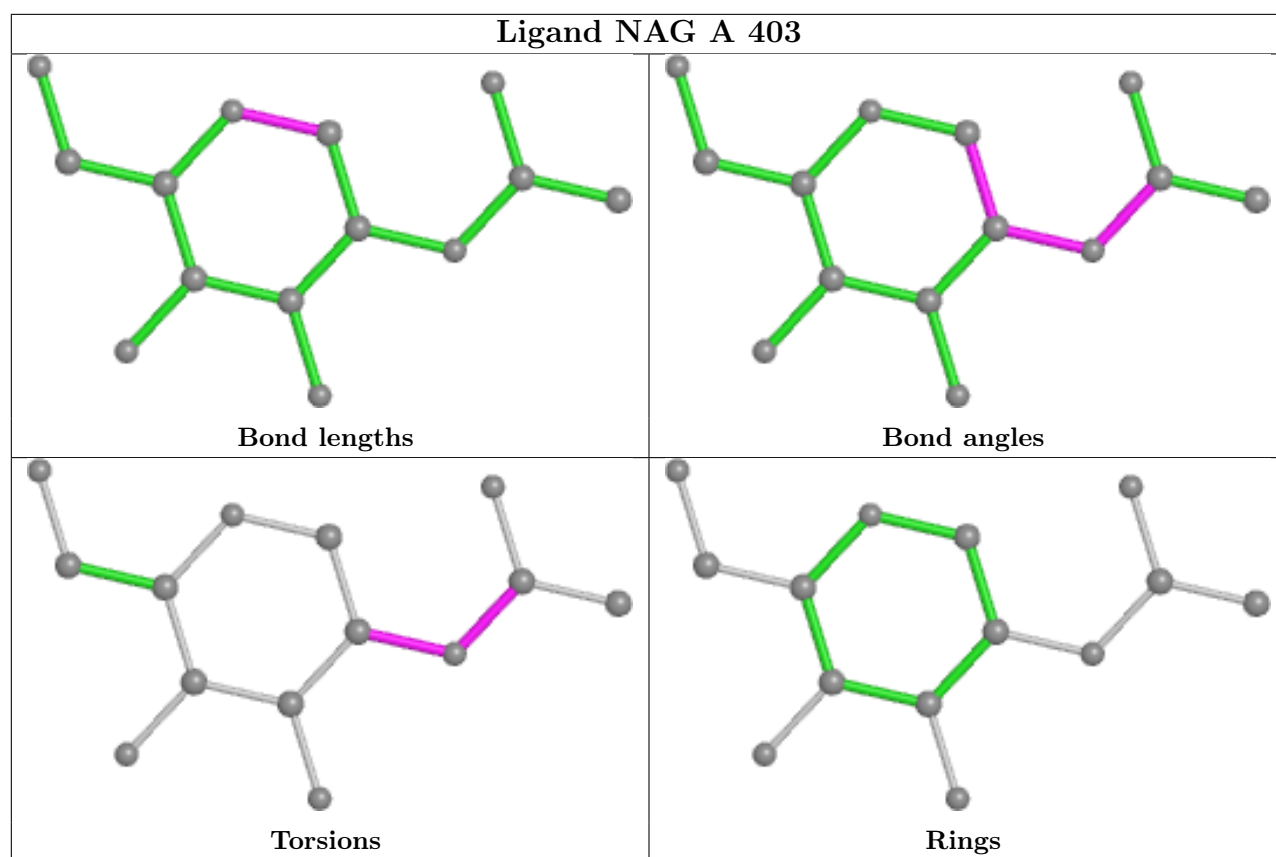


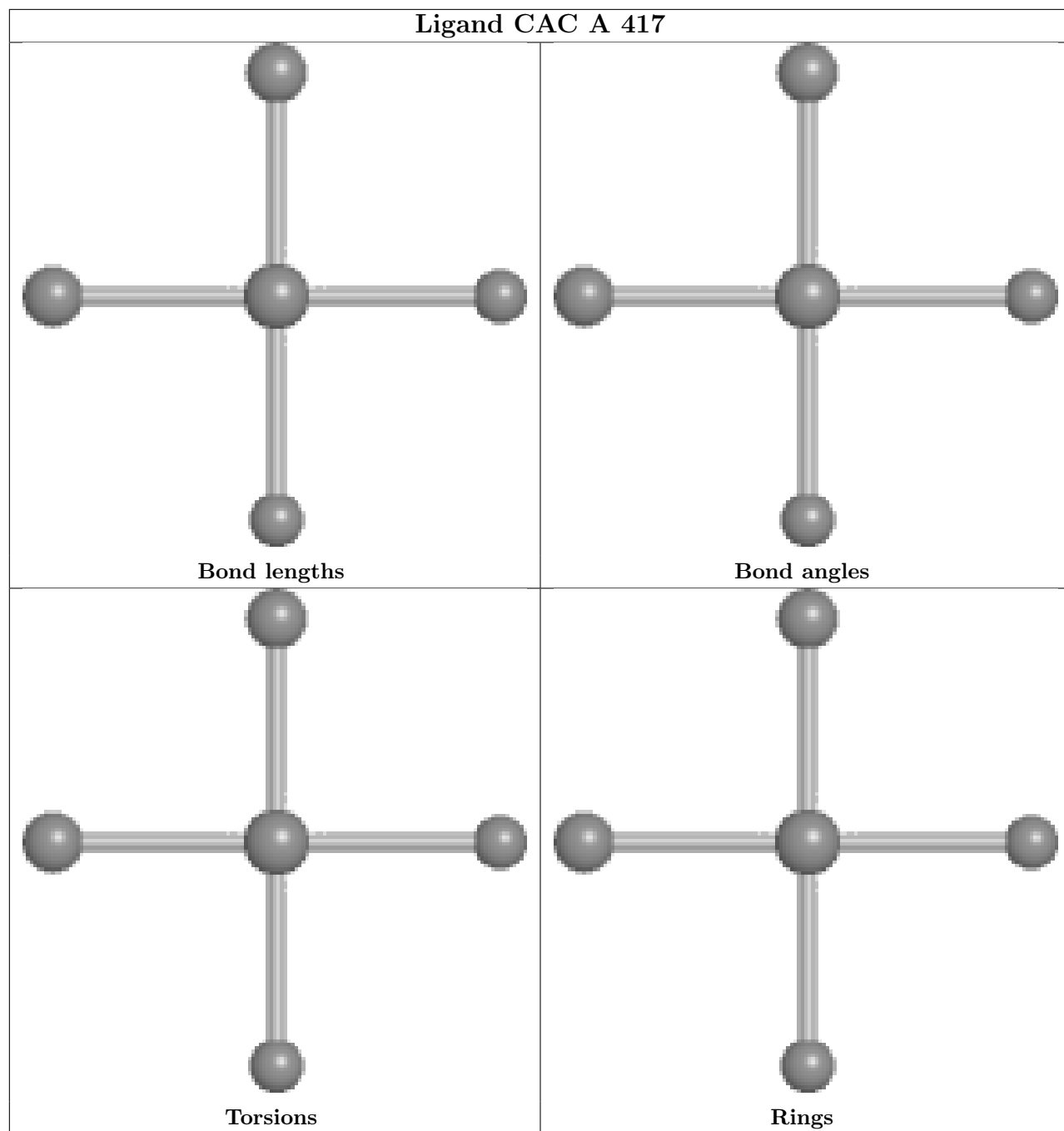




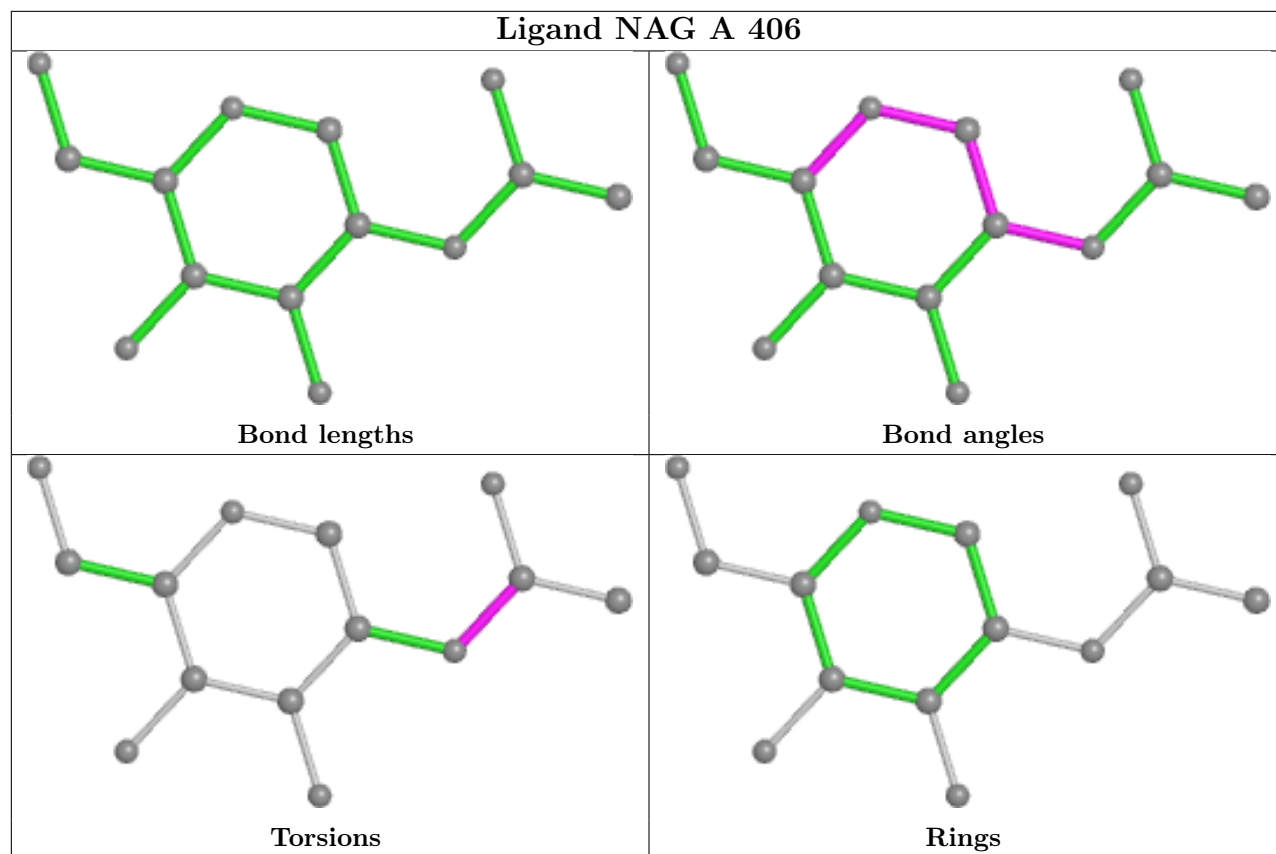


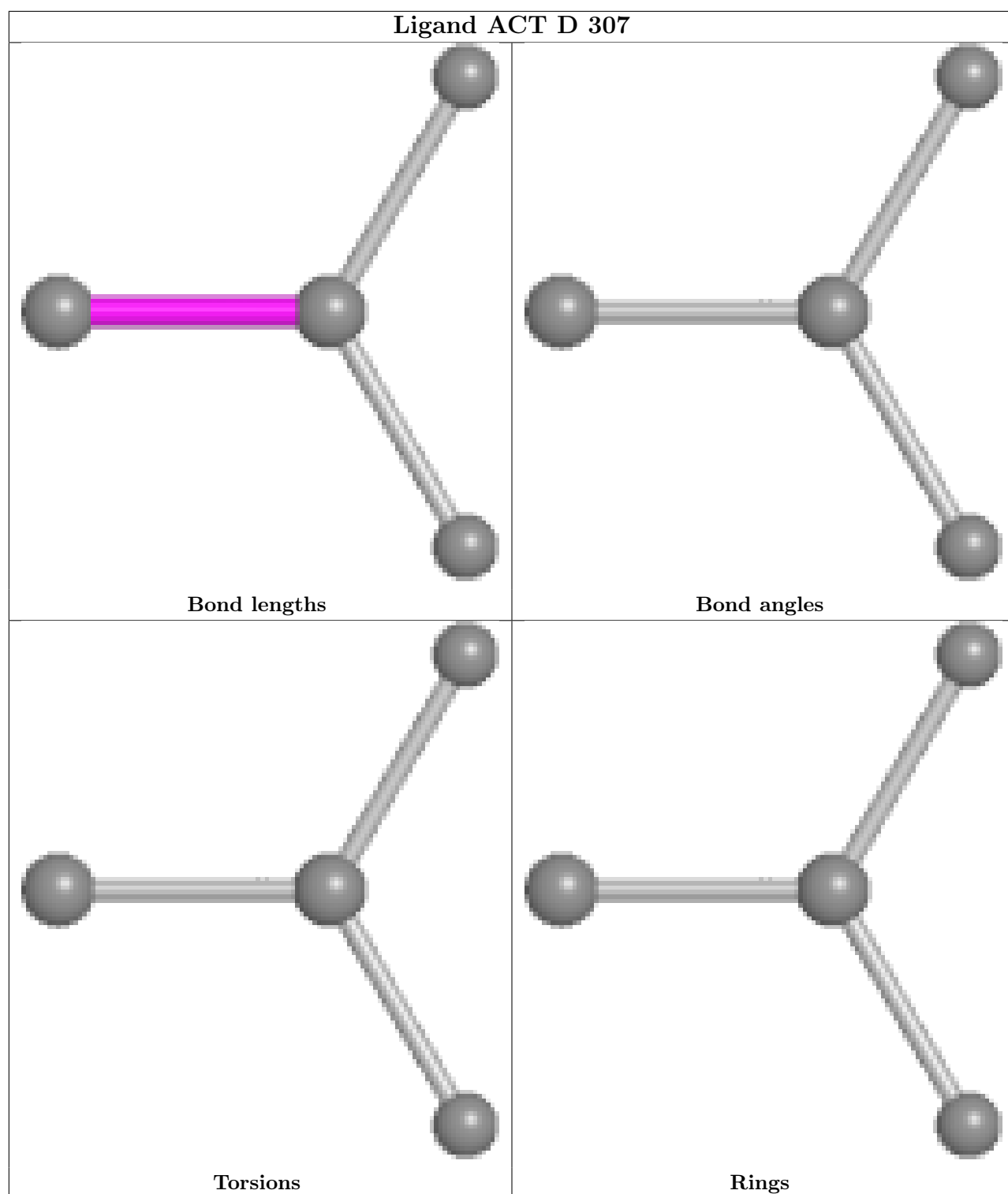


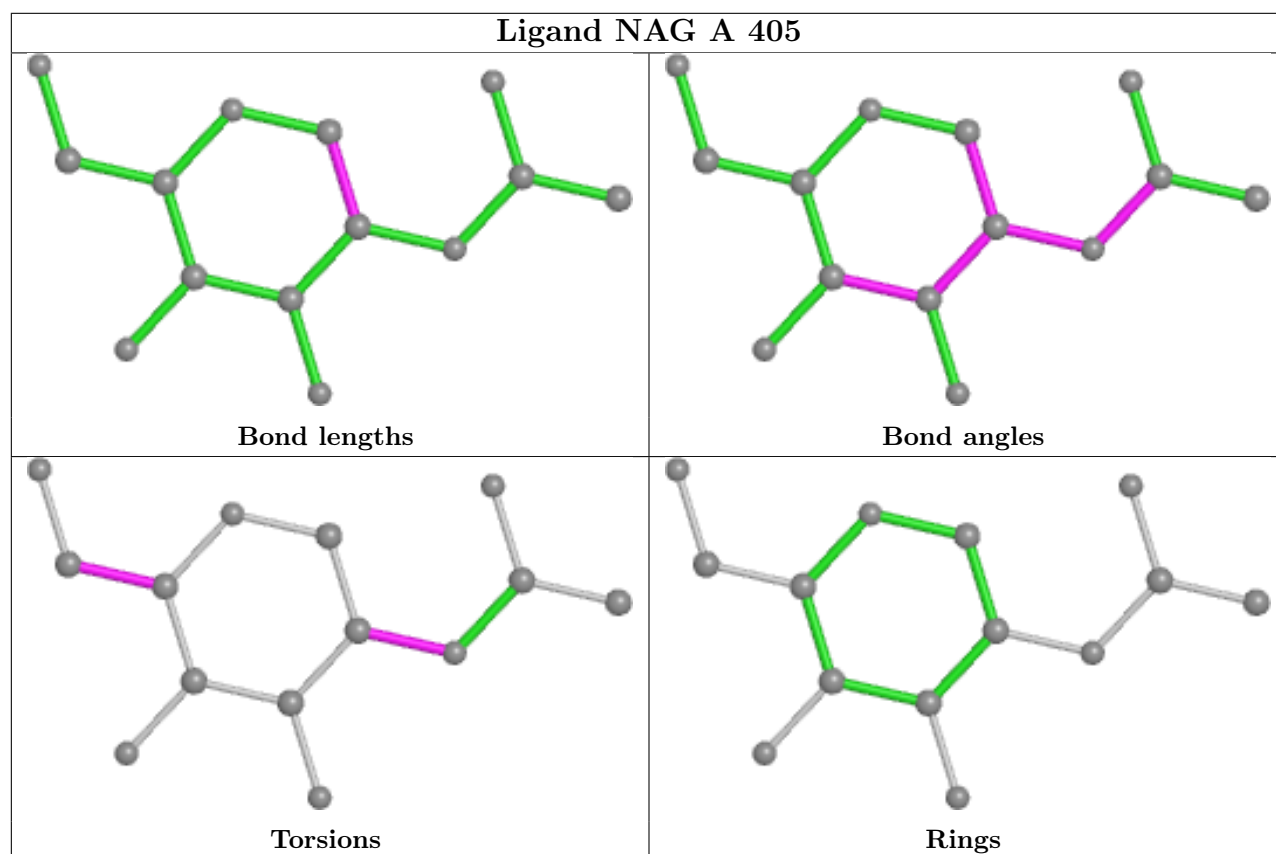
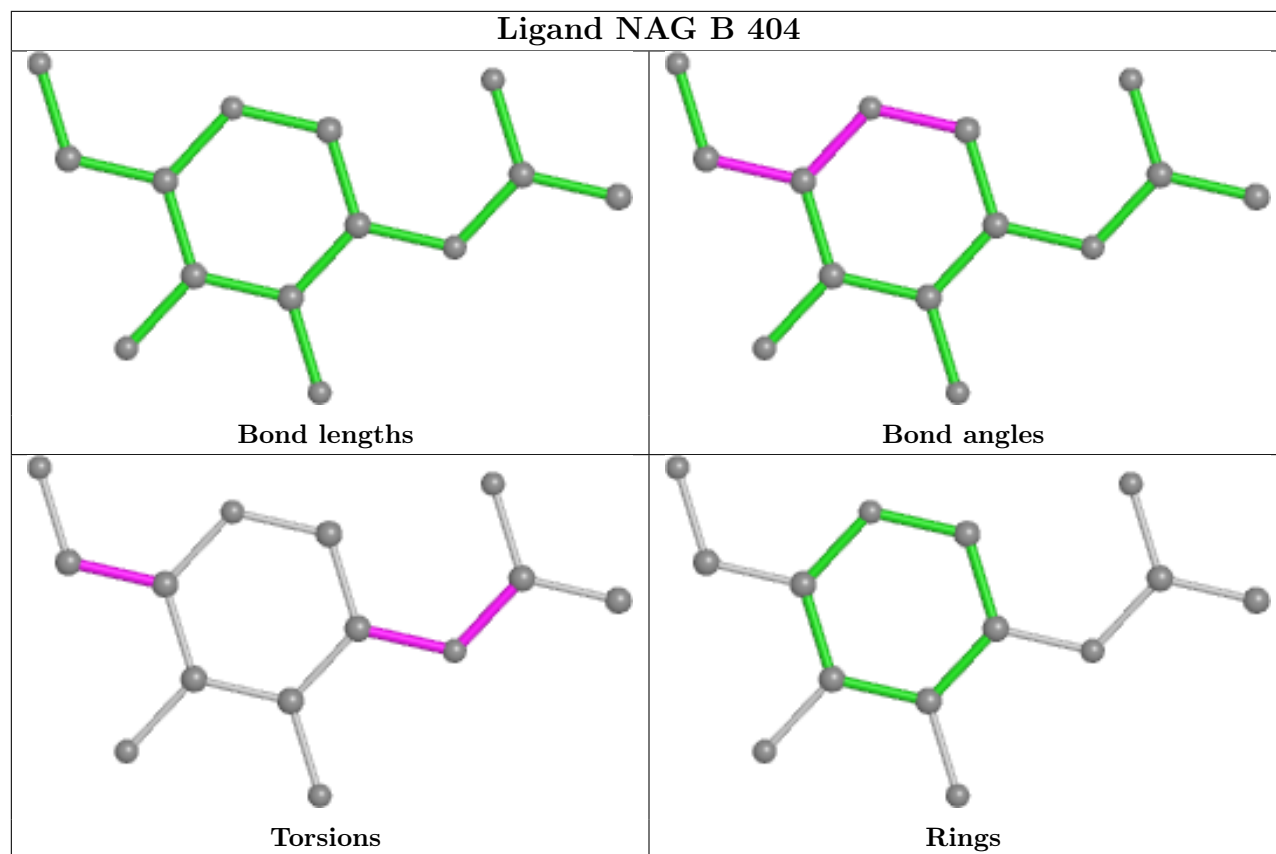


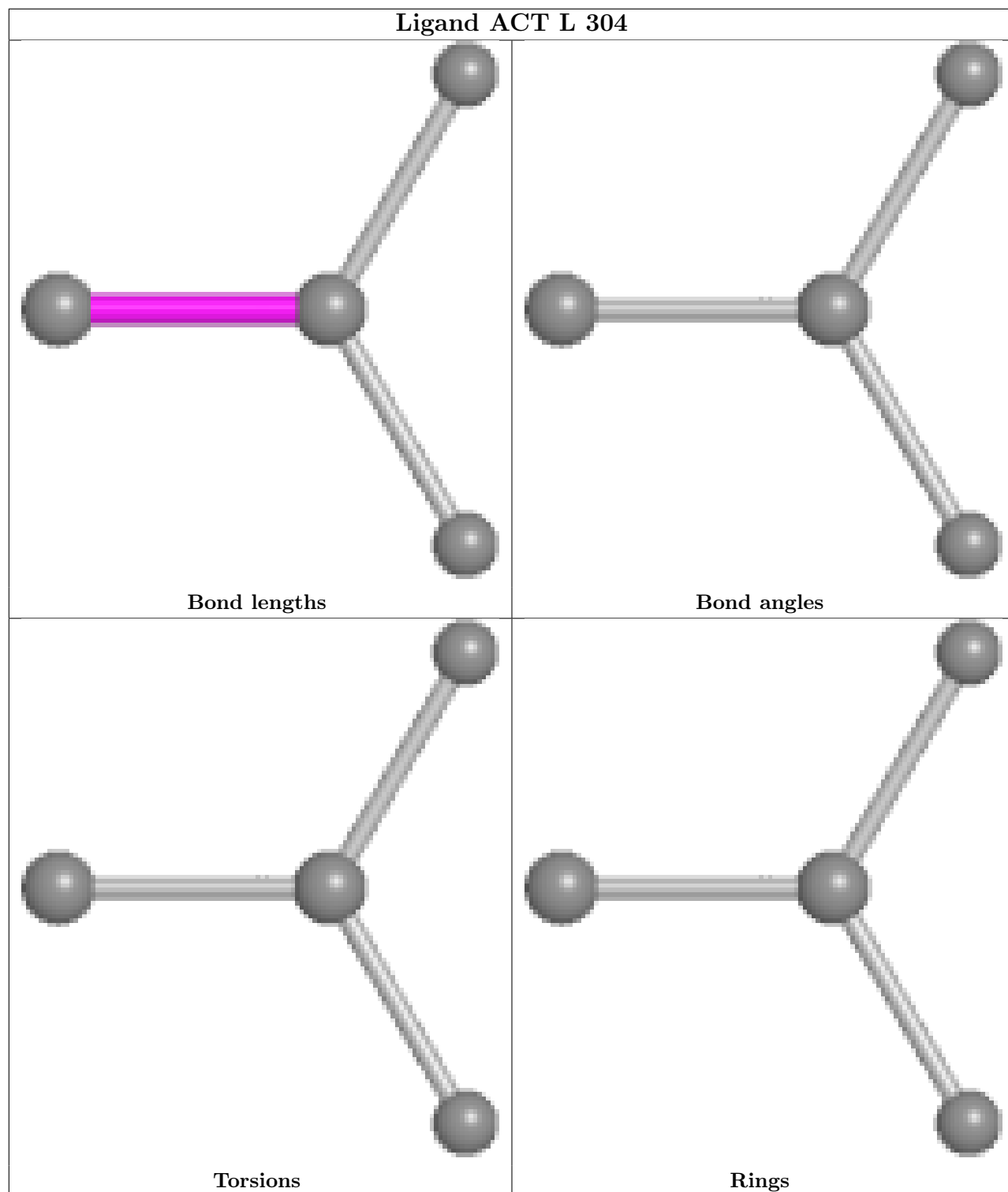


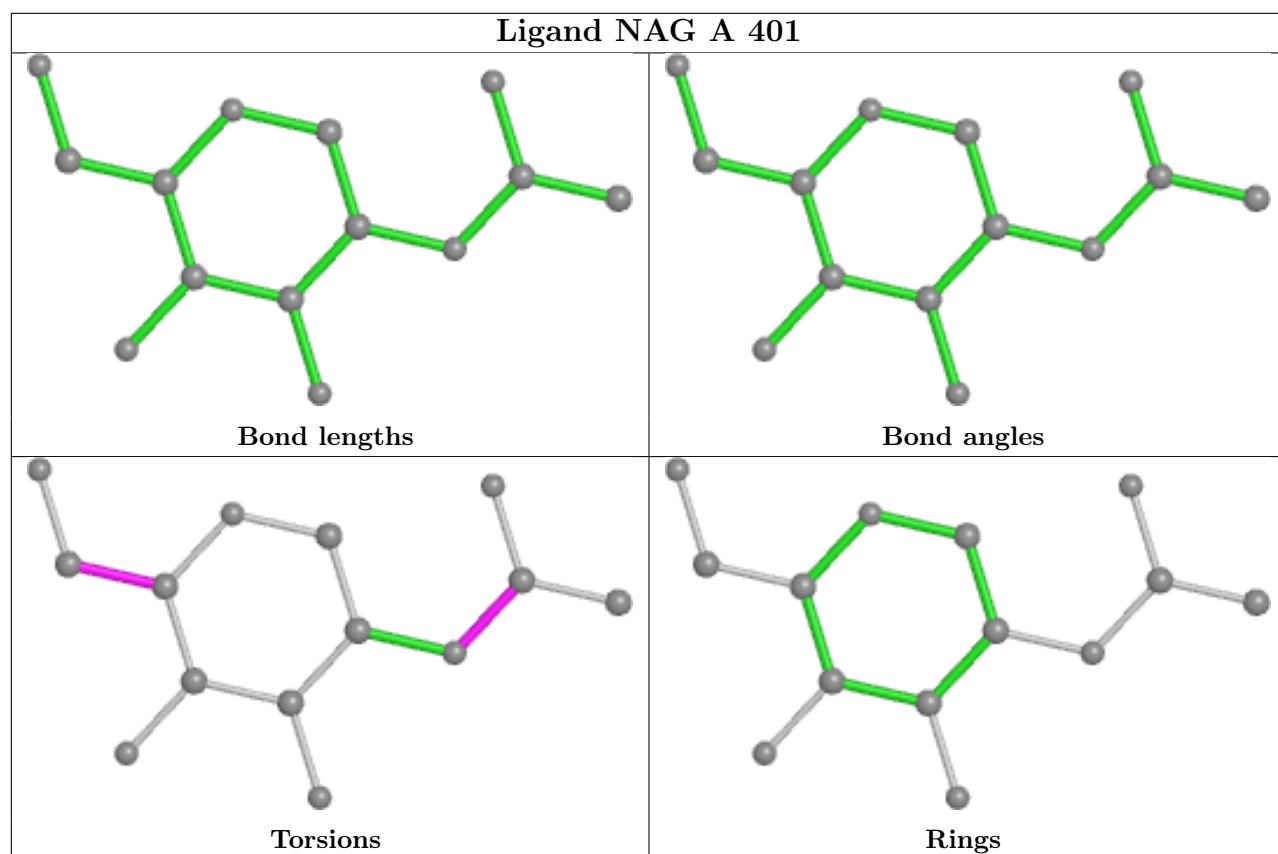
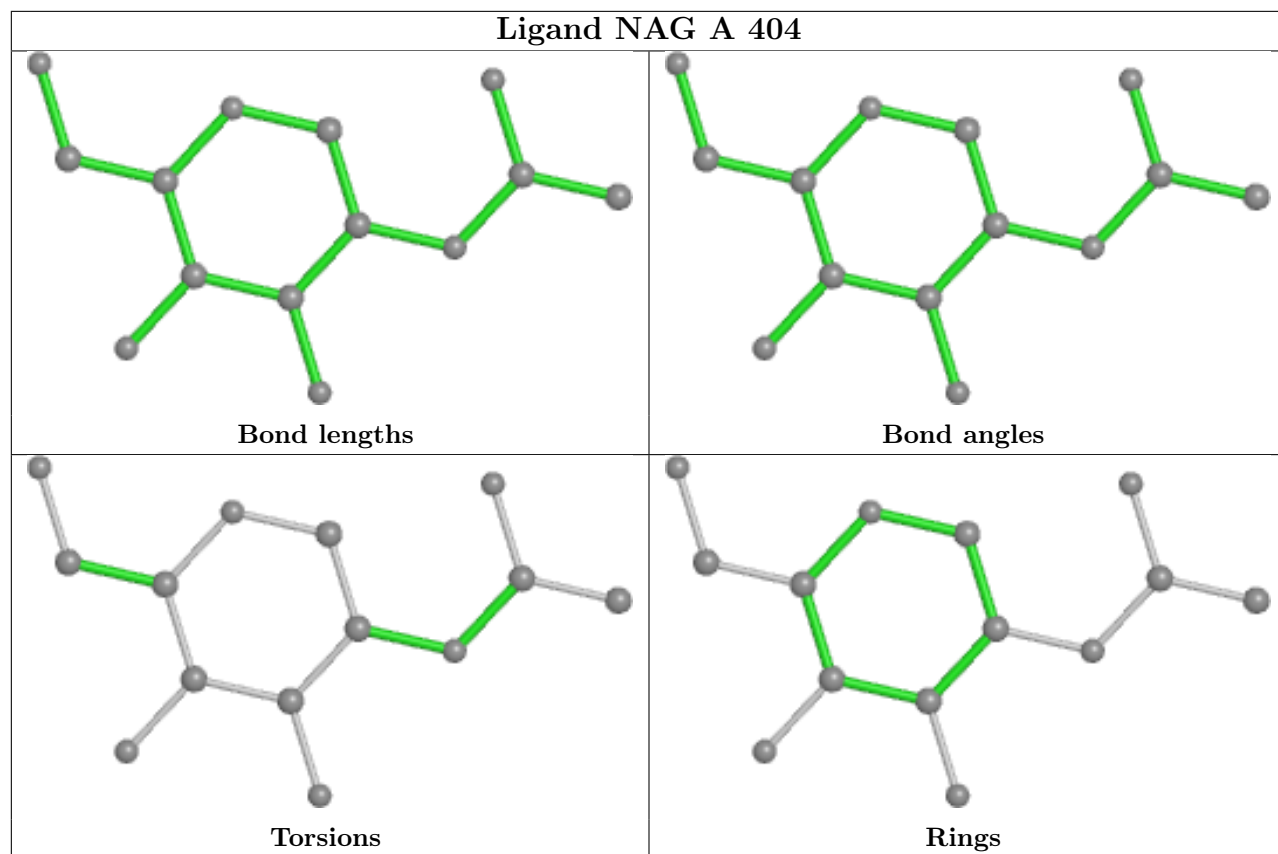


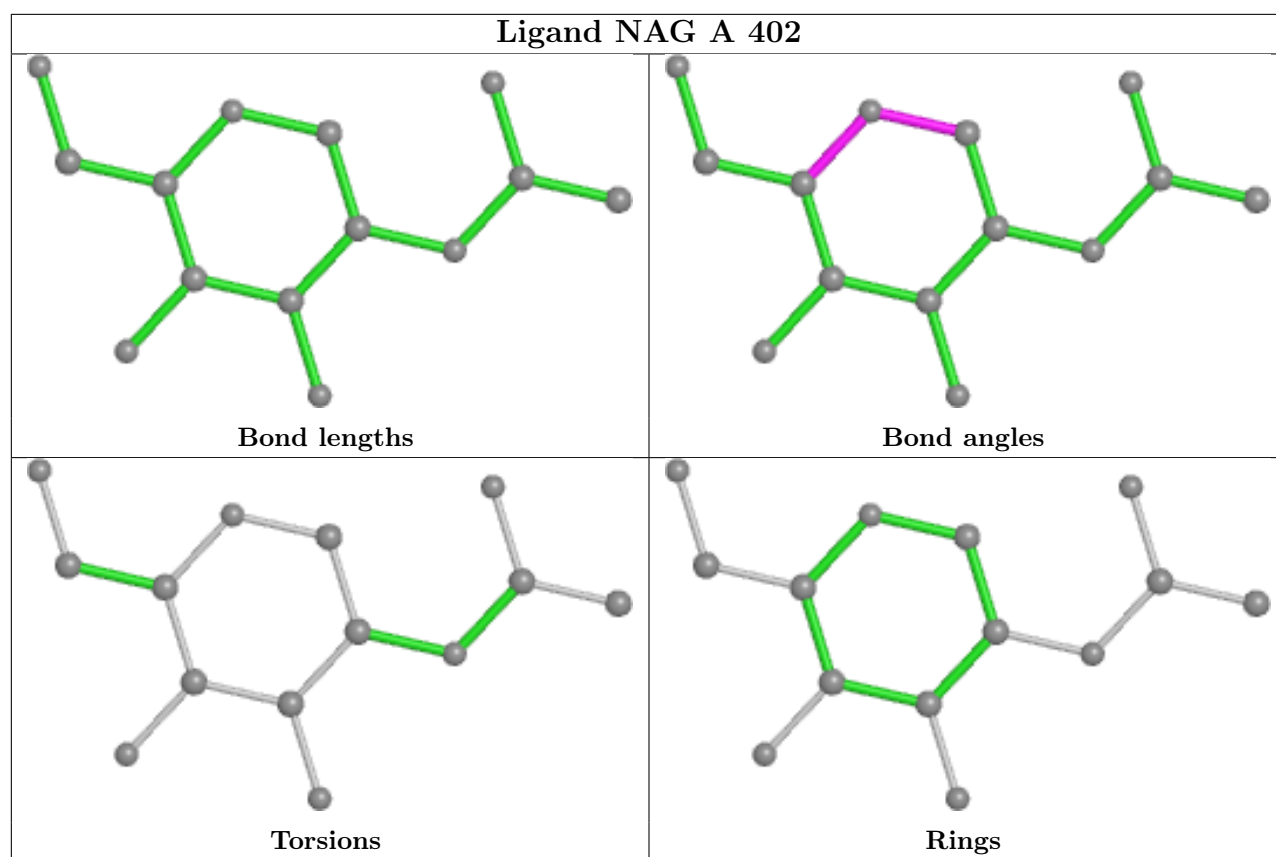


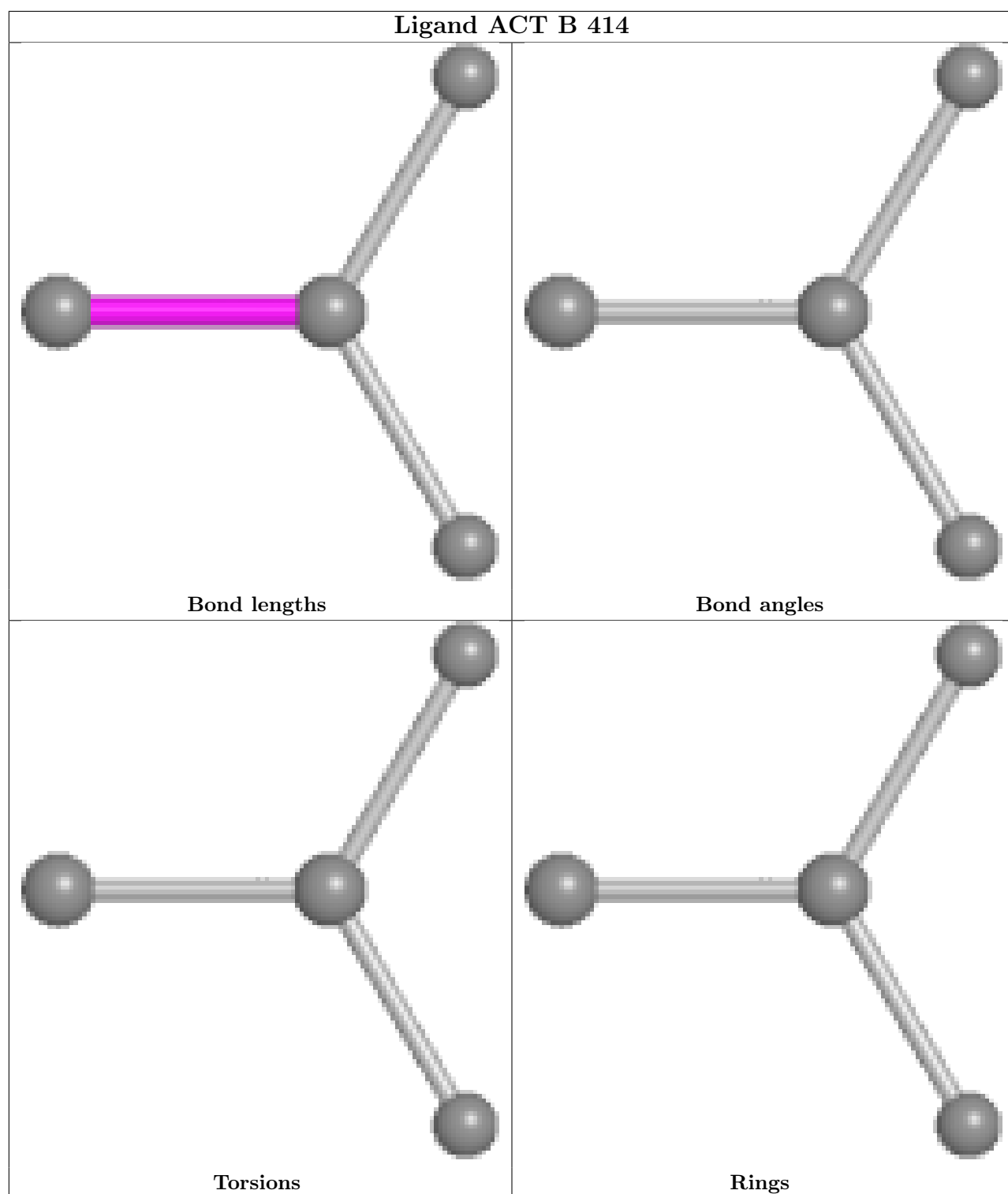


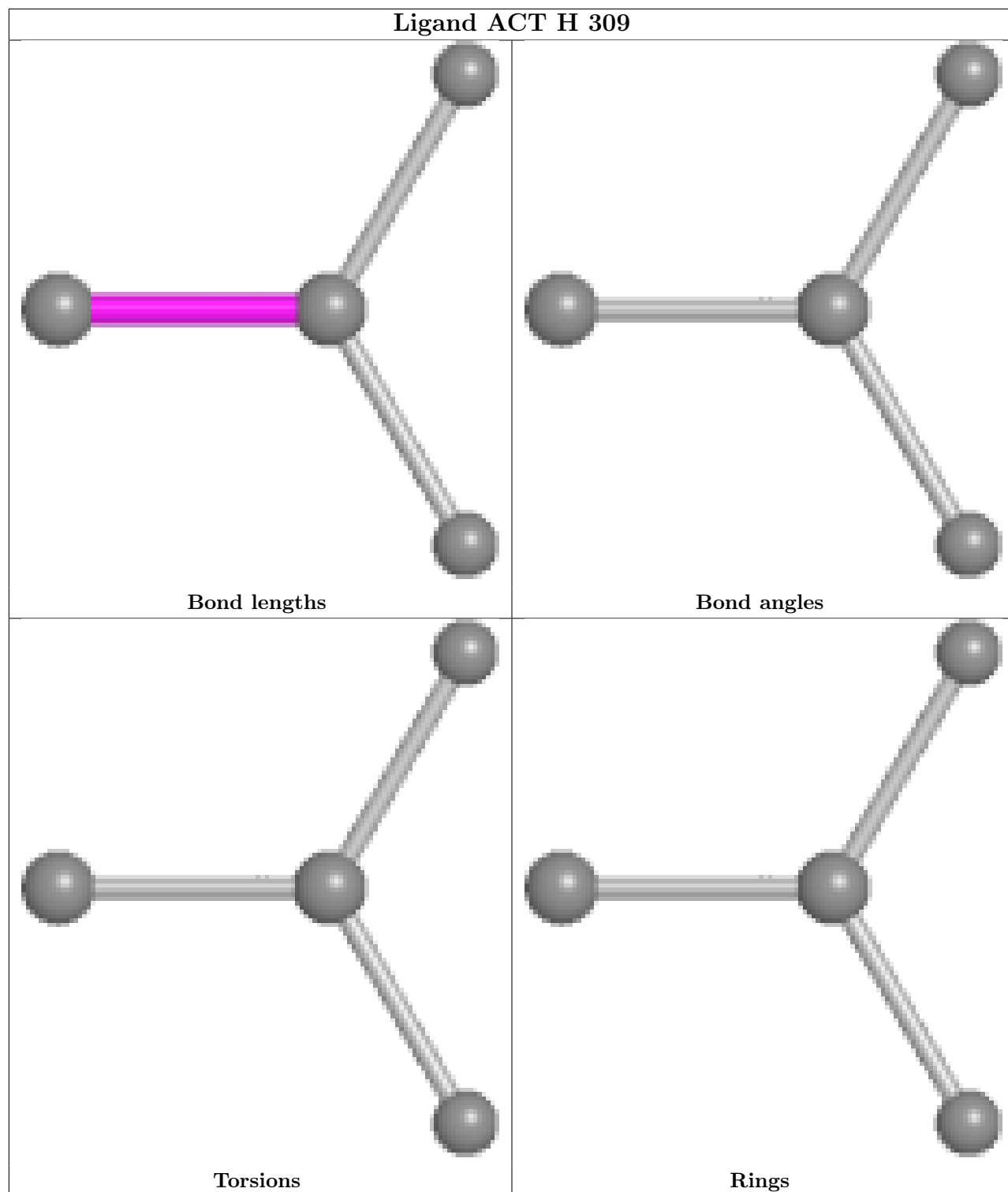




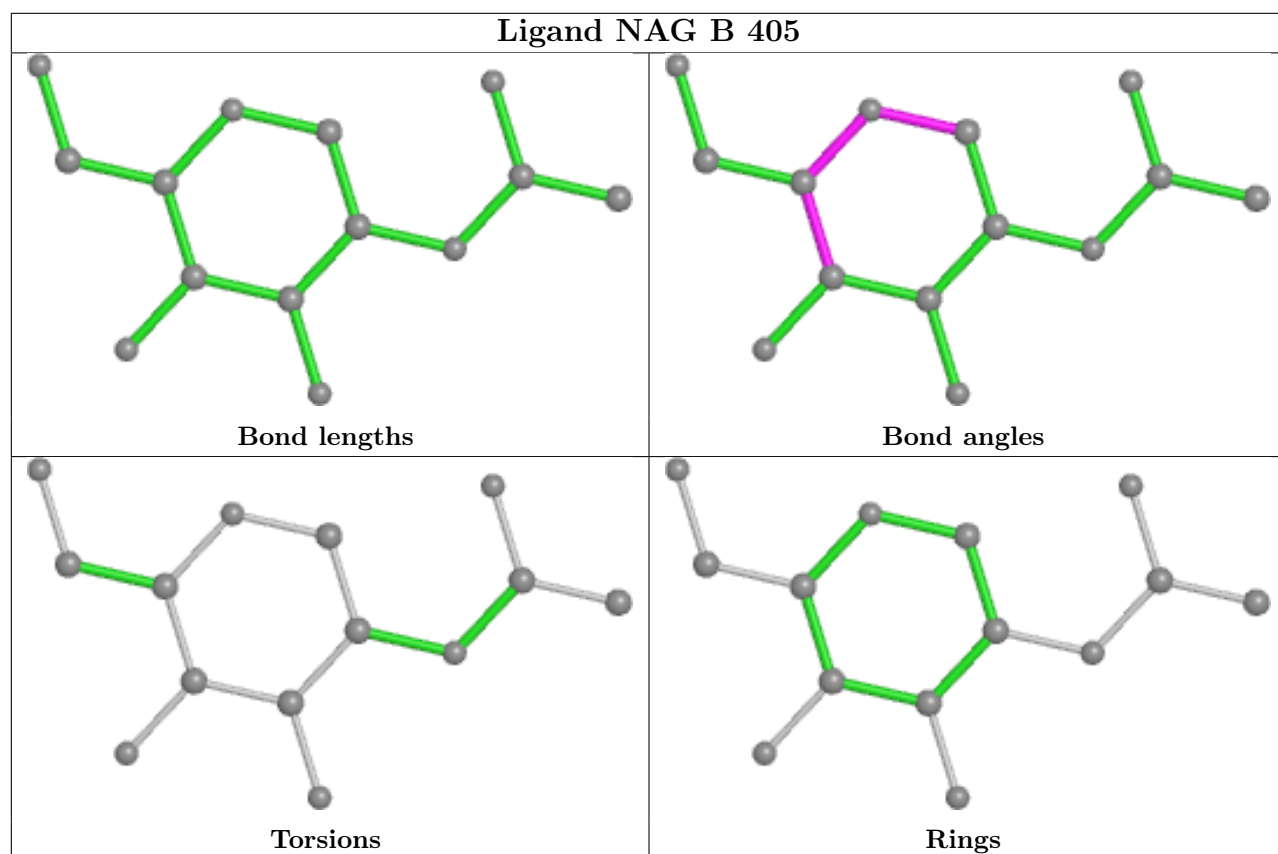
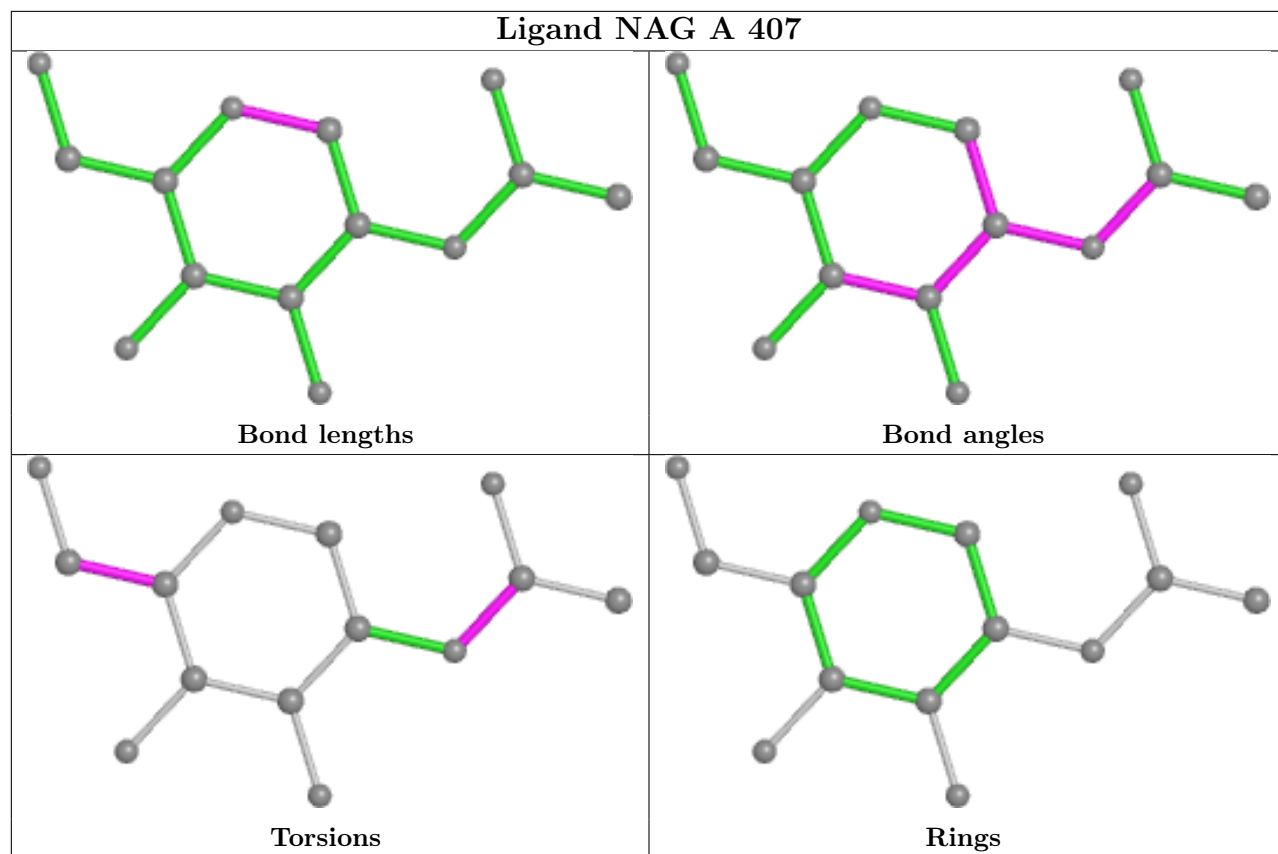


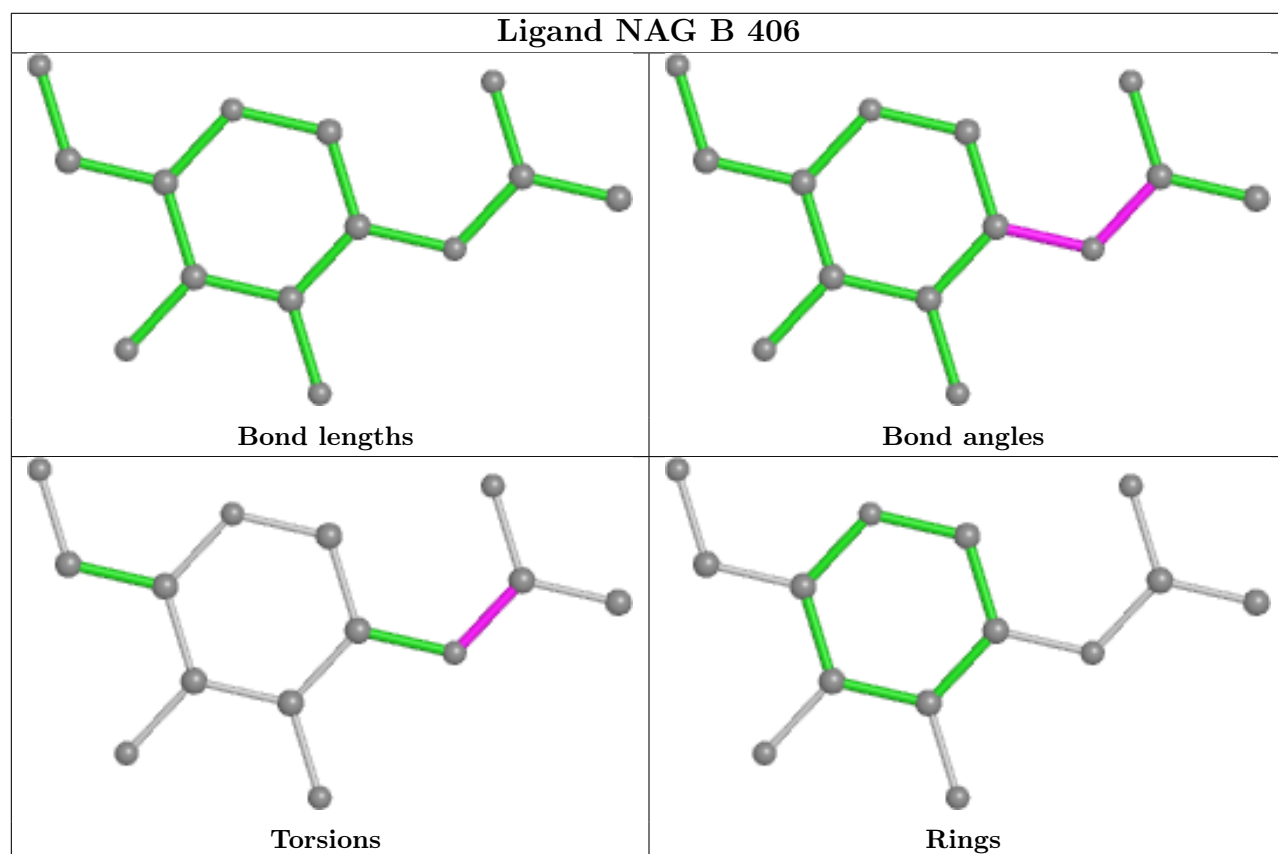
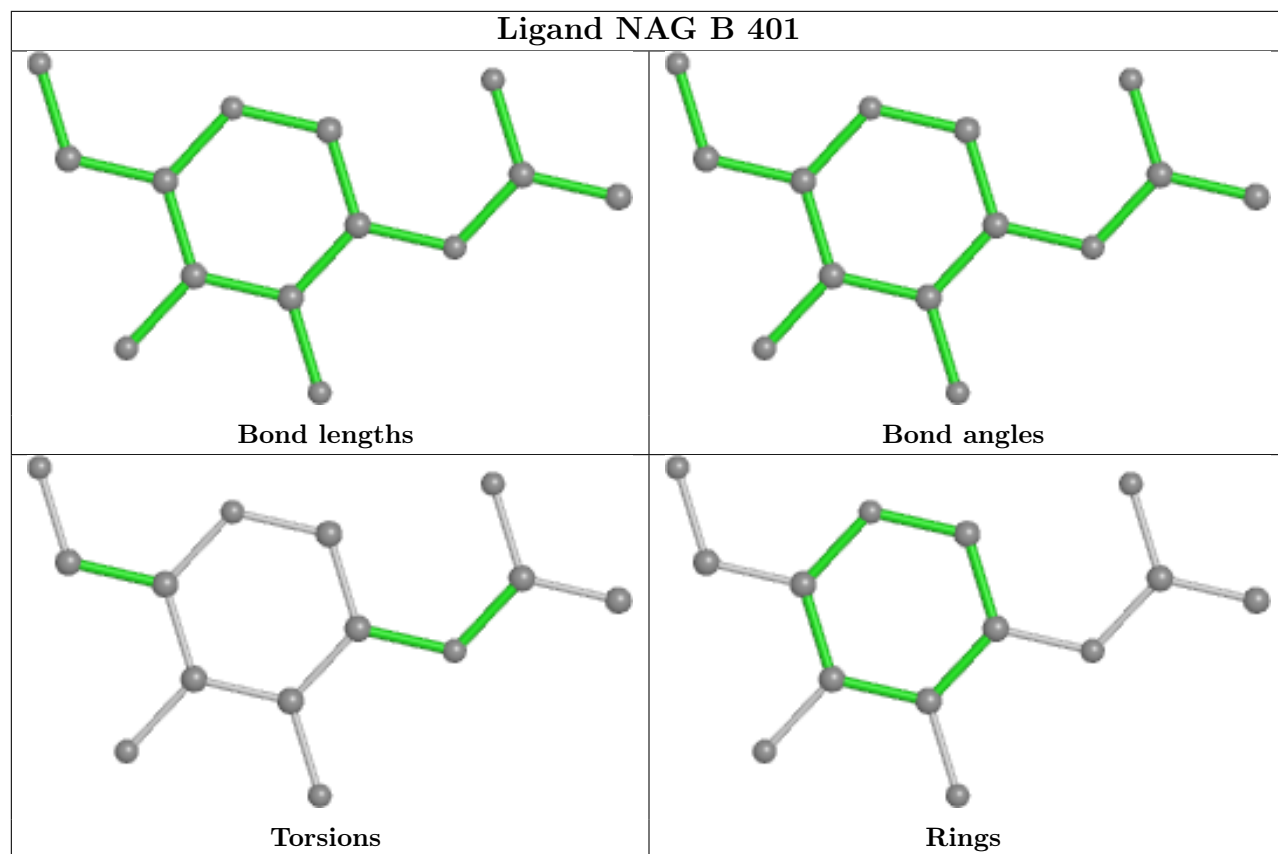












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	286/342 (83%)	0.18	4 (1%) 75 63	47, 72, 115, 158	0
1	B	273/342 (79%)	0.17	2 (0%) 87 80	42, 73, 125, 158	0
2	C	222/227 (97%)	0.10	2 (0%) 84 74	40, 57, 85, 135	0
2	H	221/227 (97%)	0.30	3 (1%) 75 63	42, 64, 93, 133	0
3	D	213/215 (99%)	0.01	0 100 100	40, 59, 79, 107	0
3	L	213/215 (99%)	0.11	0 100 100	45, 64, 94, 113	0
All	All	1428/1568 (91%)	0.15	11 (0%) 86 77	40, 65, 103, 158	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	130	SER	5.3
1	A	72	GLY	3.6
1	B	69	HIS	3.4
2	H	129	LYS	3.1
2	C	131	THR	3.1
1	A	24	LEU	3.0
2	C	130	SER	2.7
2	H	132	SER	2.7
1	A	185	ASN	2.5
1	A	76	THR	2.5
1	B	176	LEU	2.4

### 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](#)

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(Å <sup>2</sup> )	Q<0.9
4	NAG	E	2	14/15	0.80	0.32	66,101,115,120	0
4	NAG	E	1	14/15	0.89	0.28	66,84,96,98	0

### 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(Å <sup>2</sup> )	Q<0.9
6	CA	B	407	1/1	0.07	0.20	92,92,92,92	0
6	CA	A	412	1/1	0.45	0.18	95,95,95,95	0
5	NAG	B	405	14/15	0.56	0.54	84,103,114,119	0
6	CA	D	306	1/1	0.59	0.24	79,79,79,79	0
6	CA	B	409	1/1	0.66	0.18	88,88,88,88	0
6	CA	C	311	1/1	0.67	0.22	82,82,82,82	0
6	CA	D	303	1/1	0.69	0.23	84,84,84,84	0
5	NAG	A	406	14/15	0.69	0.33	85,111,120,121	0
5	NAG	B	404	14/15	0.69	0.30	91,119,131,133	0
6	CA	H	304	1/1	0.70	0.17	89,89,89,89	0
6	CA	D	305	1/1	0.71	0.18	98,98,98,98	0
7	ACT	H	308	4/4	0.72	0.39	66,66,69,76	0
5	NAG	A	401	14/15	0.77	0.32	101,126,136,136	0
5	NAG	B	402	14/15	0.77	0.28	65,88,104,110	0
8	CAC	A	417	5/5	0.77	0.28	77,95,109,172	0
6	CA	C	303	1/1	0.77	0.17	85,85,85,85	0
5	NAG	A	405	14/15	0.78	0.38	86,107,120,125	0
5	NAG	B	401	14/15	0.78	0.30	95,109,117,120	0
5	NAG	B	403	14/15	0.79	0.24	107,119,130,135	0
6	CA	B	408	1/1	0.80	0.18	71,71,71,71	0
5	NAG	A	402	14/15	0.81	0.23	96,107,118,119	0
6	CA	A	410	1/1	0.81	0.17	66,66,66,66	0
6	CA	C	307	1/1	0.82	0.34	90,90,90,90	0
6	CA	C	301	1/1	0.83	0.15	73,73,73,73	0
7	ACT	A	416	4/4	0.83	0.25	70,75,80,86	0

*Continued on next page...*

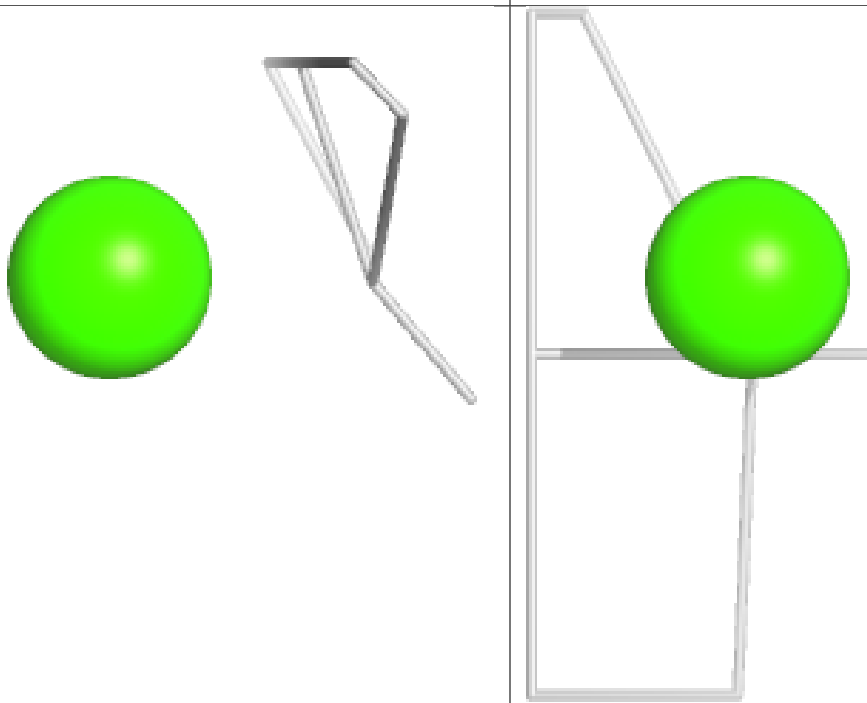
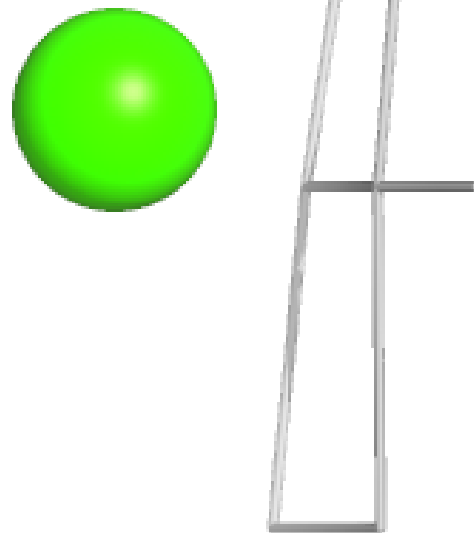
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	406	14/15	0.83	0.30	91,108,115,117	0
7	ACT	L	304	4/4	0.84	0.27	61,61,62,67	0
6	CA	C	302	1/1	0.86	0.14	77,77,77,77	0
6	CA	H	306	1/1	0.86	0.08	103,103,103,103	0
6	CA	C	305	1/1	0.86	0.10	72,72,72,72	0
5	NAG	A	403	14/15	0.86	0.28	91,102,106,107	0
6	CA	L	301	1/1	0.86	0.14	81,81,81,81	0
5	NAG	A	404	14/15	0.87	0.22	71,79,86,94	0
5	NAG	A	407	14/15	0.87	0.20	77,82,96,101	0
6	CA	D	302	1/1	0.87	0.14	80,80,80,80	0
7	ACT	B	413	4/4	0.87	0.26	58,60,63,69	0
6	CA	C	306	1/1	0.88	0.14	73,73,73,73	0
6	CA	C	309	1/1	0.88	0.14	82,82,82,82	0
6	CA	H	305	1/1	0.88	0.32	87,87,87,87	0
6	CA	H	307	1/1	0.89	0.20	72,72,72,72	0
6	CA	L	303	1/1	0.89	0.21	83,83,83,83	0
6	CA	A	409	1/1	0.89	0.11	60,60,60,60	0
9	PGE	C	312	10/10	0.89	0.36	39,48,54,61	0
7	ACT	D	307	4/4	0.90	0.27	47,54,54,57	0
7	ACT	A	415	4/4	0.90	0.19	42,52,55,58	0
6	CA	B	412	1/1	0.90	0.15	100,100,100,100	0
7	ACT	B	414	4/4	0.91	0.21	71,77,80,82	0
7	ACT	H	309	4/4	0.91	0.42	50,61,64,84	0
6	CA	C	304	1/1	0.91	0.21	78,78,78,78	0
7	ACT	A	414	4/4	0.91	0.22	58,68,68,69	0
6	CA	C	308	1/1	0.91	0.16	84,84,84,84	0
6	CA	A	411	1/1	0.92	0.12	74,74,74,74	0
6	CA	H	302	1/1	0.92	0.11	71,71,71,71	0
6	CA	H	301	1/1	0.94	0.16	64,64,64,64	0
6	CA	H	303	1/1	0.94	0.23	74,74,74,74	0
6	CA	D	301	1/1	0.94	0.17	65,65,65,65	0
6	CA	A	408	1/1	0.94	0.13	61,61,61,61	0
6	CA	B	411	1/1	0.94	0.20	83,83,83,83	0
6	CA	L	302	1/1	0.94	0.10	75,75,75,75	0
6	CA	A	413	1/1	0.95	0.18	80,80,80,80	0
6	CA	C	310	1/1	0.96	0.30	68,68,68,68	0
6	CA	B	410	1/1	0.97	0.07	72,72,72,72	0
6	CA	D	304	1/1	0.97	0.24	66,66,66,66	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.

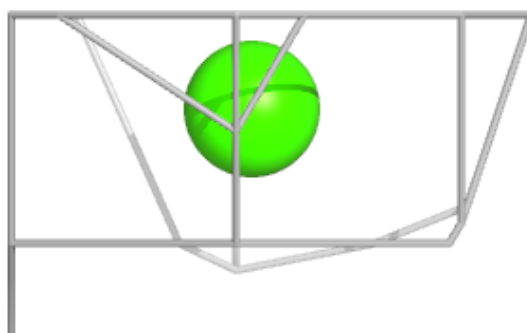
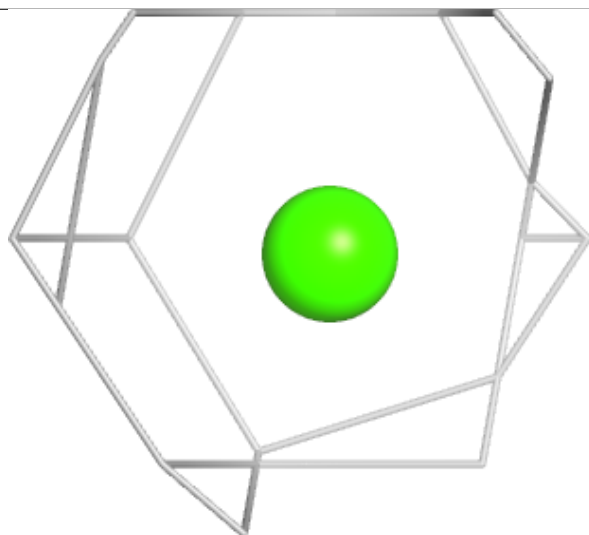
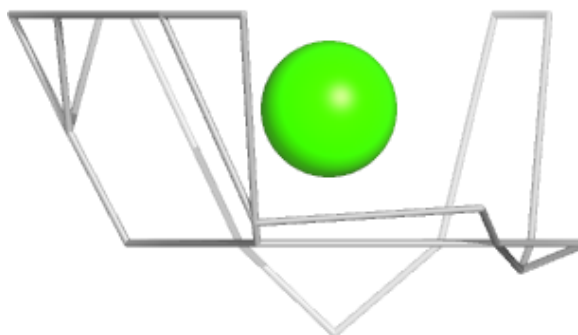
**Electron density around CA B 407:**

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



**Electron density around CA A 412:**

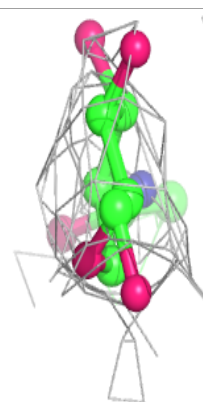
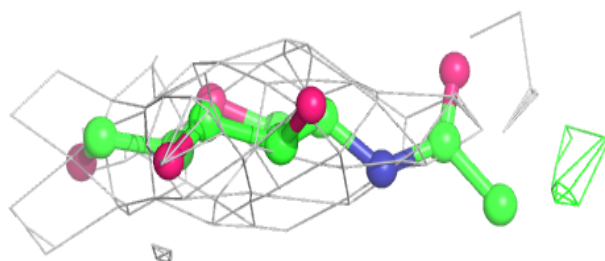
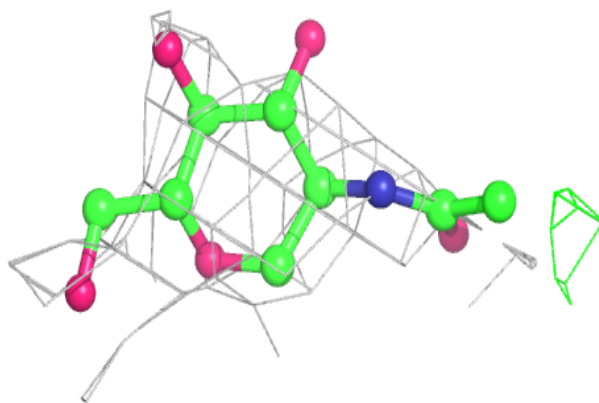
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





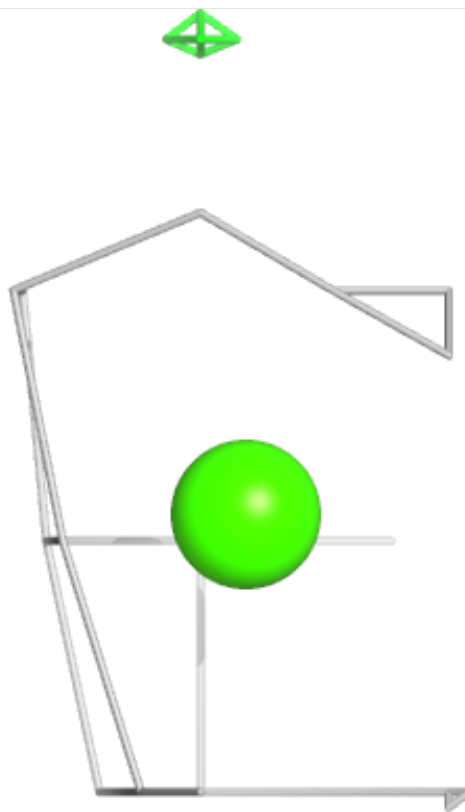
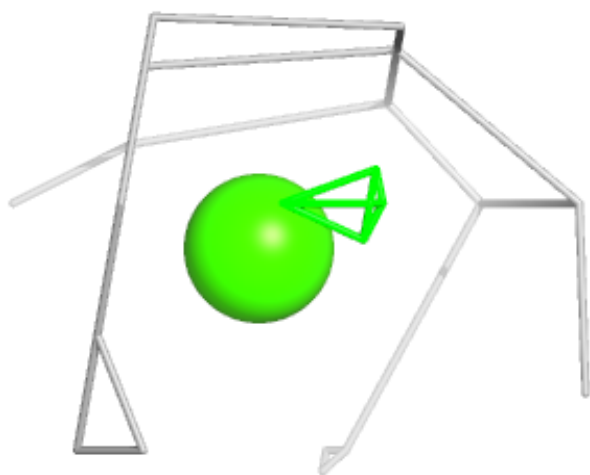
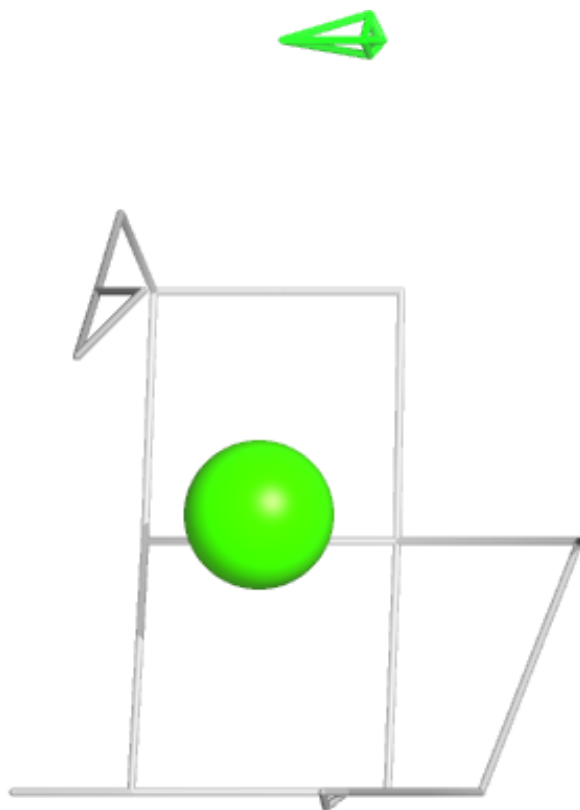
**Electron density around NAG B 405:**

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



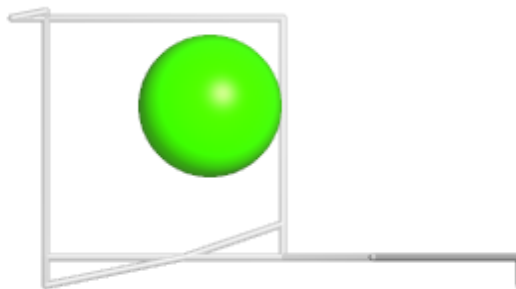
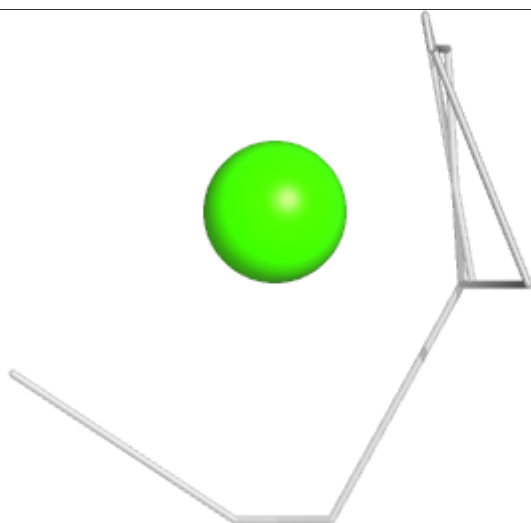
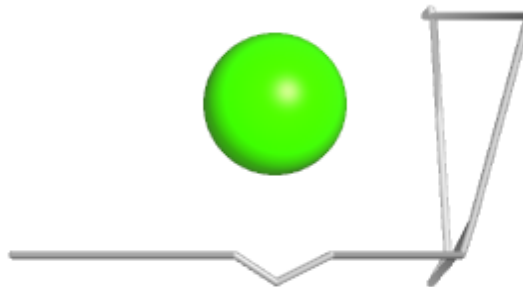
**Electron density around CA D 306:**

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



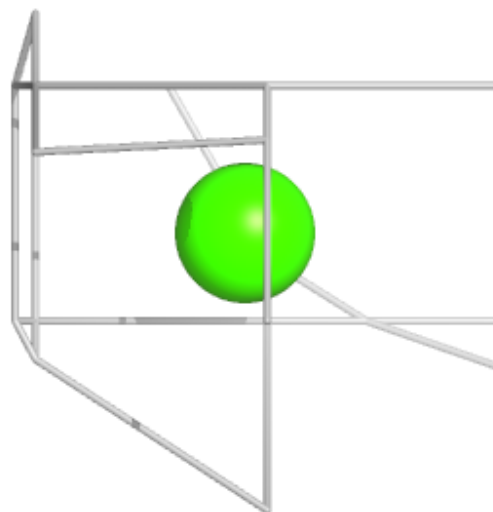
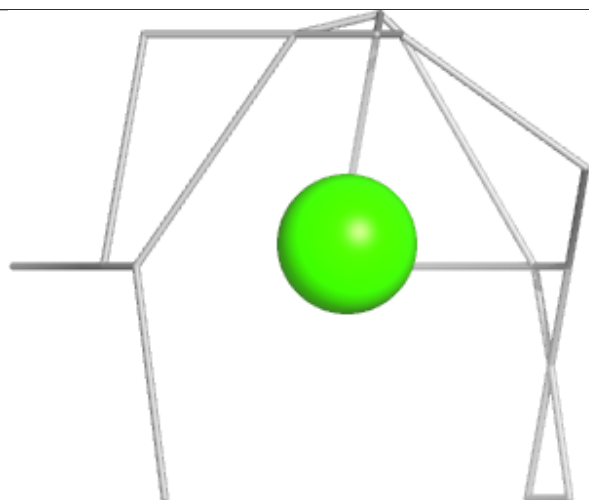
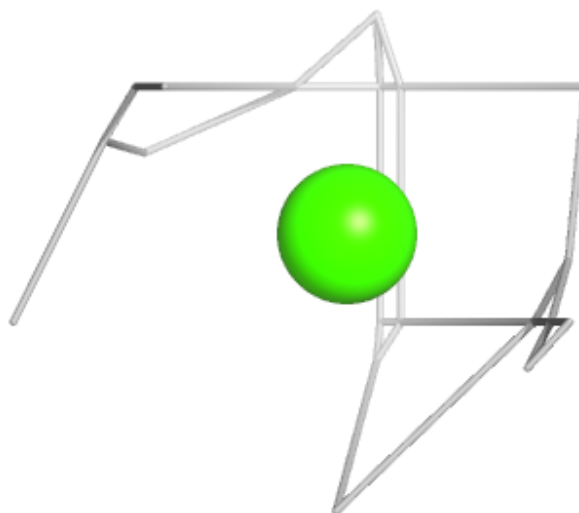
**Electron density around CA B 409:**

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and green (positive)



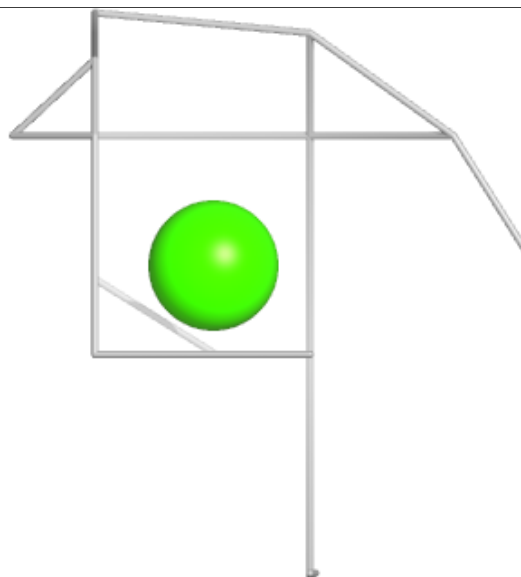
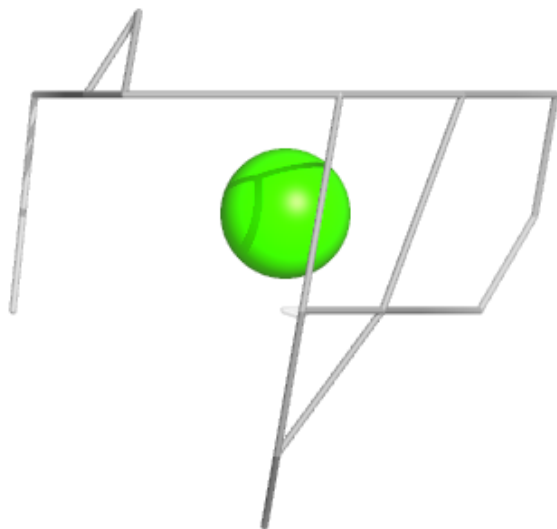
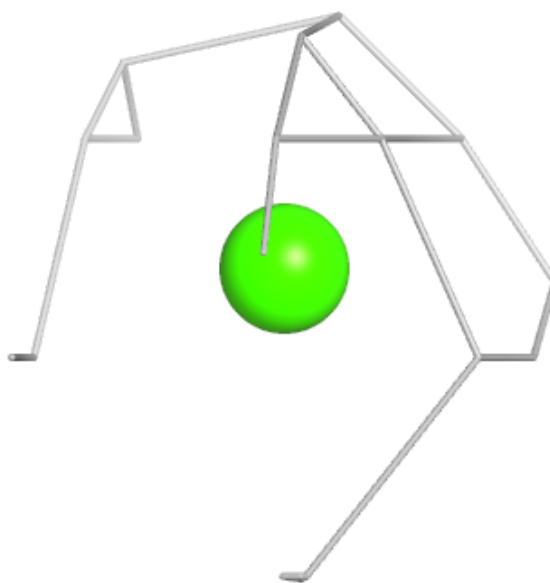
**Electron density around CA C 311:**

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



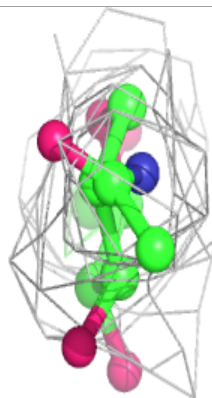
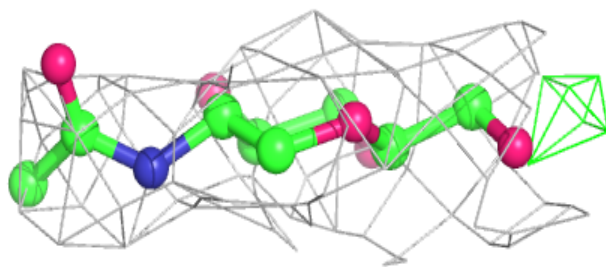
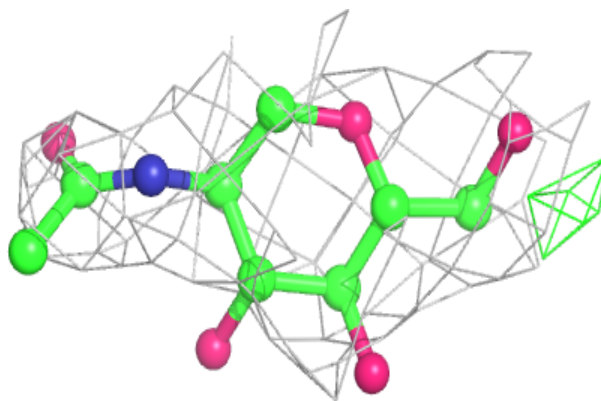
**Electron density around CA D 303:**

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



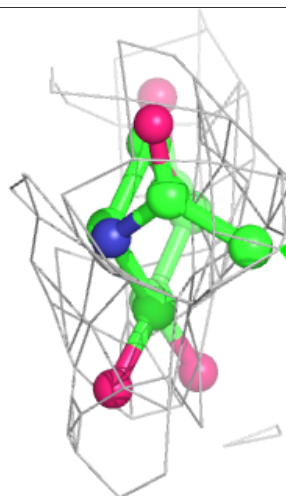
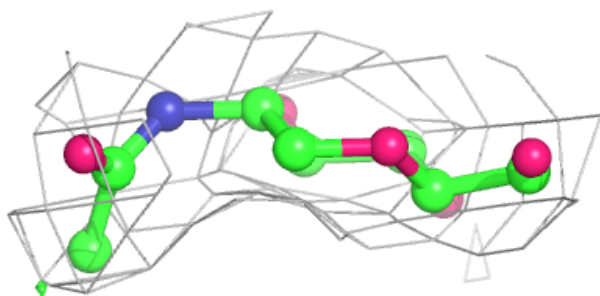
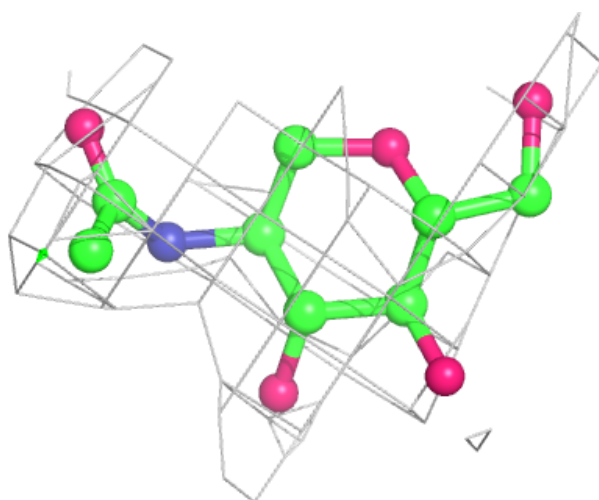
**Electron density around NAG A 406:**

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



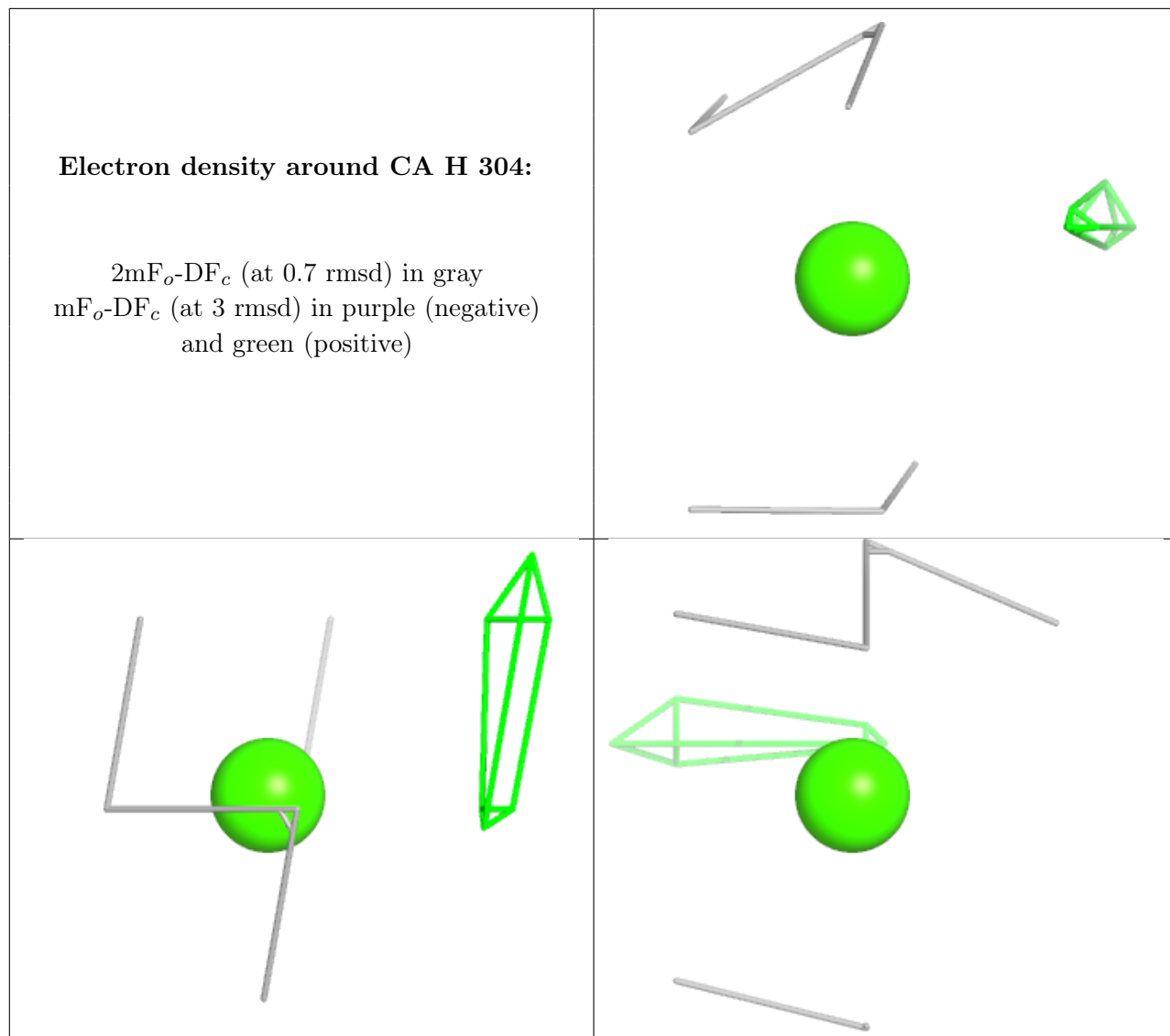
**Electron density around NAG B 404:**

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and green (positive)



**Electron density around CA H 304:**

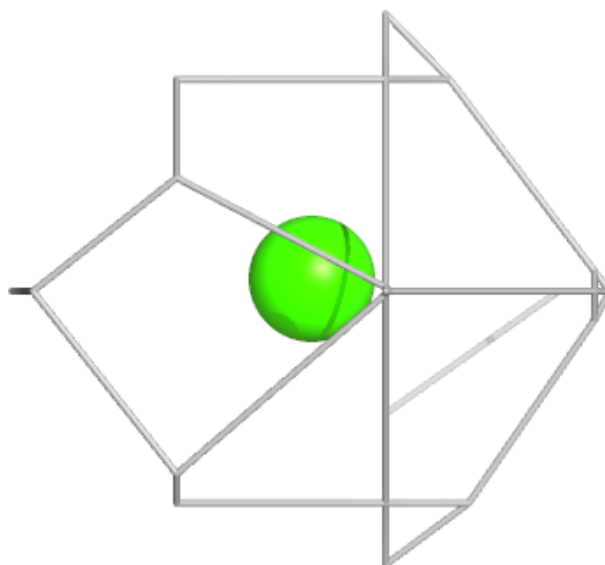
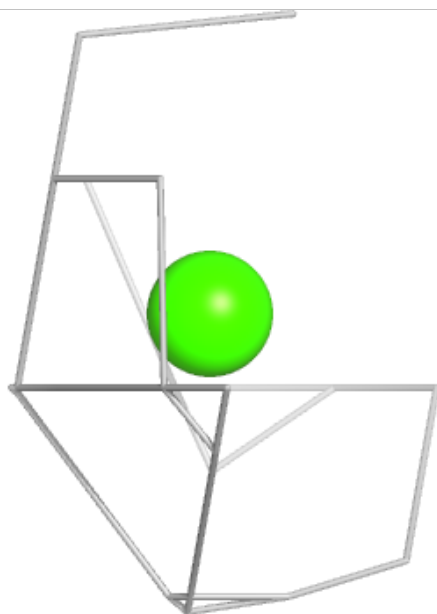
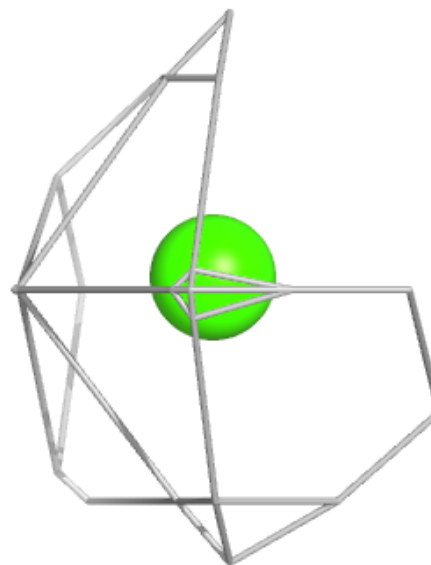
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





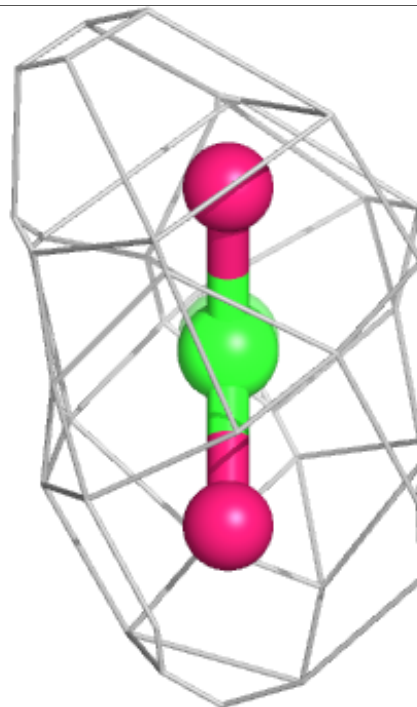
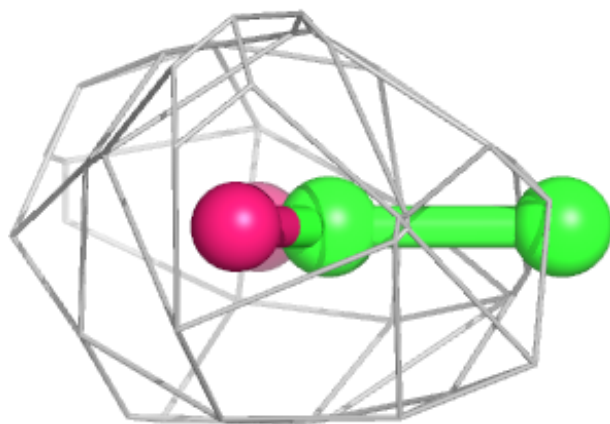
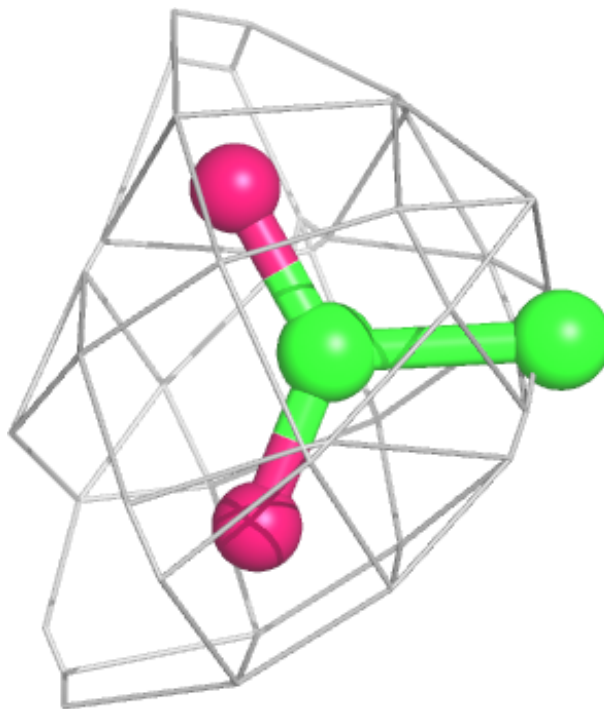
**Electron density around CA D 305:**

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



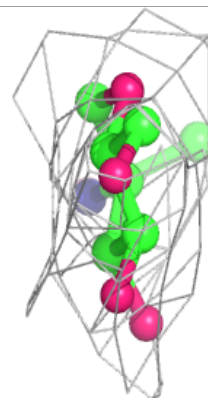
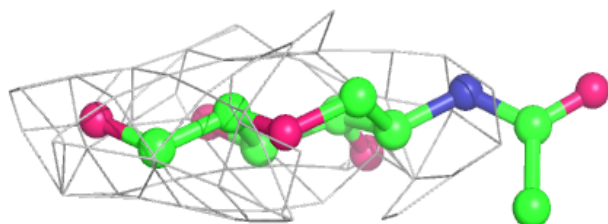
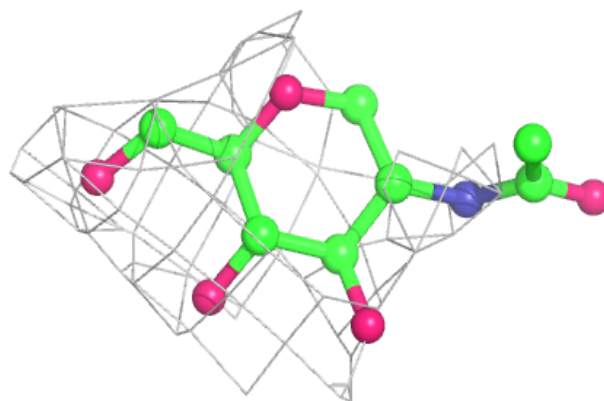
**Electron density around ACT H 308:**

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

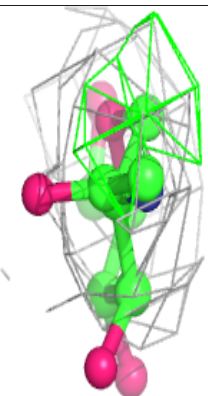
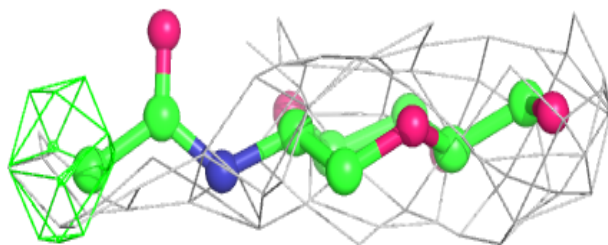
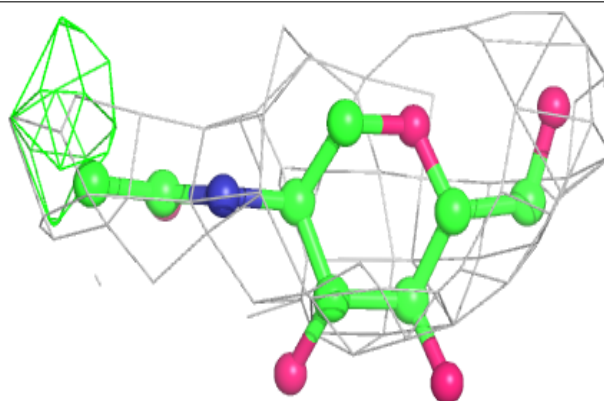


**Electron density around NAG A 401:**

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

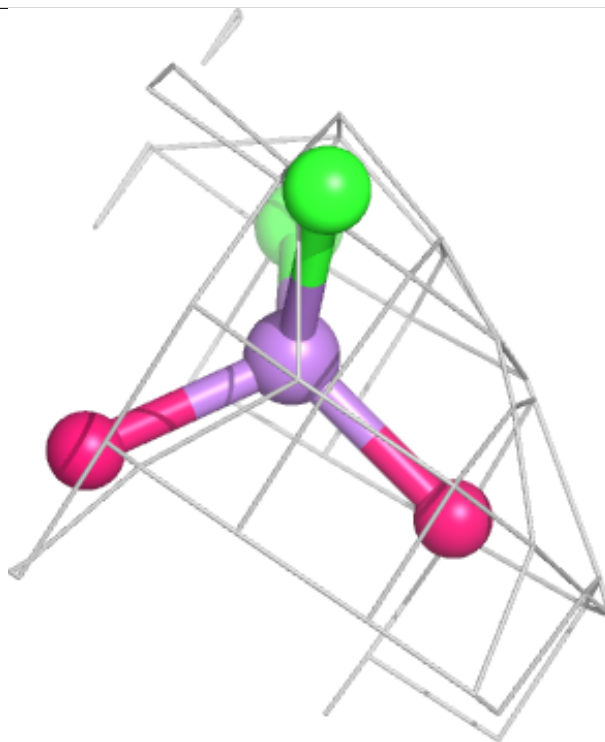
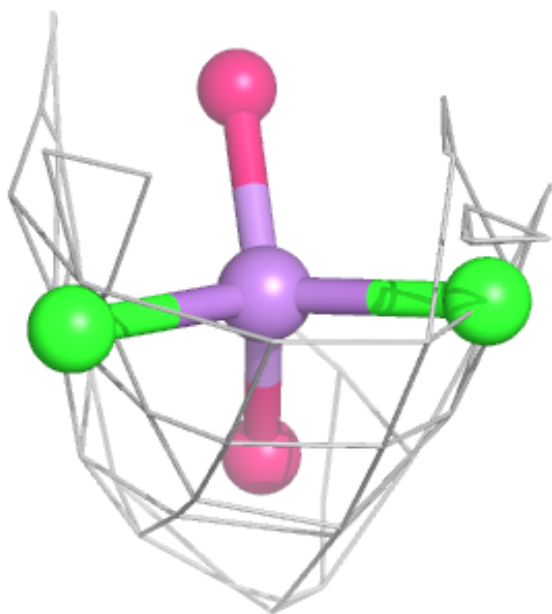
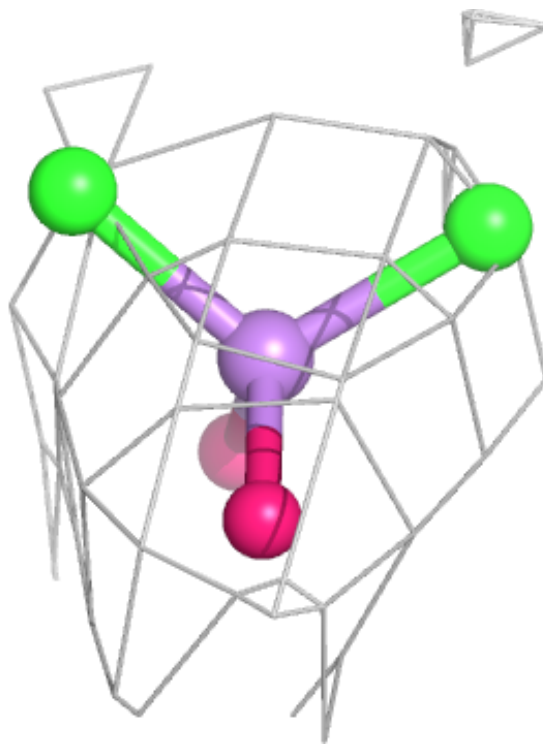
**Electron density around NAG B 402:**

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



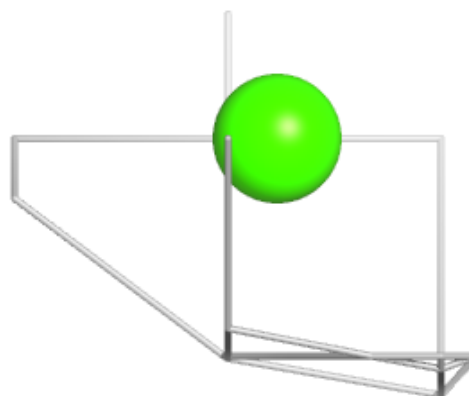
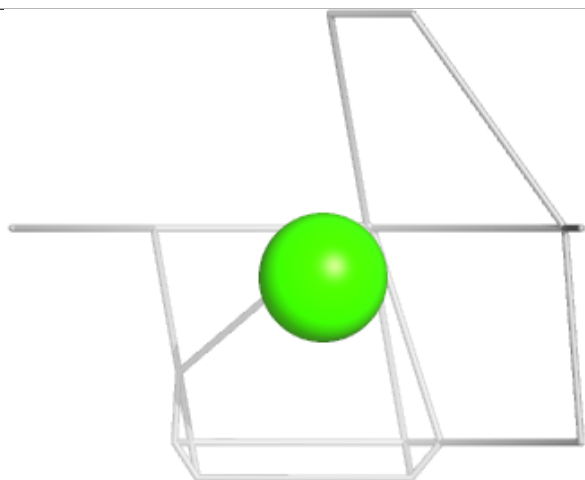
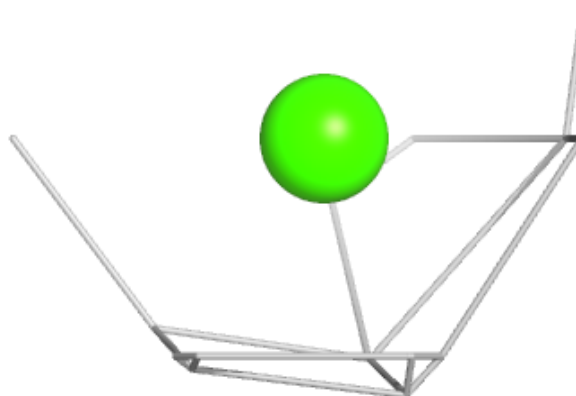
**Electron density around CAC A 417:**

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



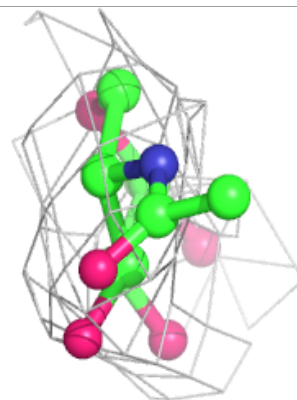
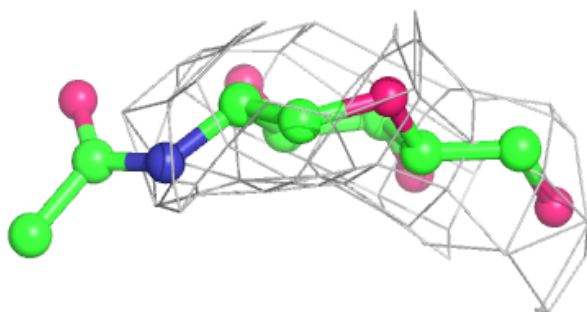
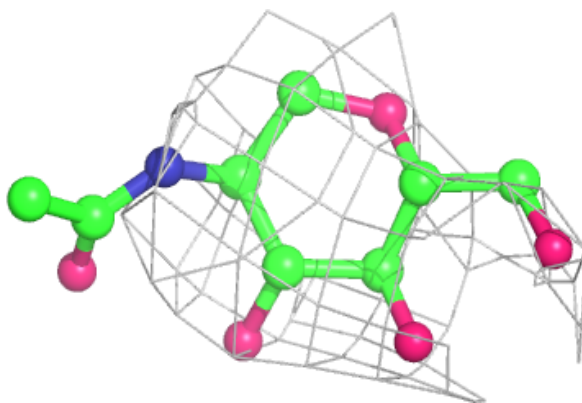
**Electron density around CA C 303:**

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

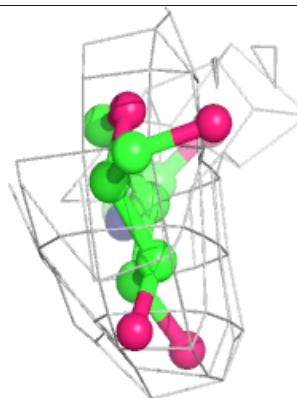
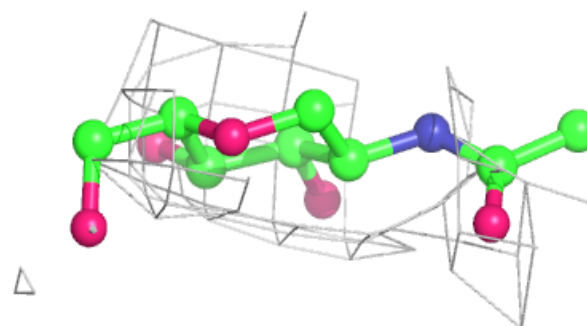
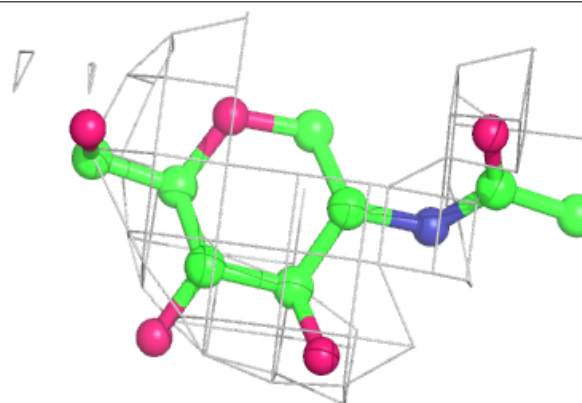


**Electron density around NAG A 405:**

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

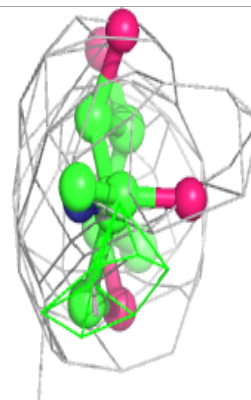
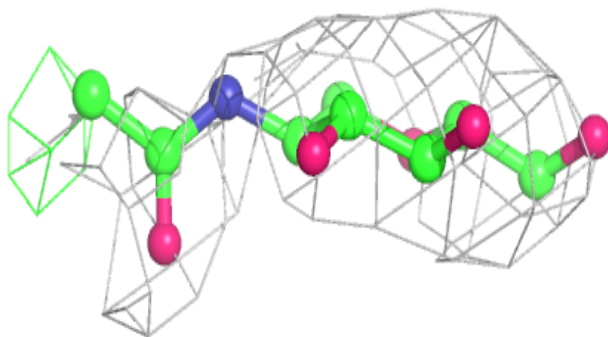
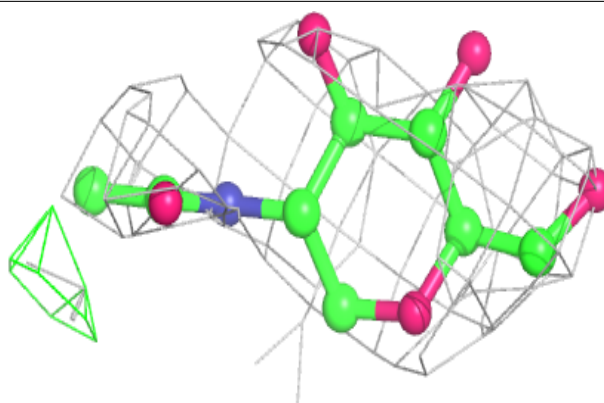
**Electron density around NAG B 401:**

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



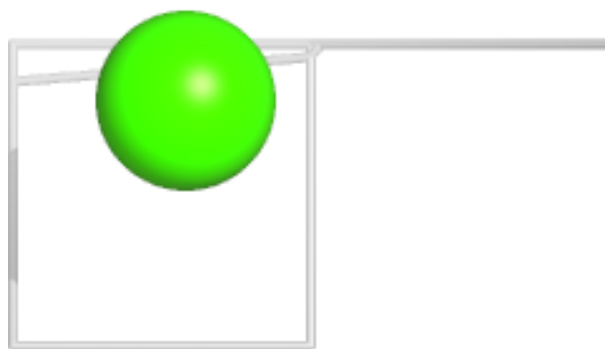
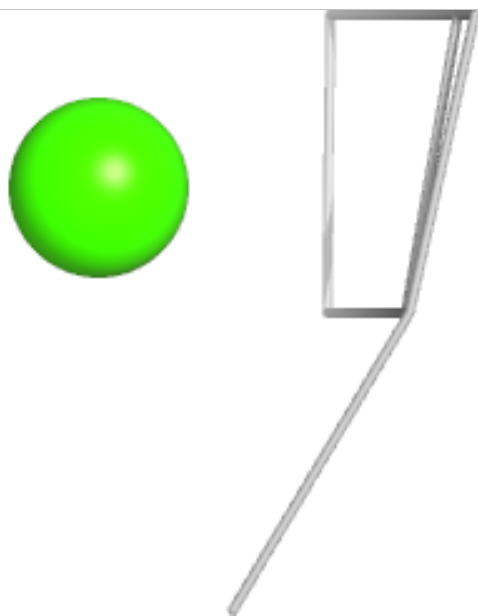
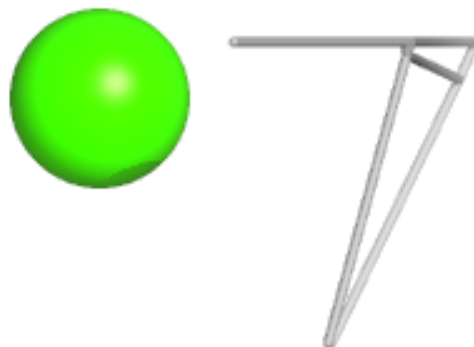
**Electron density around NAG B 403:**

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



**Electron density around CA B 408:**

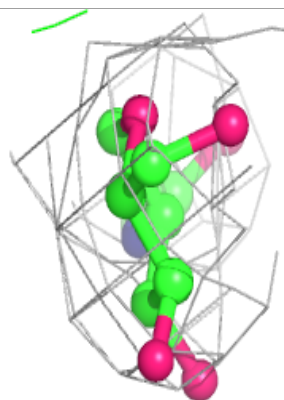
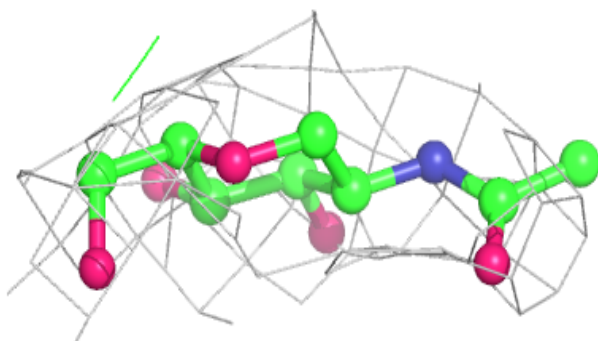
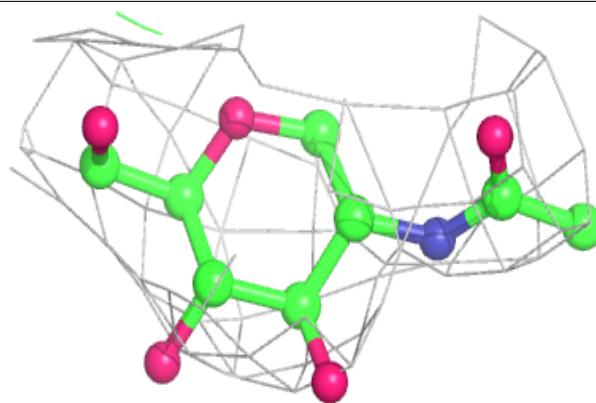
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





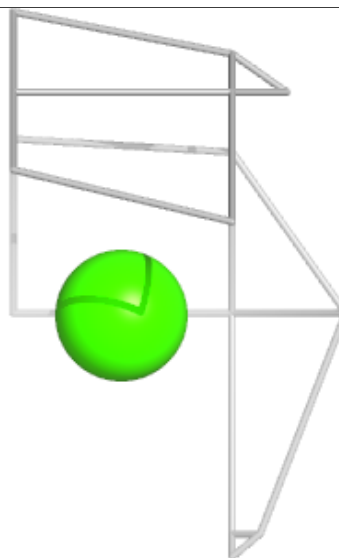
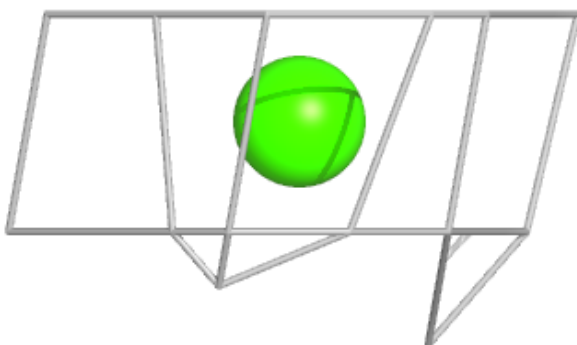
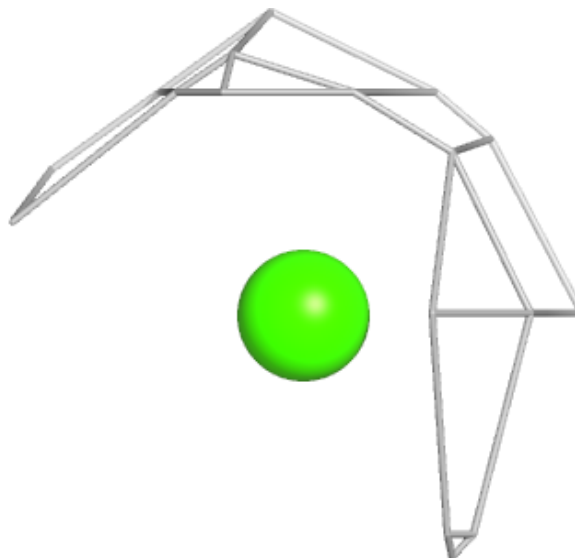
**Electron density around NAG A 402:**

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



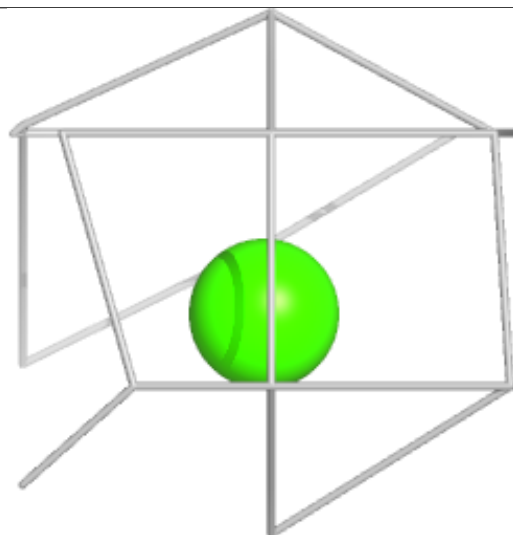
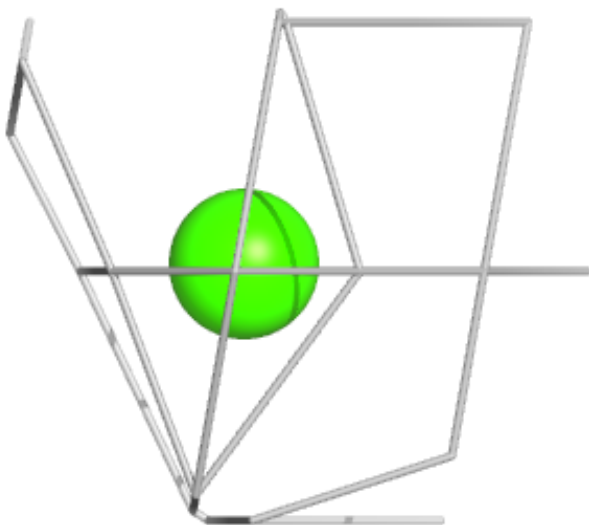
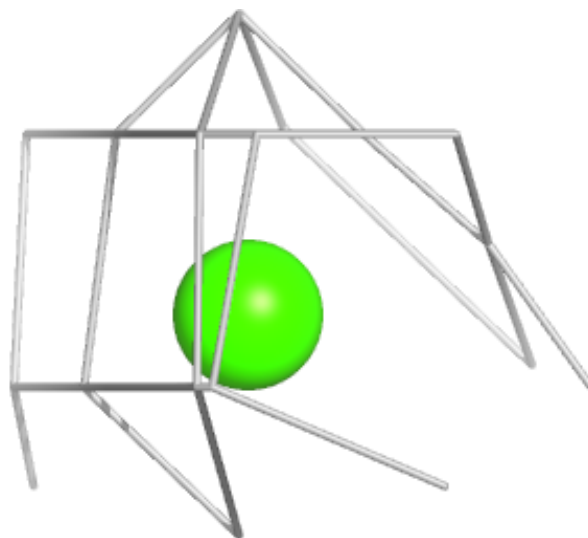
**Electron density around CA A 410:**

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



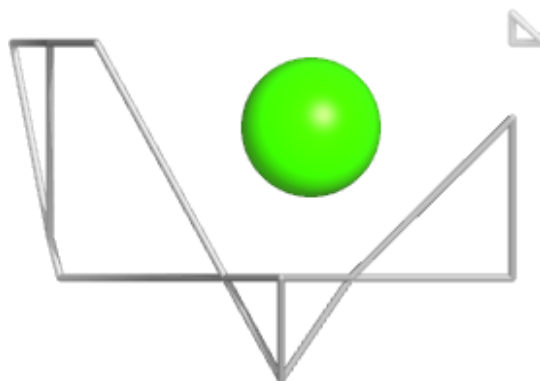
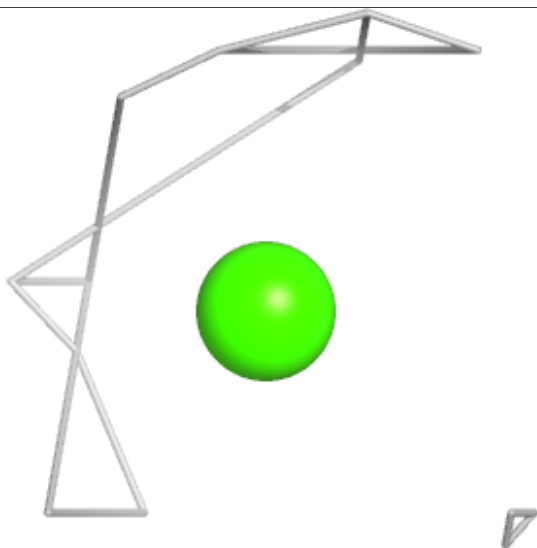
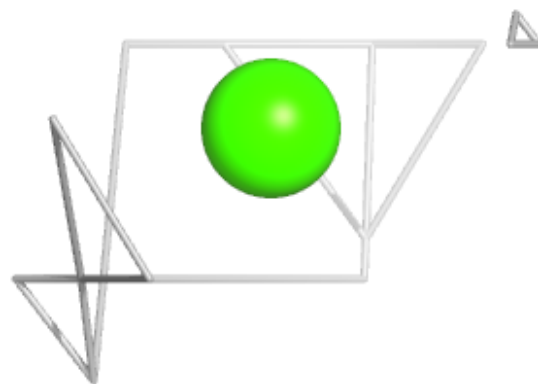
**Electron density around CA C 307:**

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



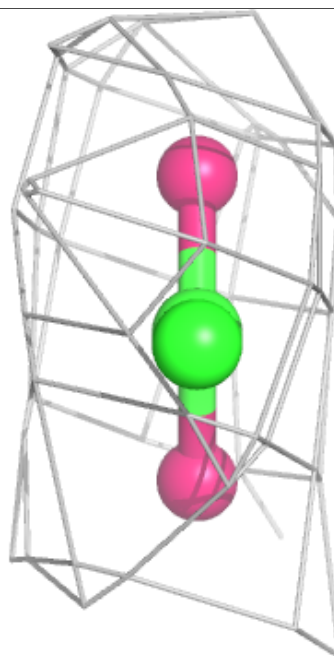
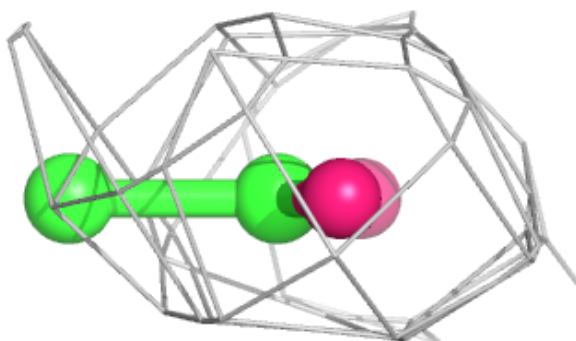
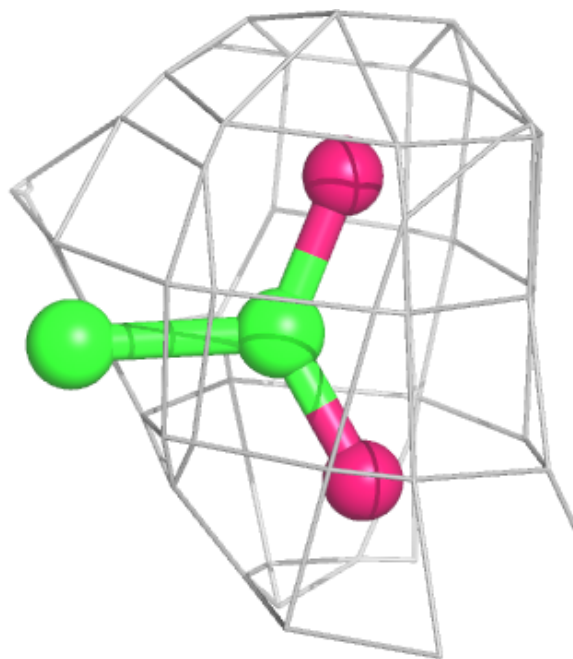
**Electron density around CA C 301:**

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



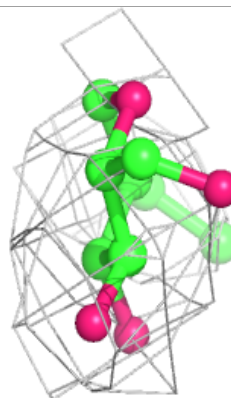
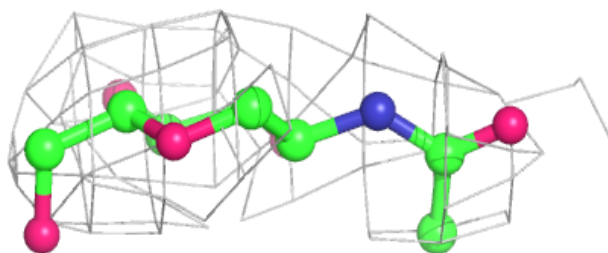
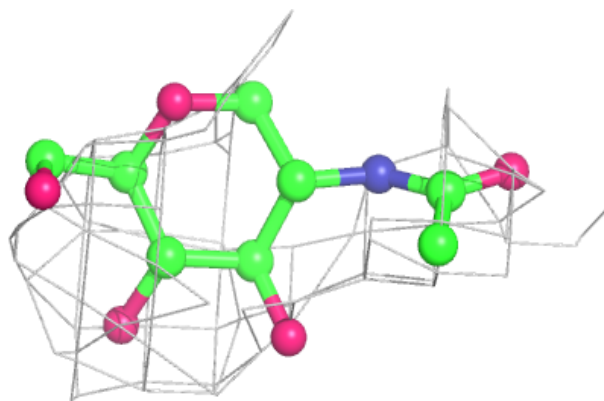
**Electron density around ACT A 416:**

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



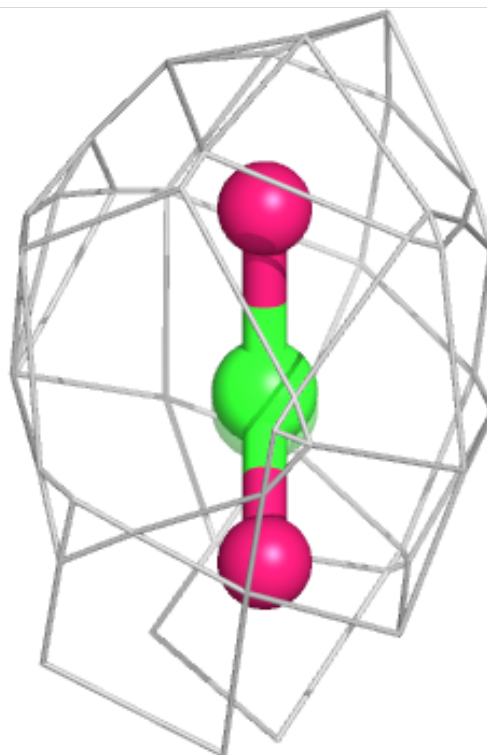
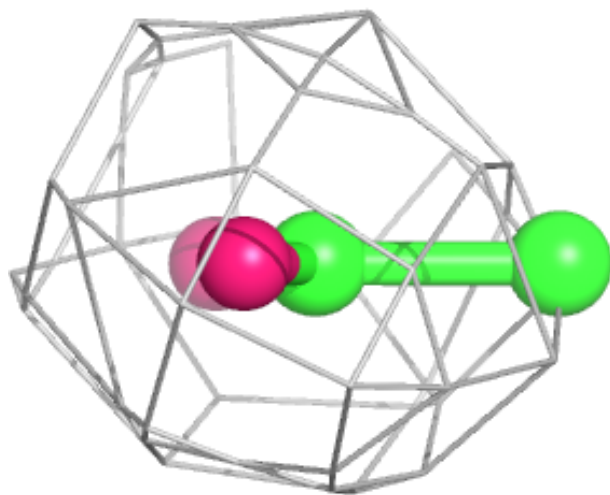
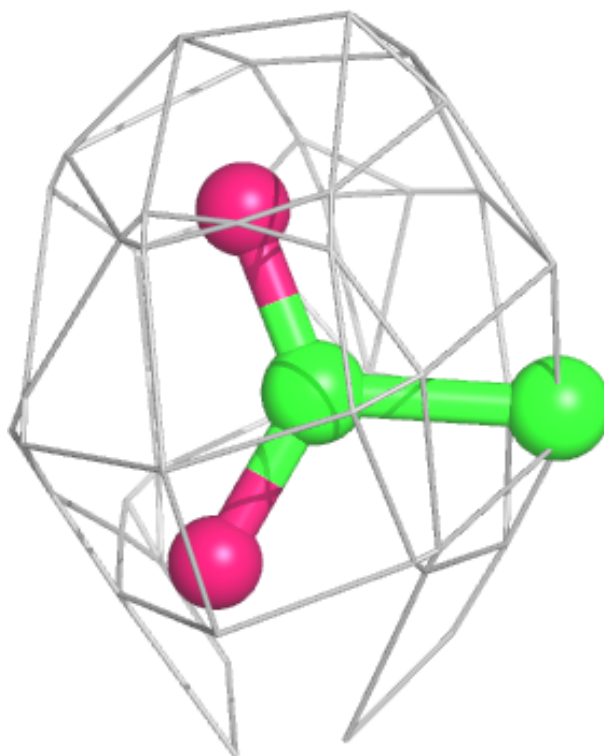
**Electron density around NAG B 406:**

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



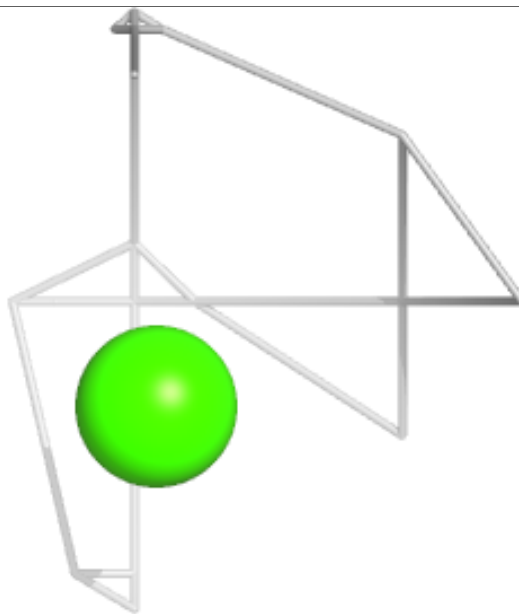
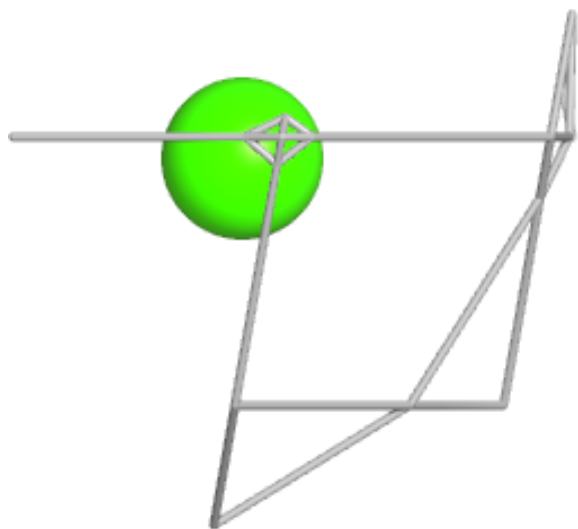
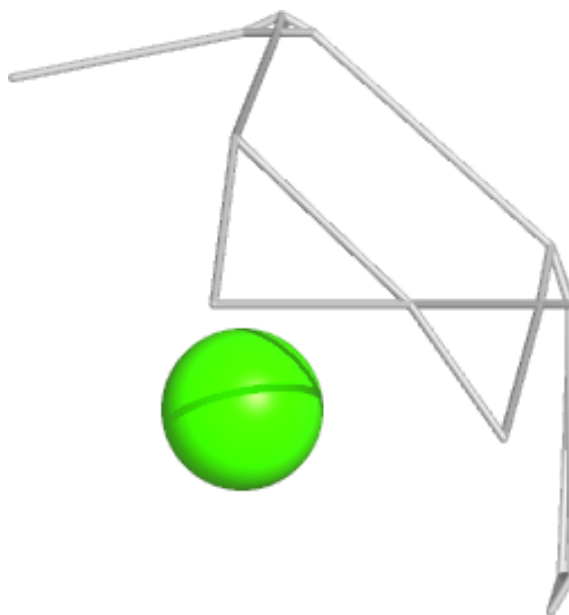
**Electron density around ACT L 304:**

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



**Electron density around CA C 302:**

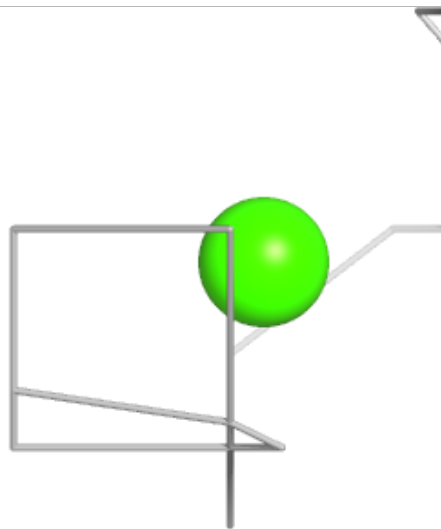
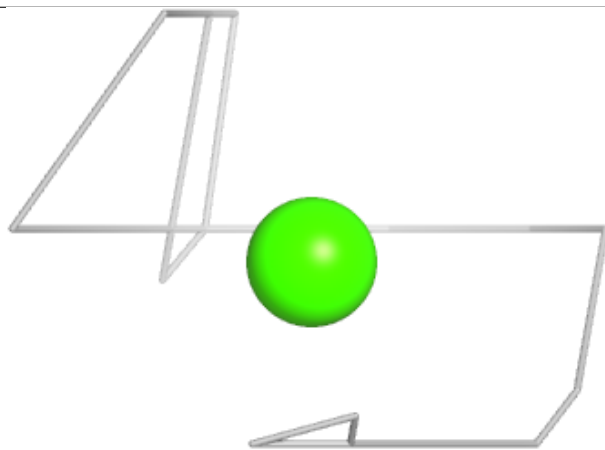
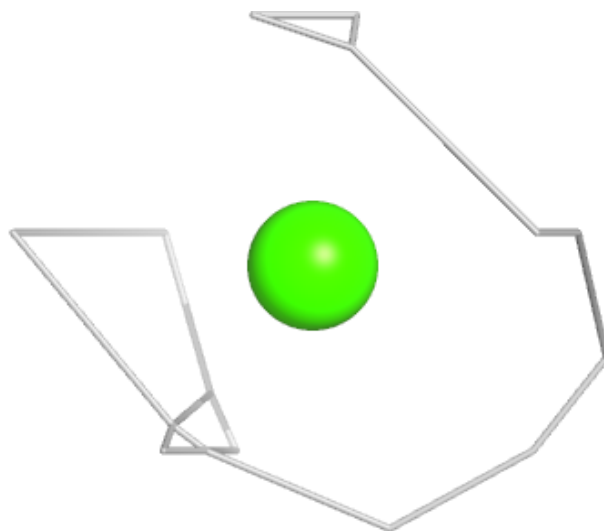
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





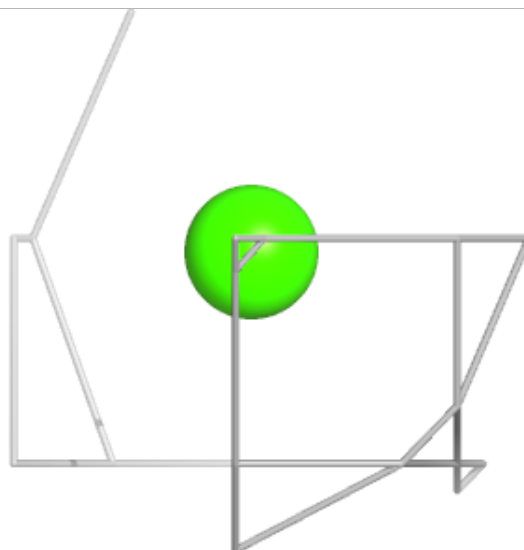
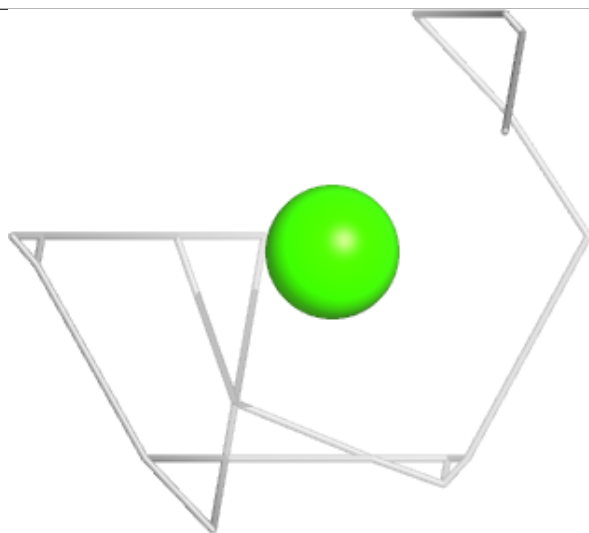
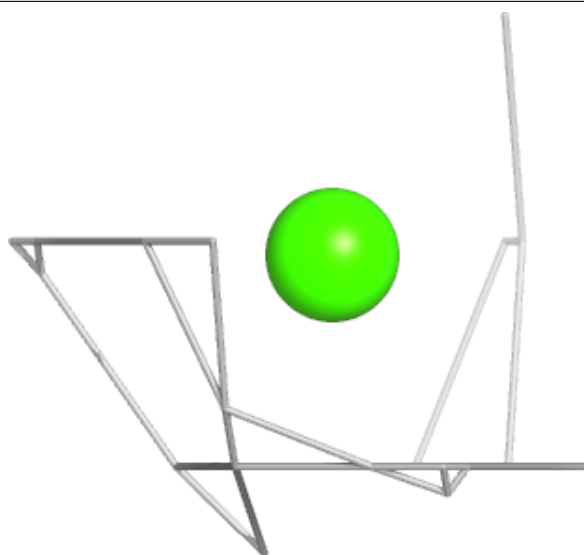
**Electron density around CA H 306:**

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



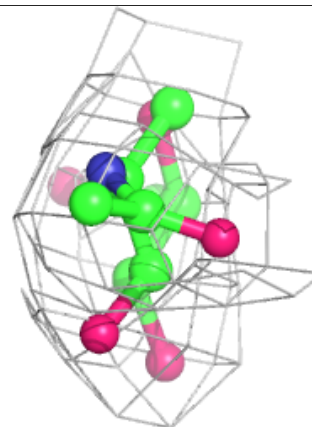
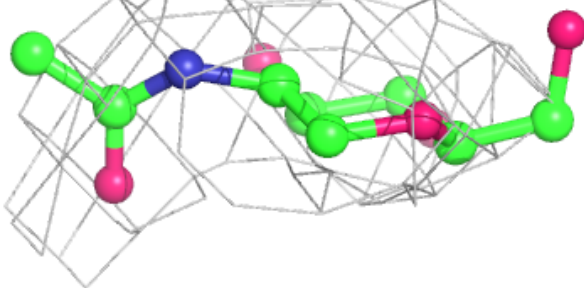
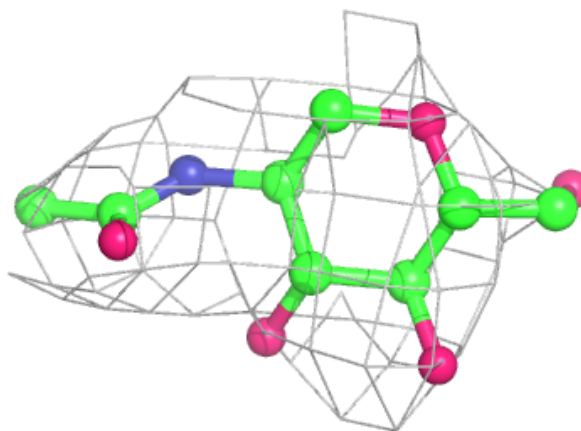
**Electron density around CA C 305:**

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



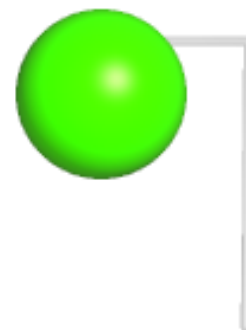
**Electron density around NAG A 403:**

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



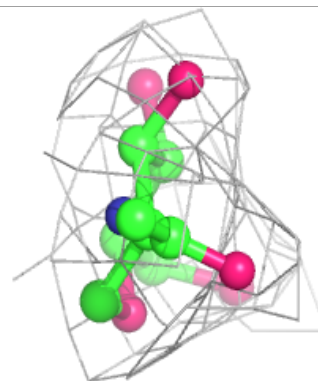
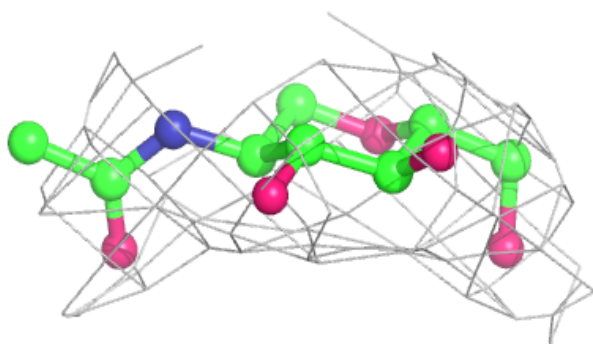
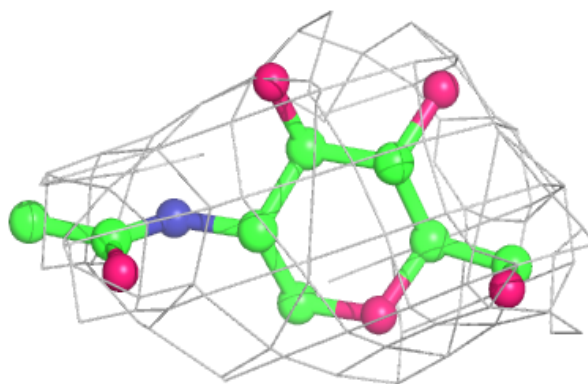
**Electron density around CA L 301:**

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

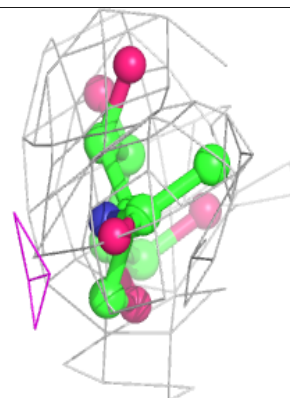
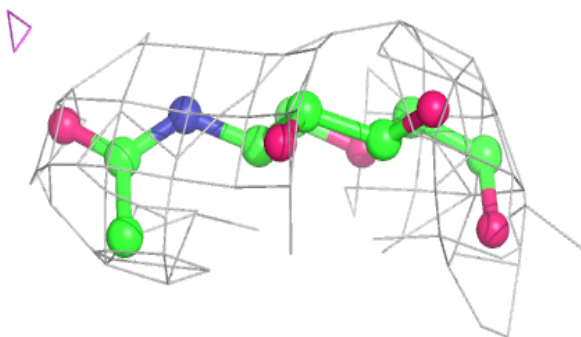
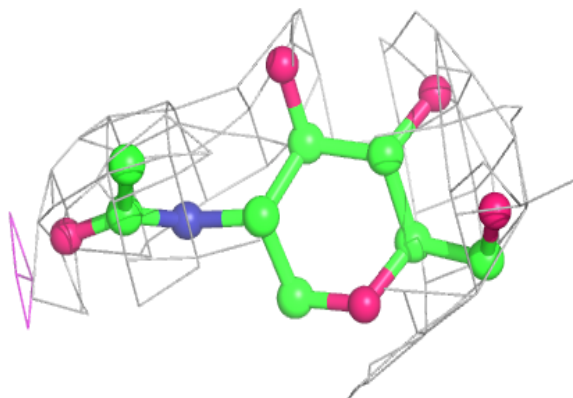


**Electron density around NAG A 404:**

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

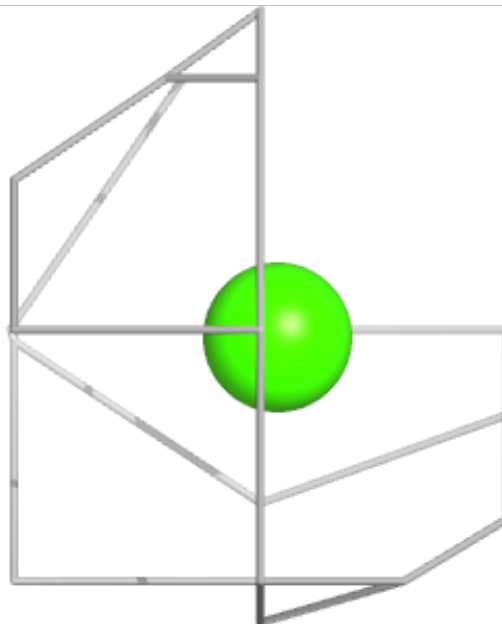
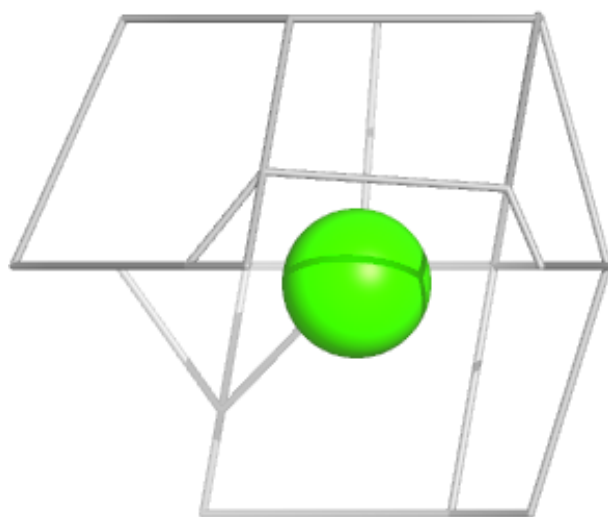
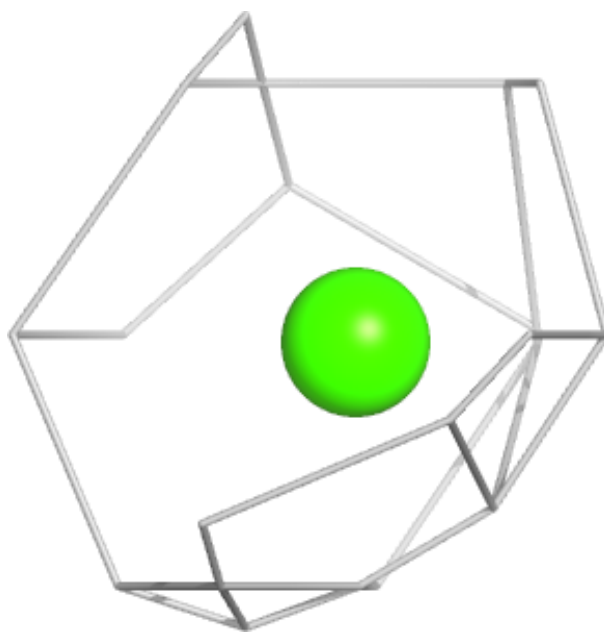
**Electron density around NAG A 407:**

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



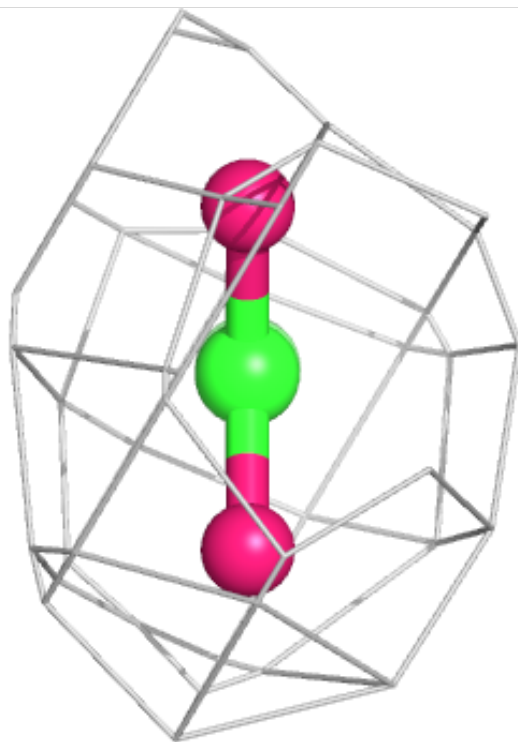
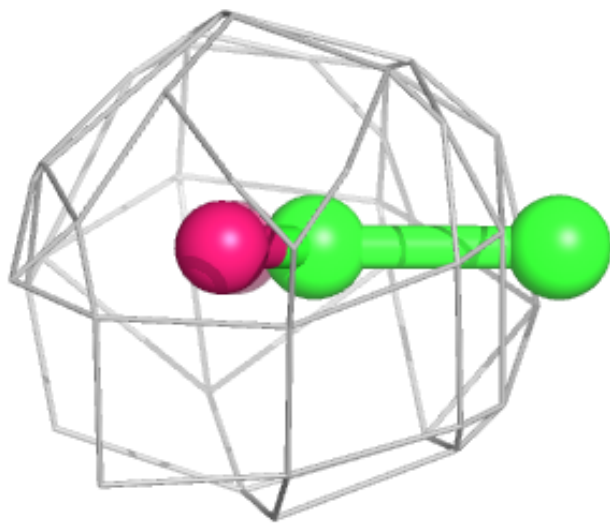
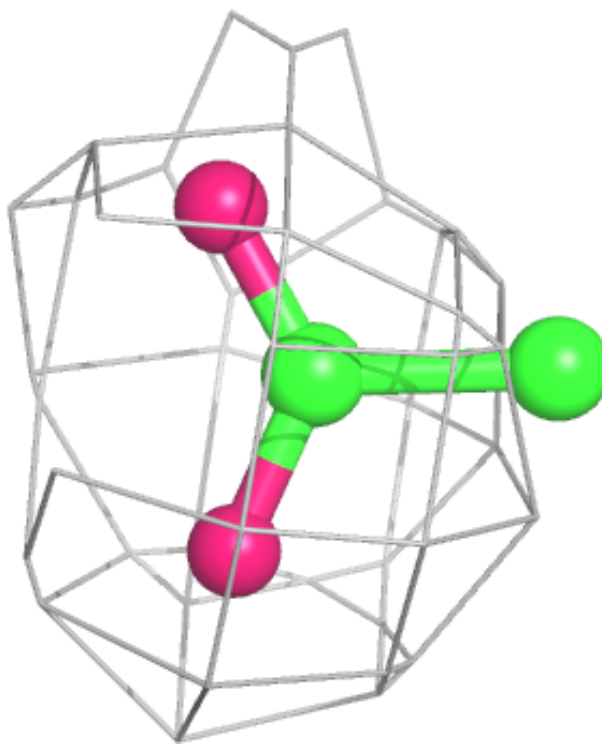
**Electron density around CA D 302:**

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



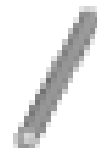
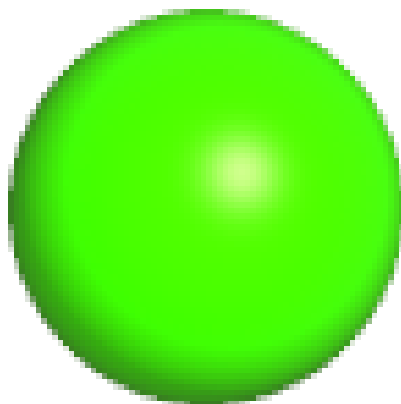
**Electron density around ACT B 413:**

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



**Electron density around CA C 306:**

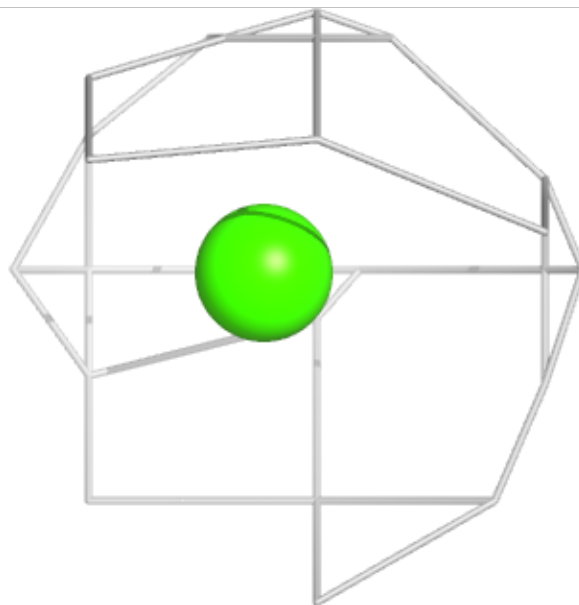
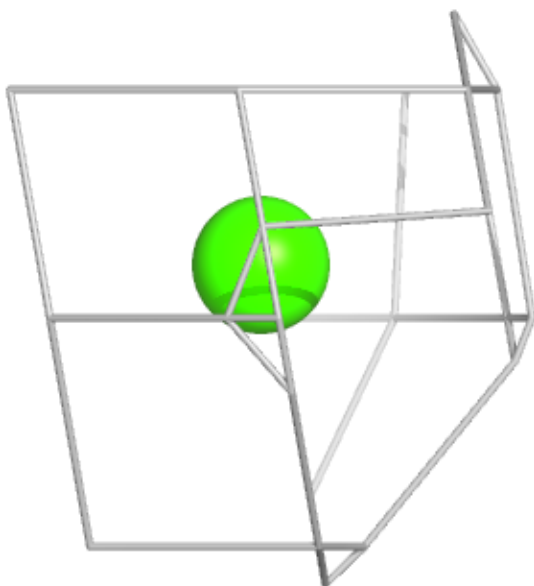
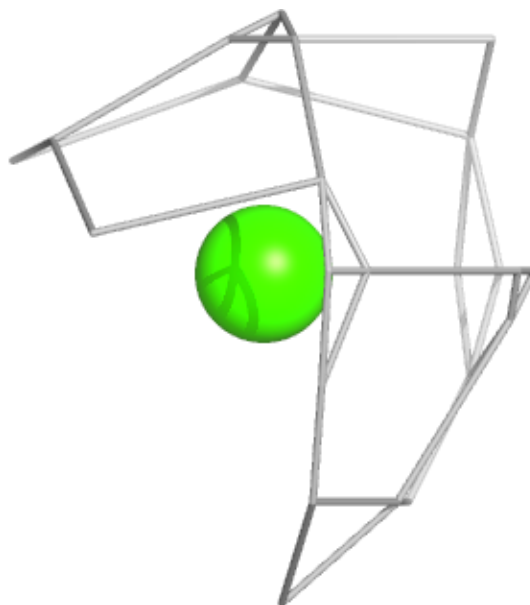
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





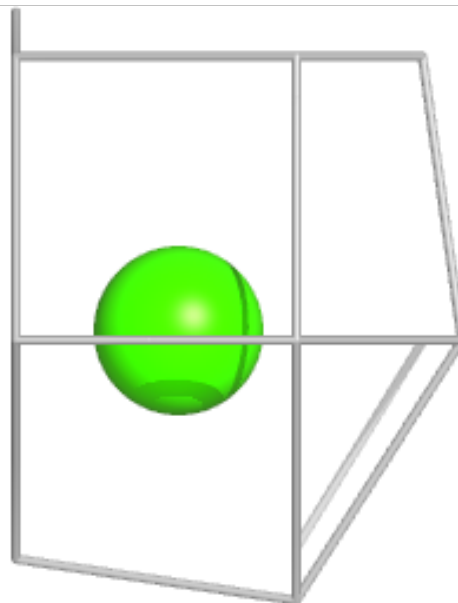
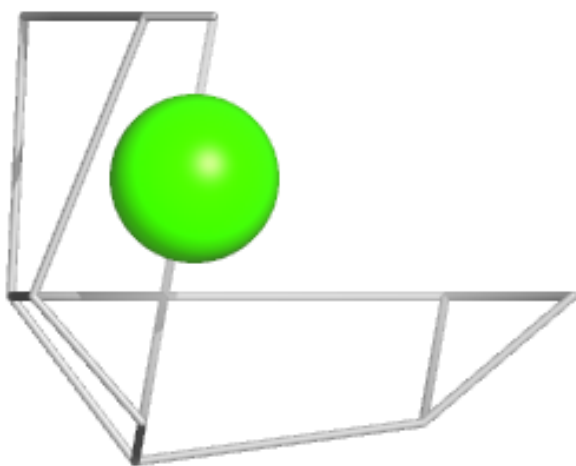
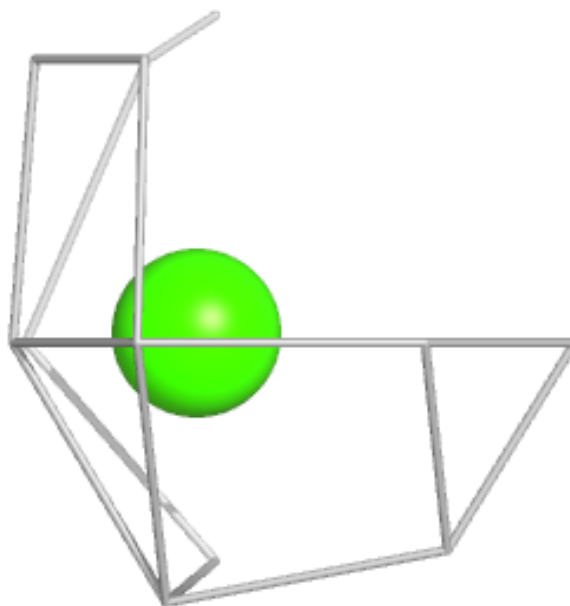
**Electron density around CA C 309:**

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



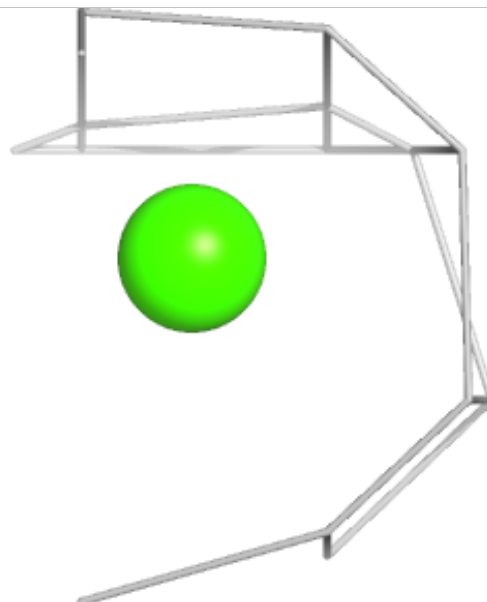
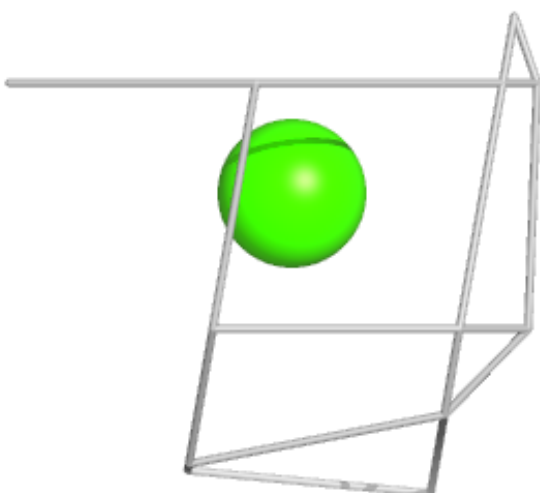
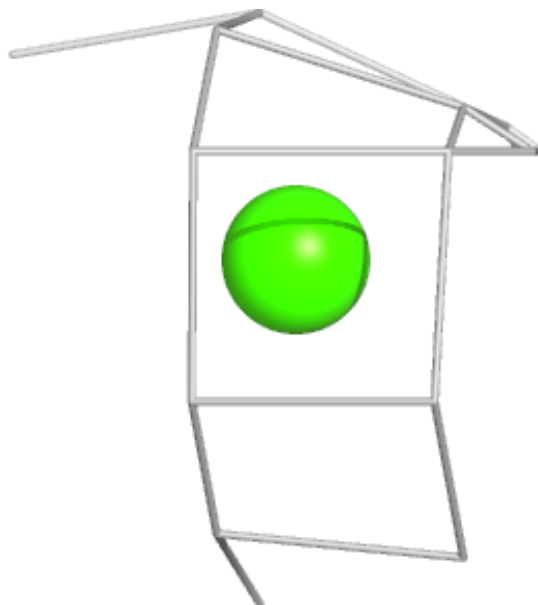
**Electron density around CA H 305:**

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



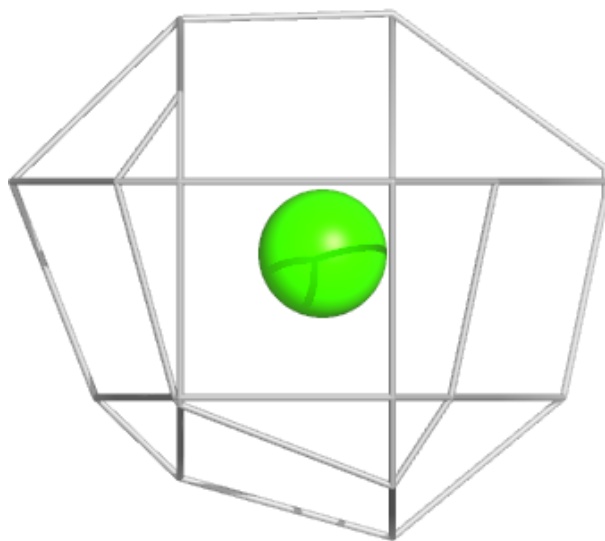
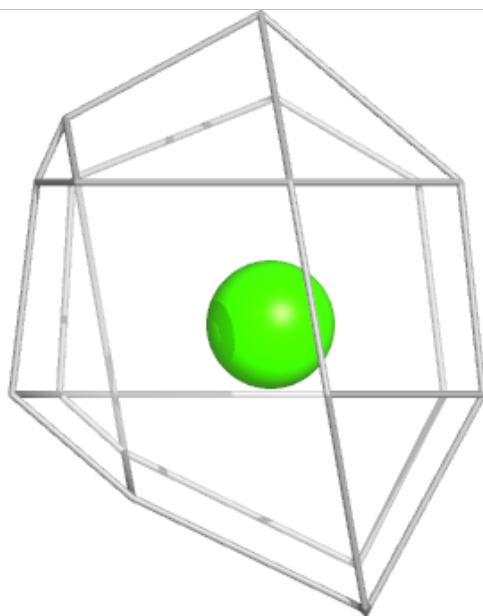
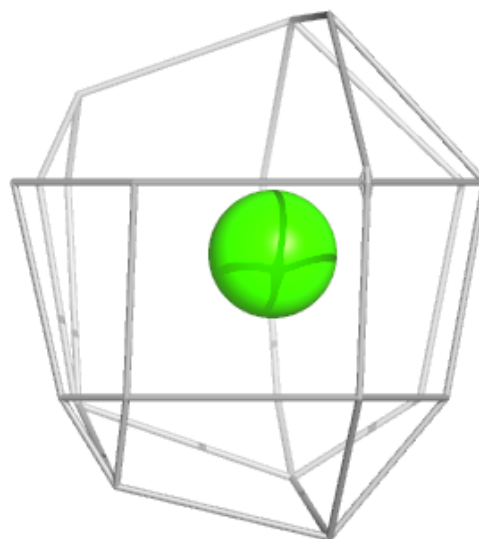
**Electron density around CA H 307:**

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



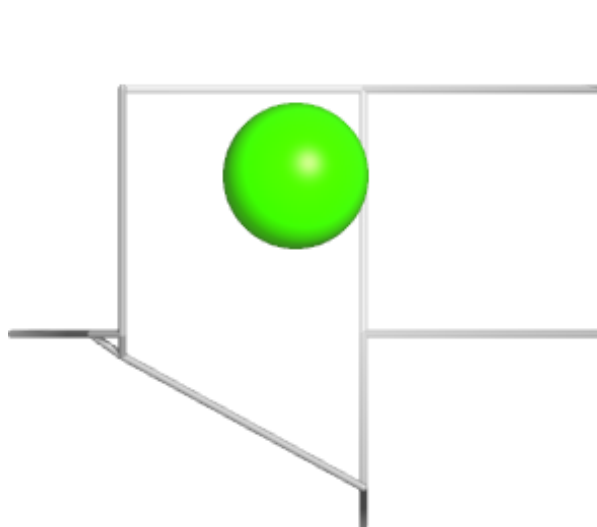
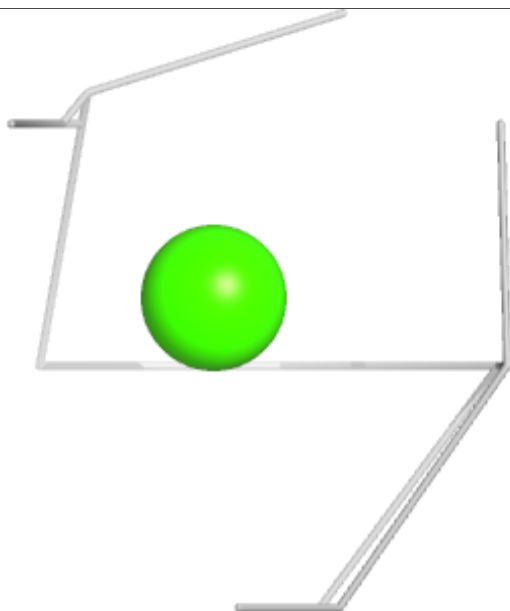
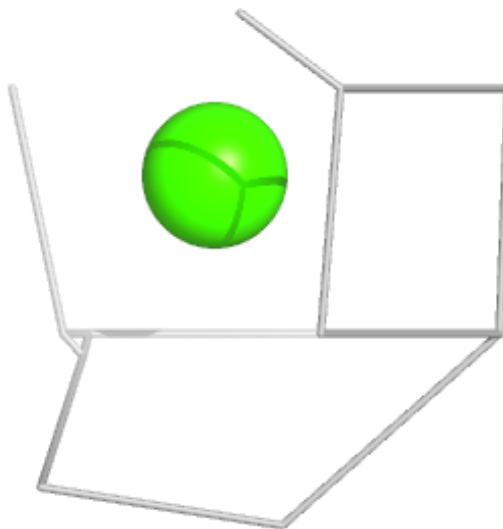
**Electron density around CA L 303:**

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



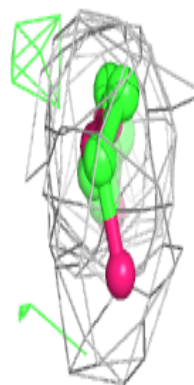
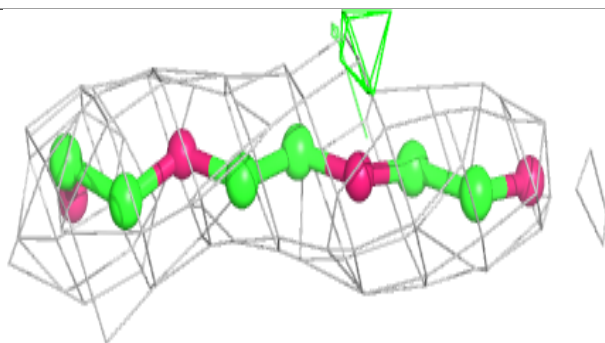
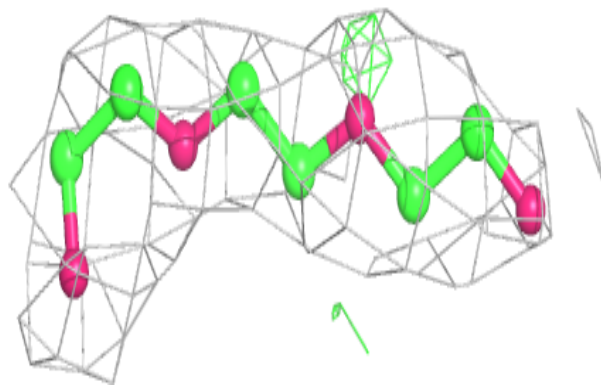
**Electron density around CA A 409:**

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



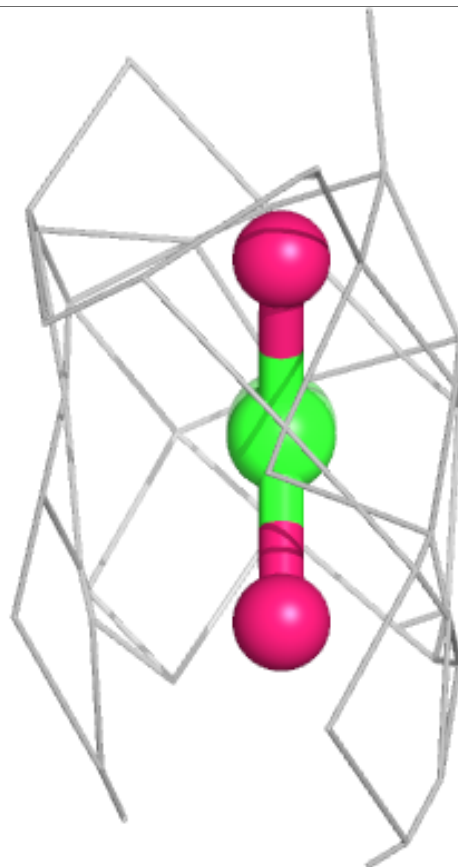
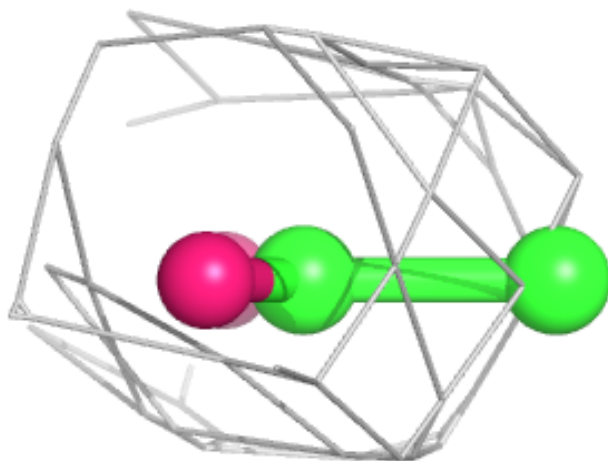
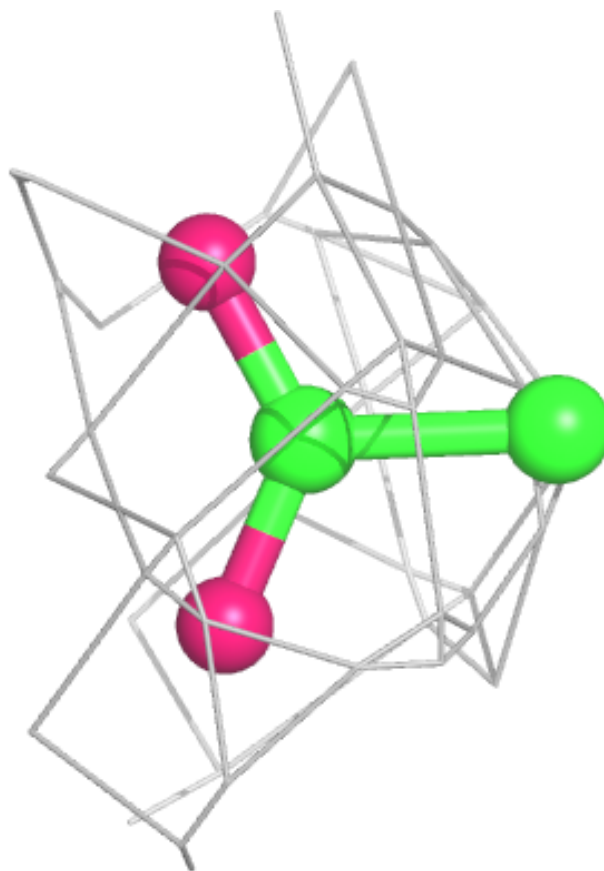
**Electron density around PGE C 312:**

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



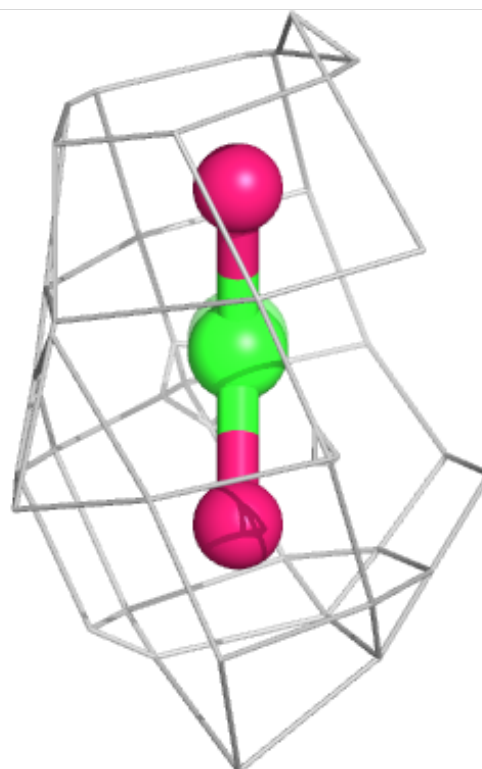
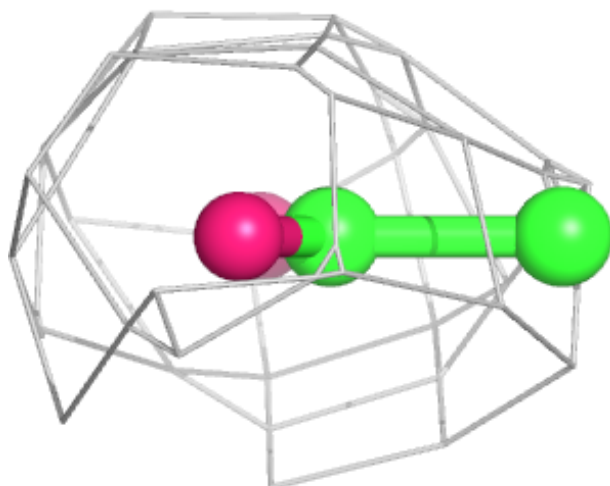
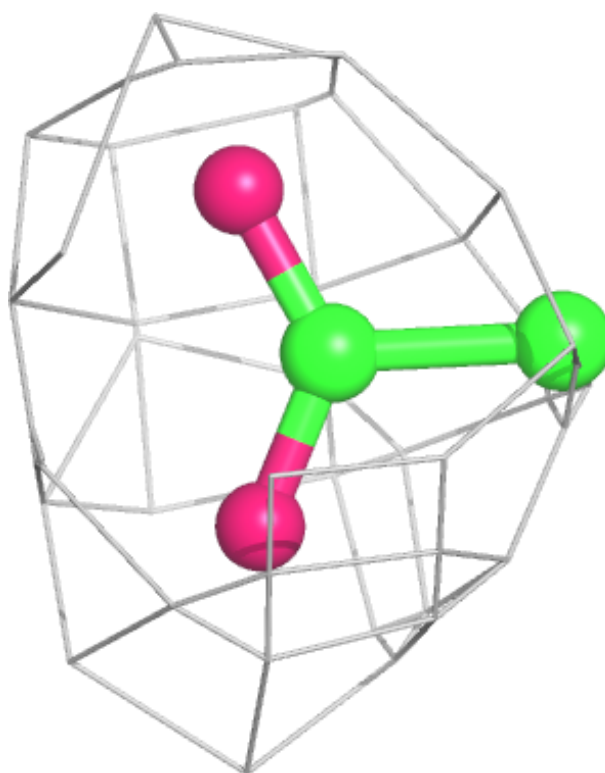
**Electron density around ACT D 307:**

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



**Electron density around ACT A 415:**

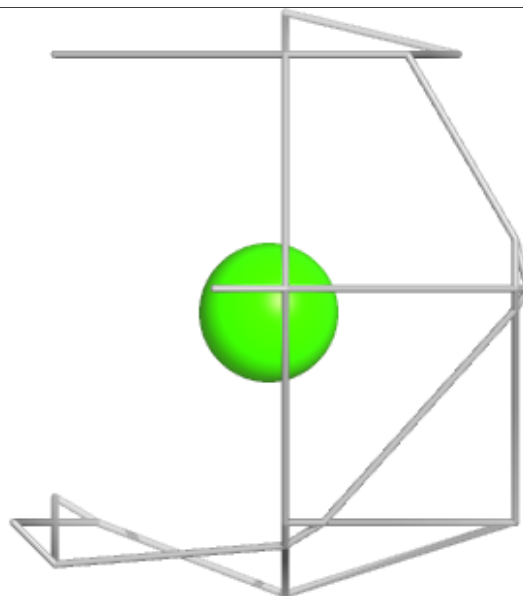
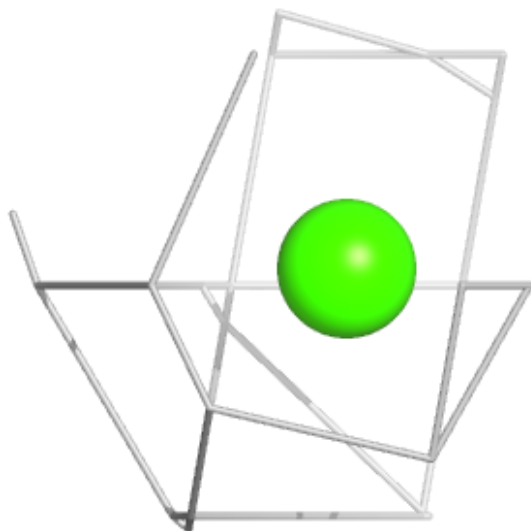
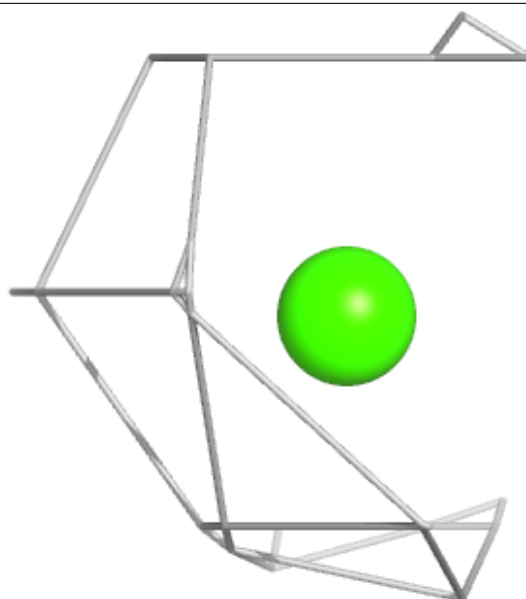
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





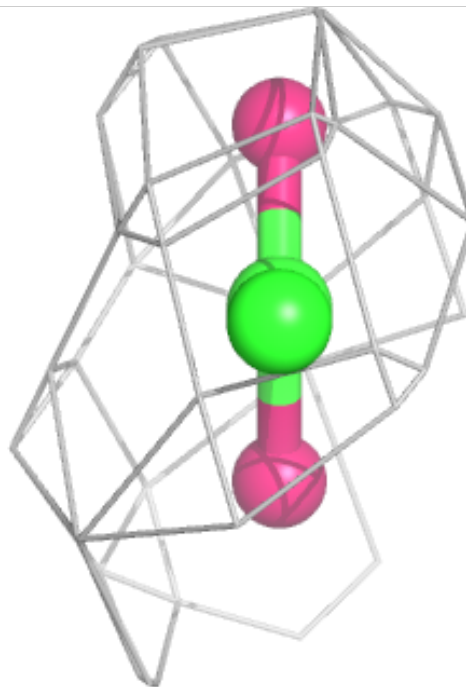
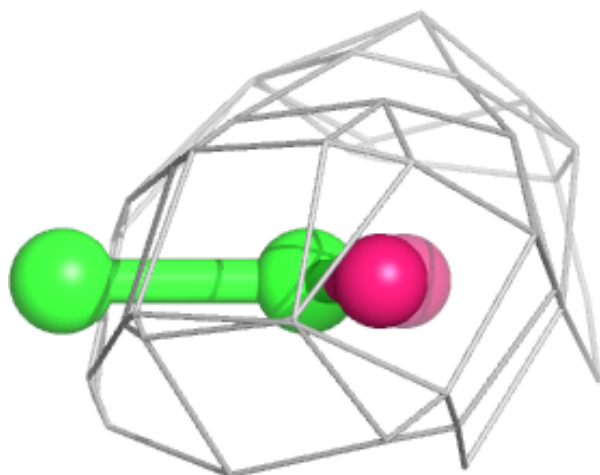
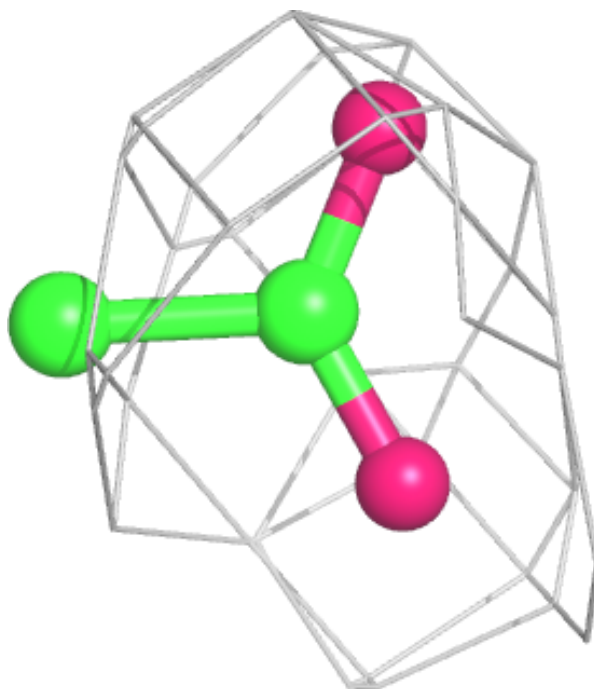
**Electron density around CA B 412:**

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



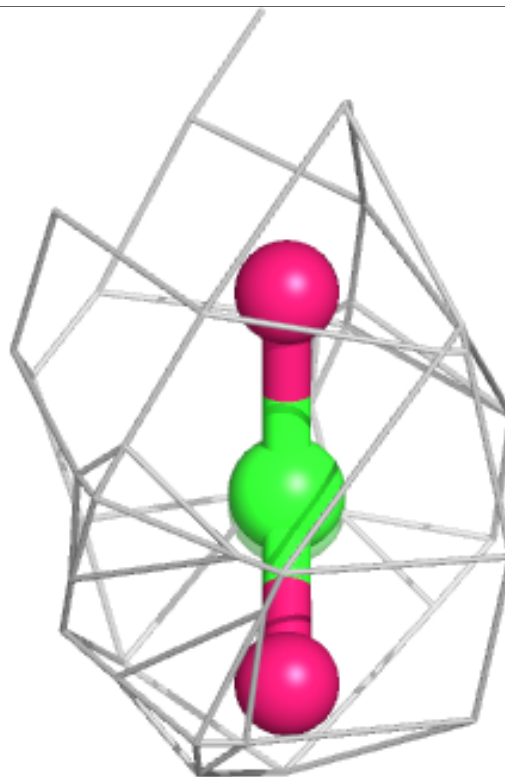
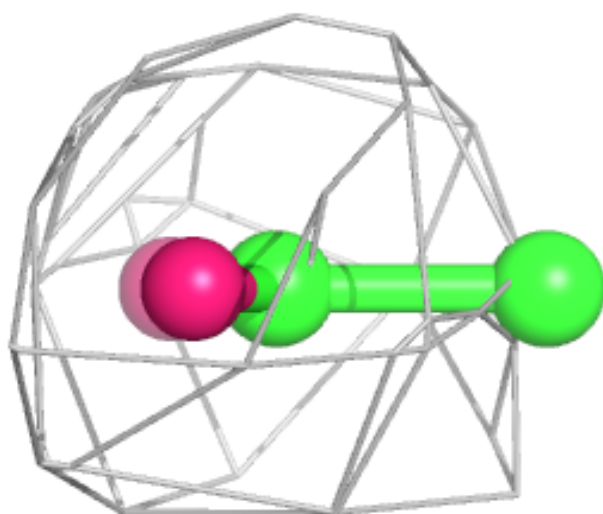
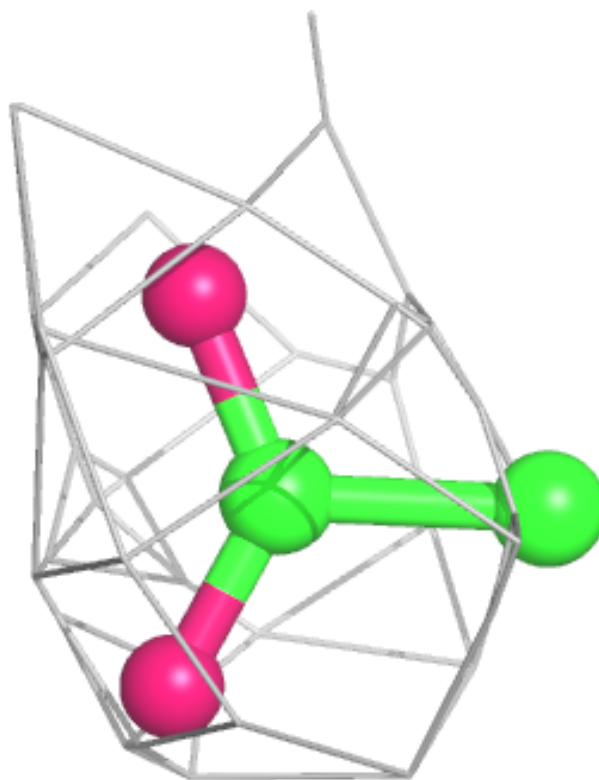
**Electron density around ACT B 414:**

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



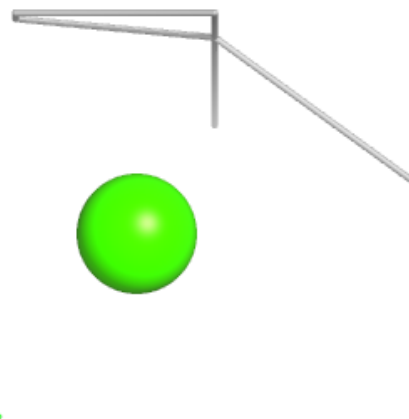
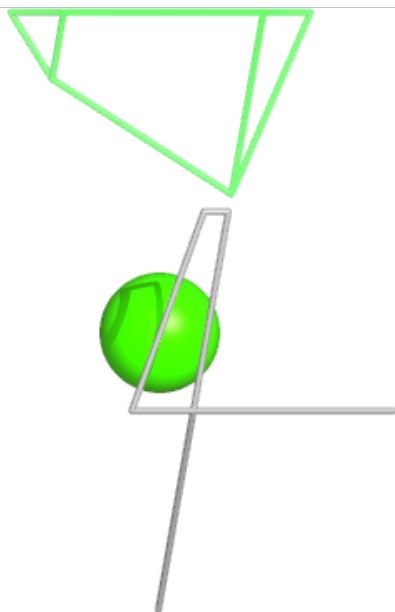
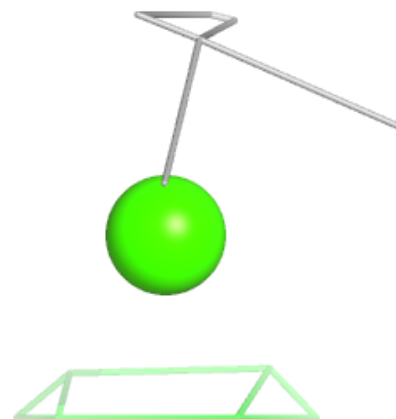
**Electron density around ACT H 309:**

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



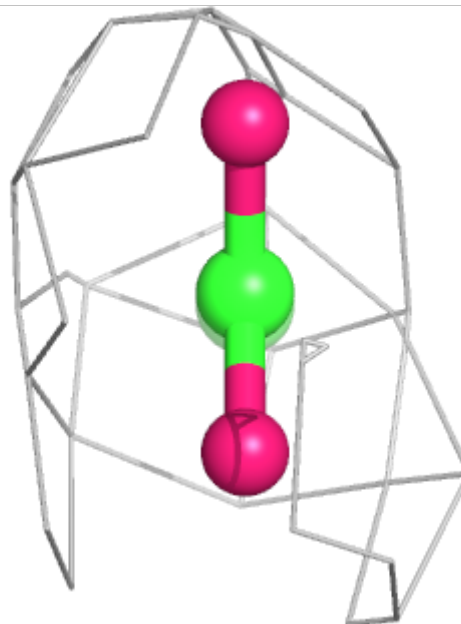
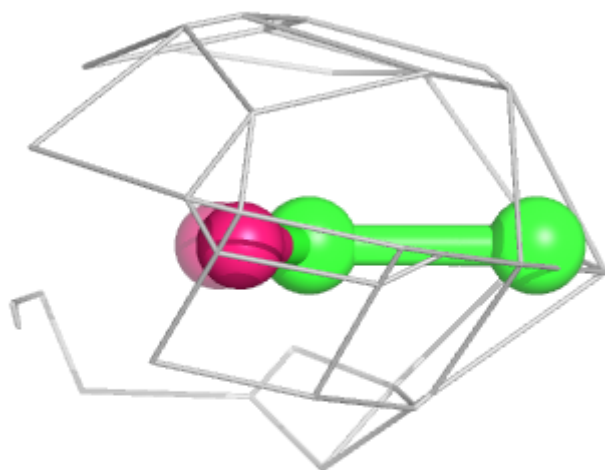
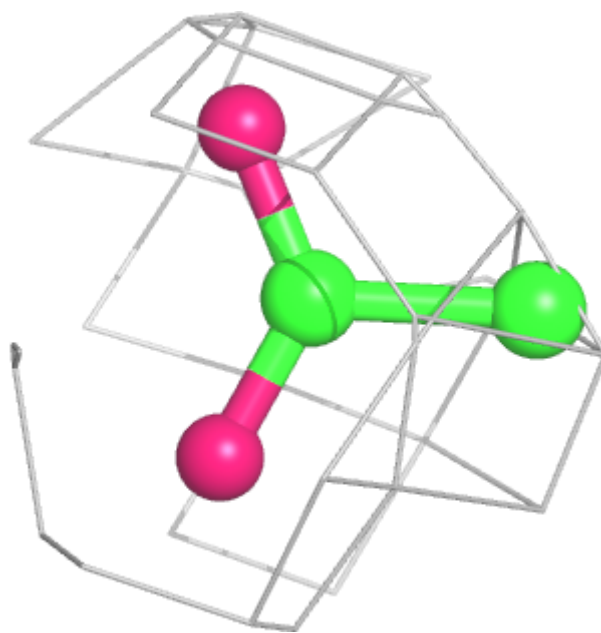
**Electron density around CA C 304:**

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



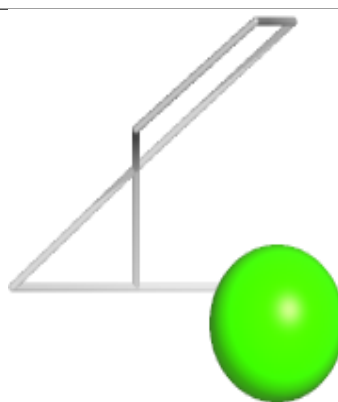
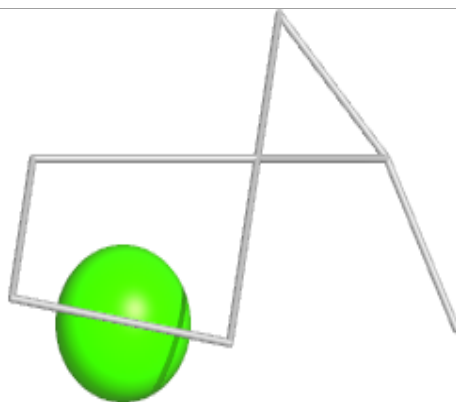
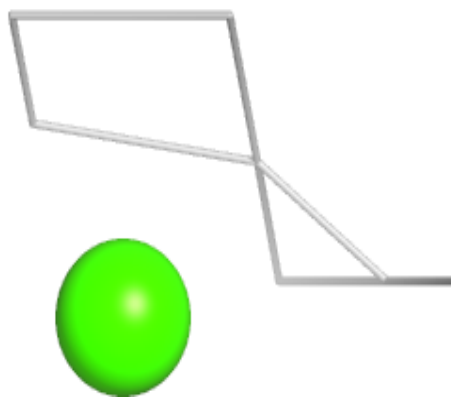
**Electron density around ACT A 414:**

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



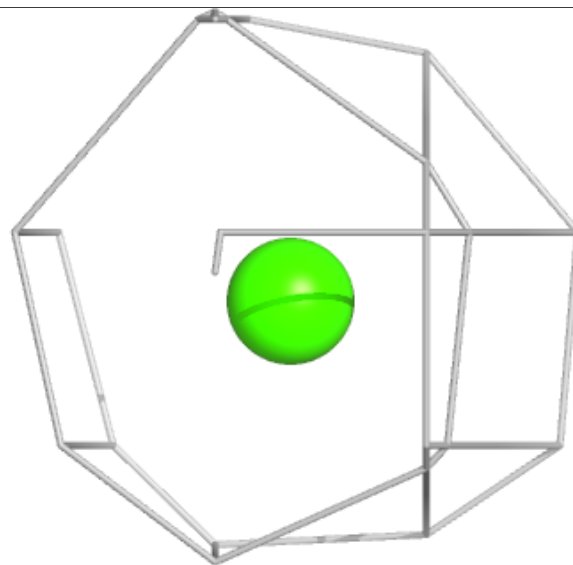
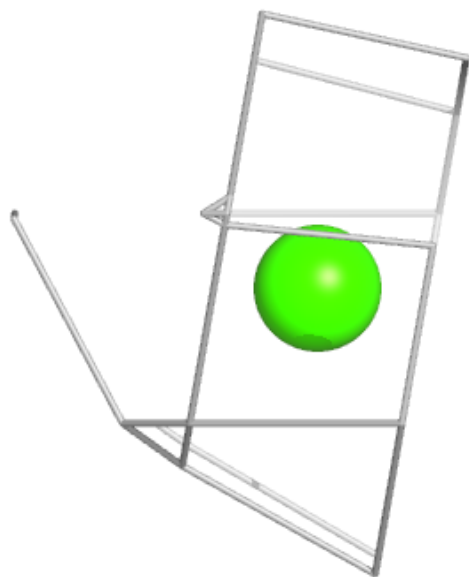
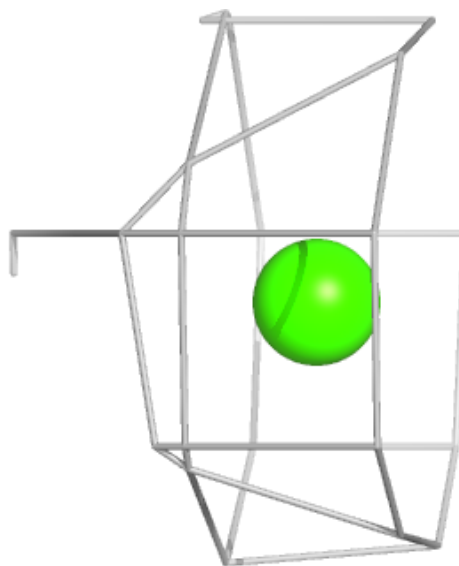
**Electron density around CA C 308:**

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



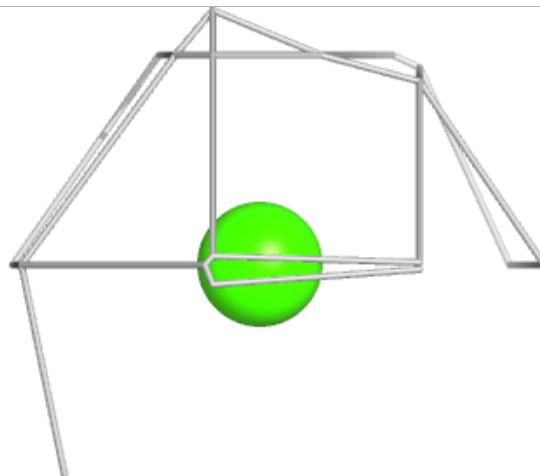
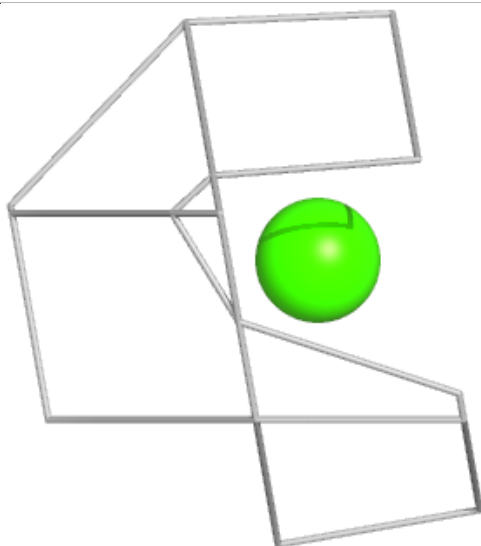
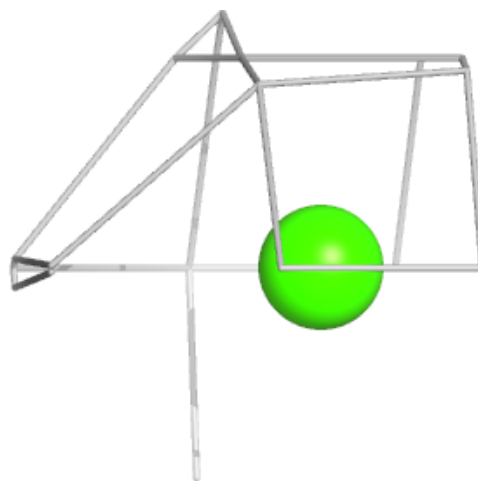
**Electron density around CA A 411:**

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



**Electron density around CA H 302:**

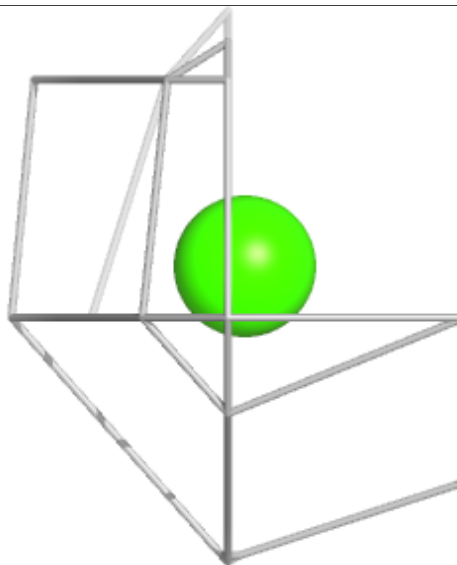
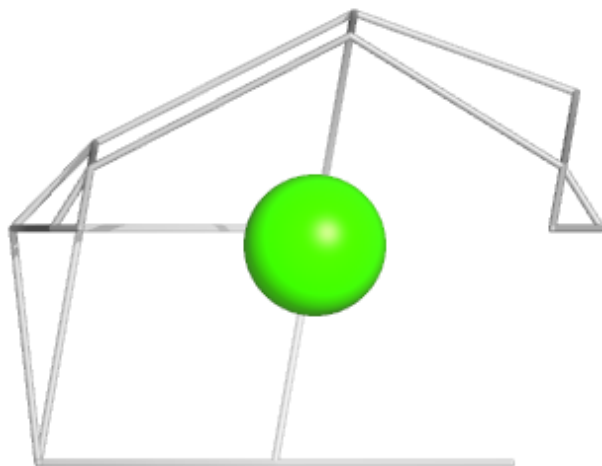
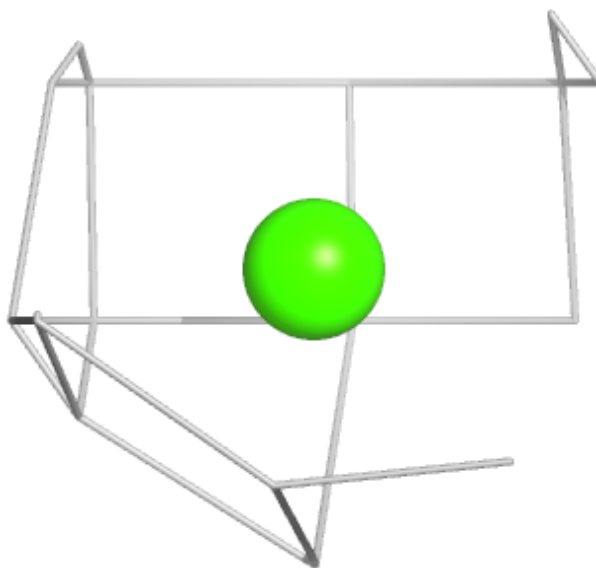
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





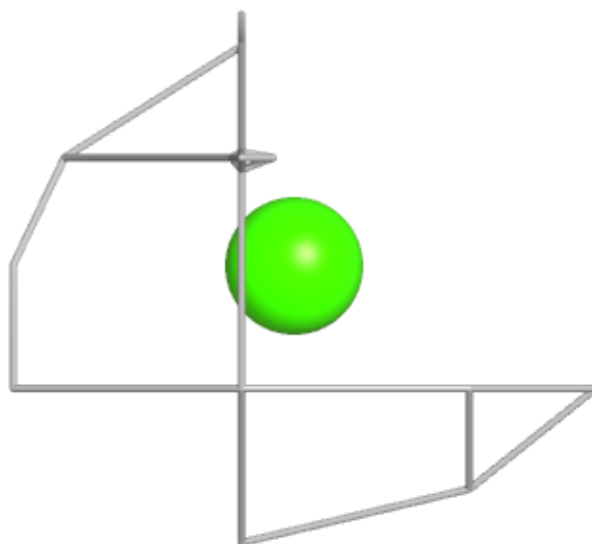
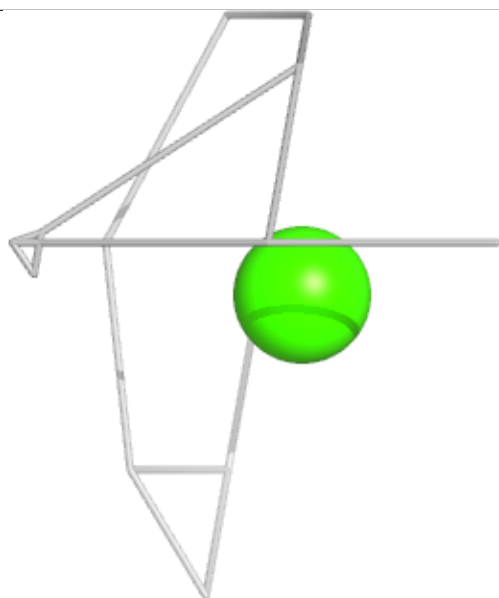
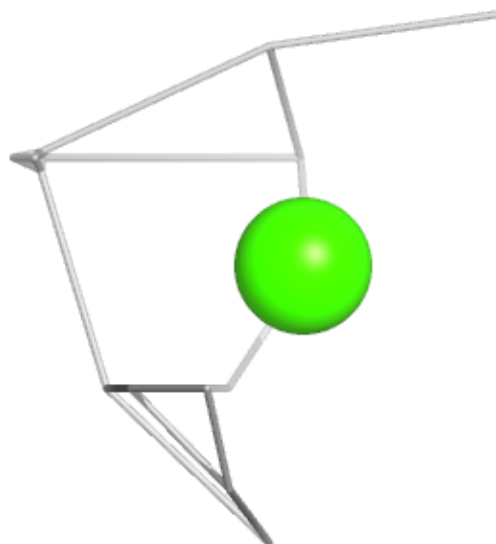
**Electron density around CA H 301:**

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



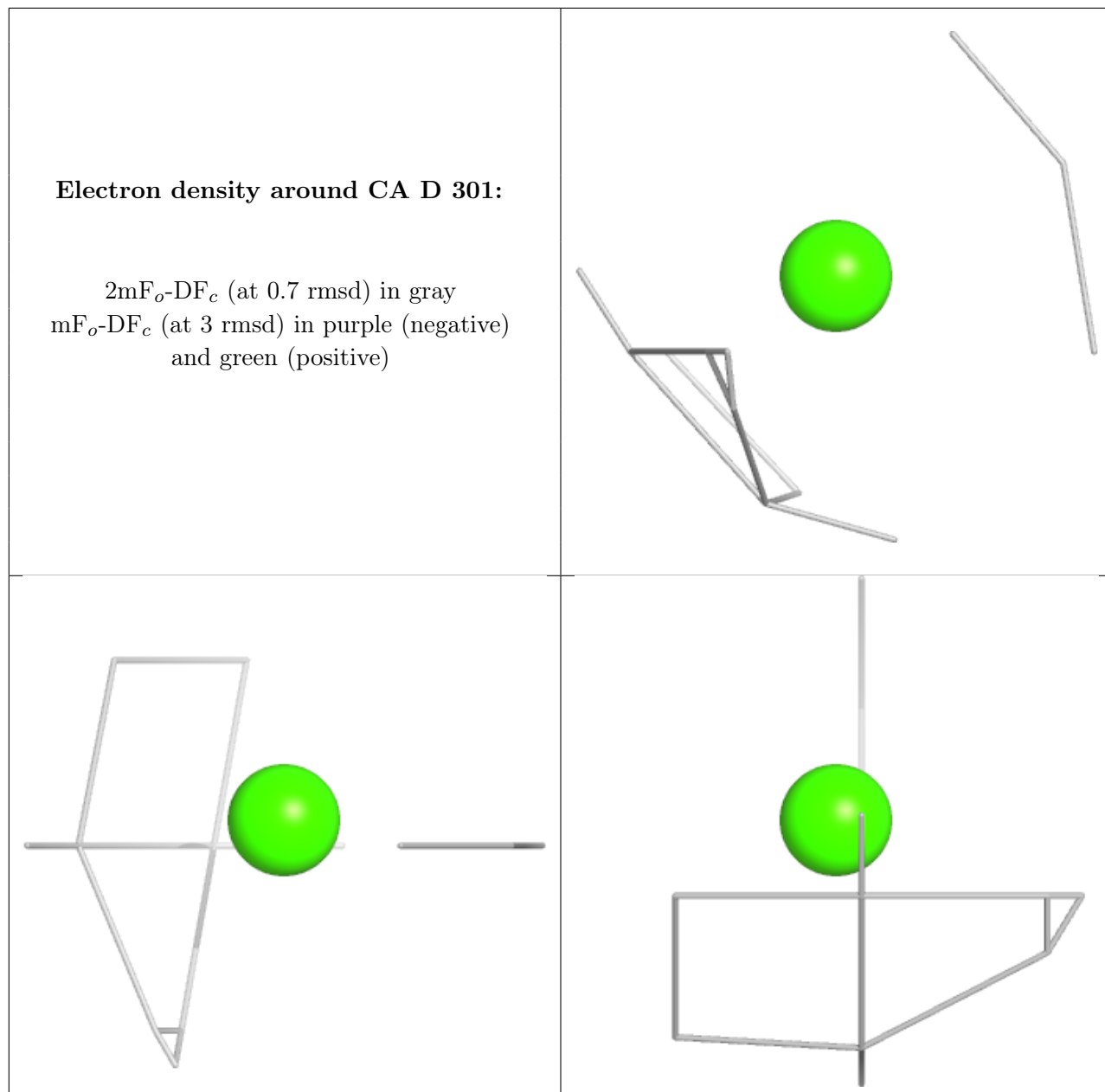
**Electron density around CA H 303:**

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



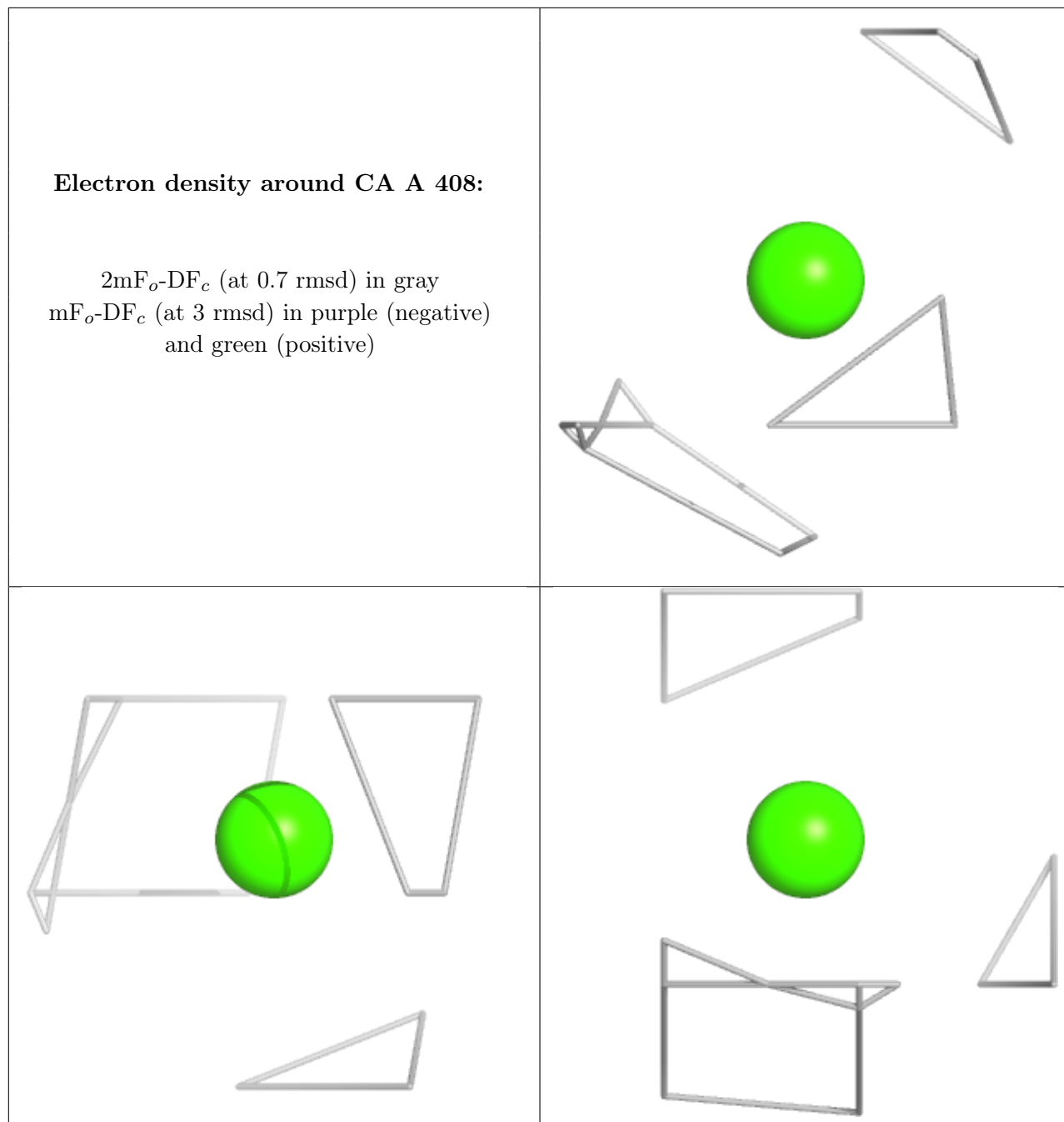
**Electron density around CA D 301:**

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



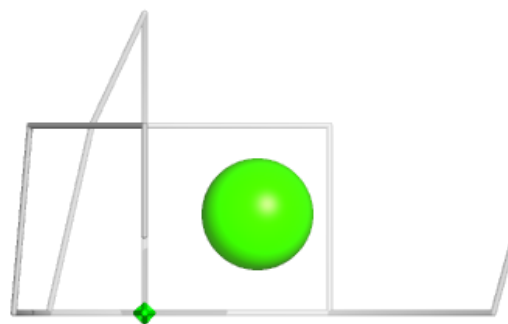
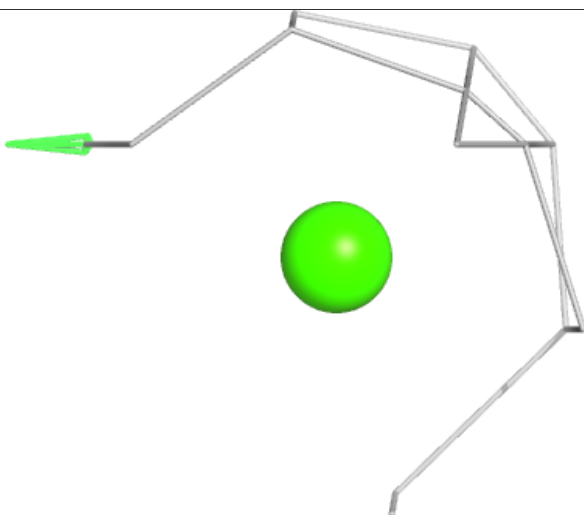
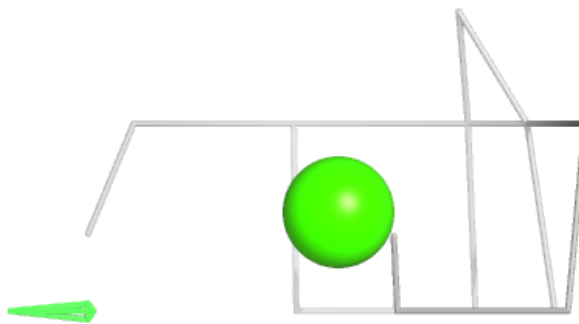
**Electron density around CA A 408:**

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



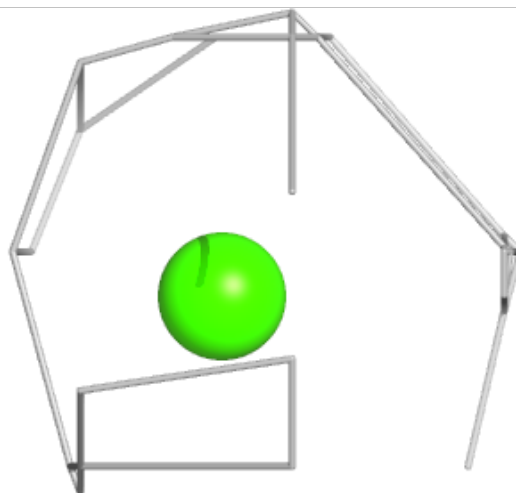
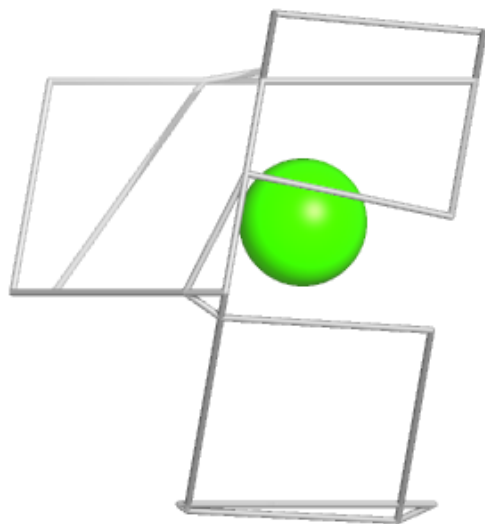
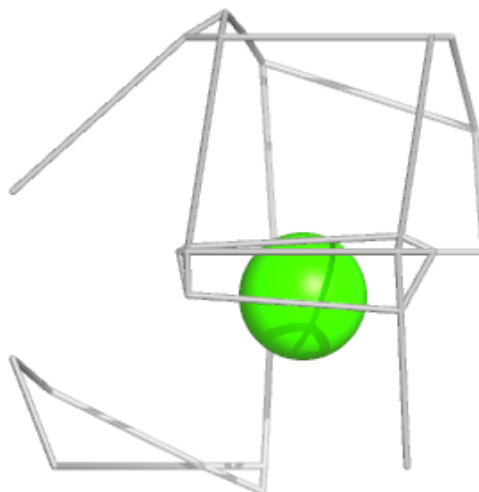
**Electron density around CA B 411:**

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



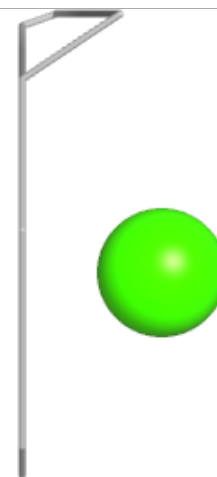
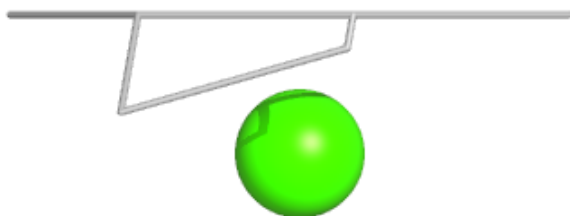
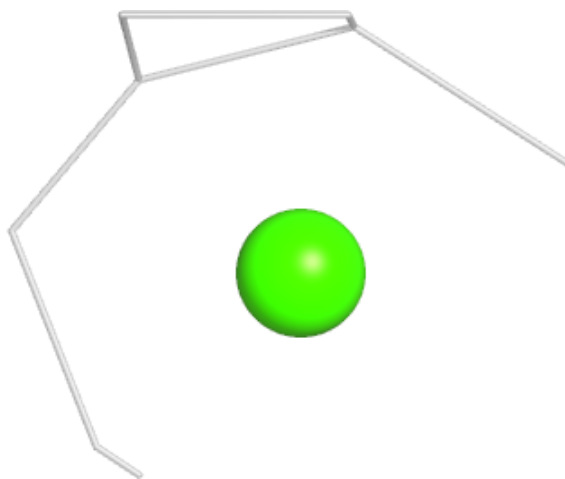
**Electron density around CA L 302:**

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



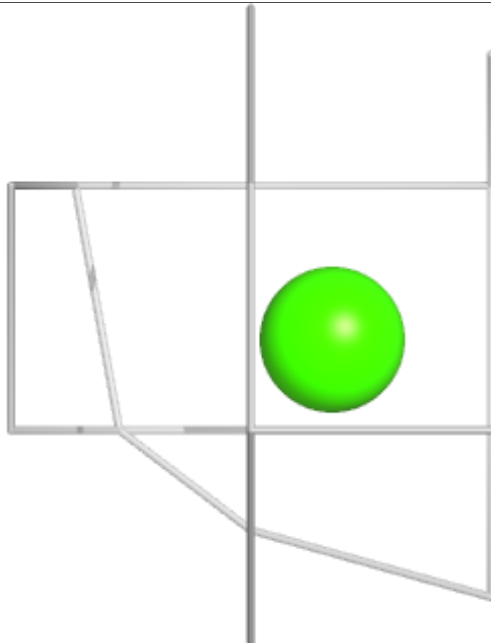
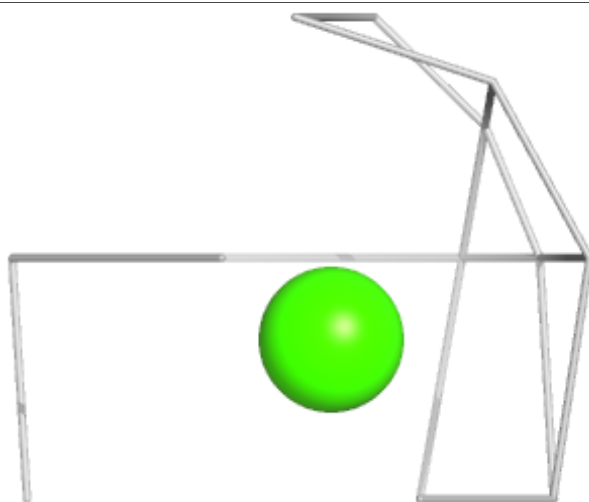
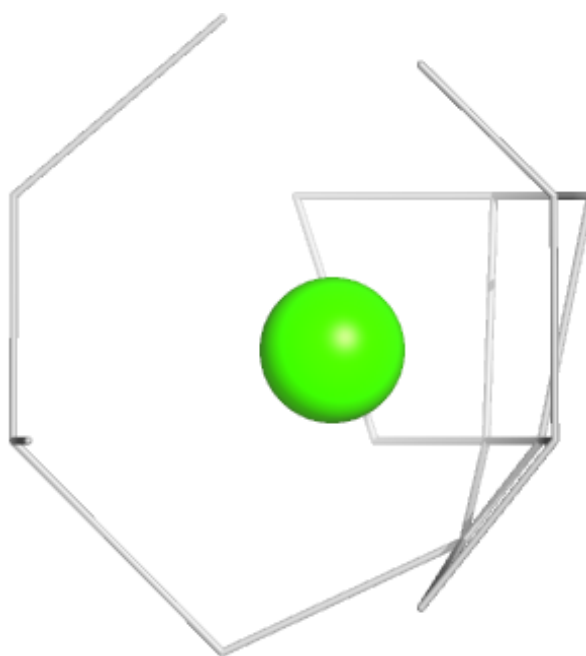
**Electron density around CA A 413:**

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



**Electron density around CA C 310:**

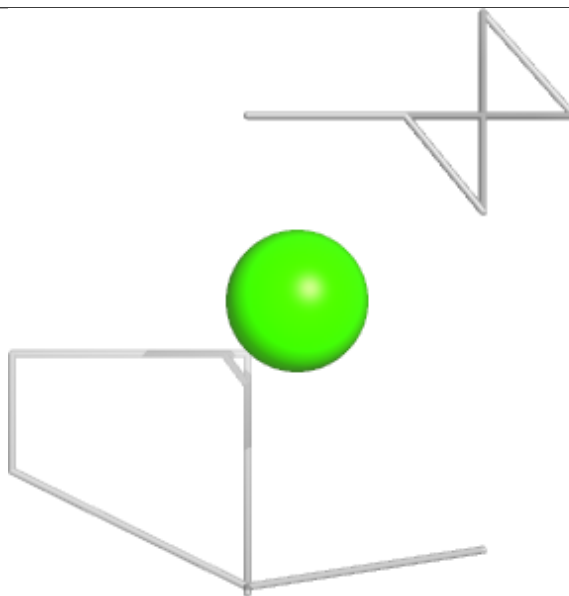
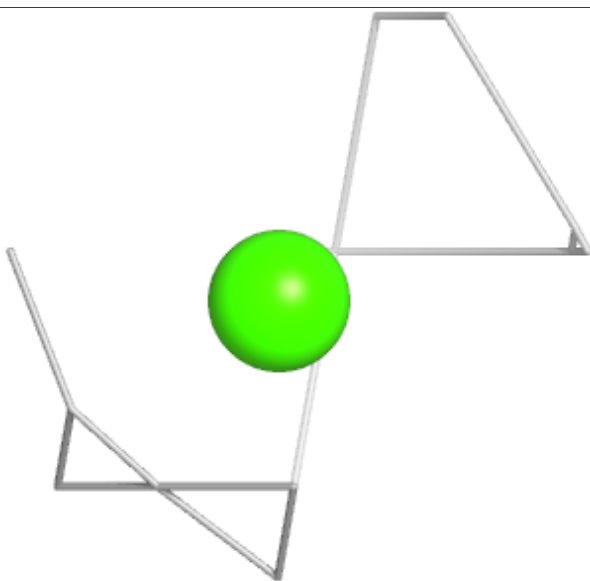
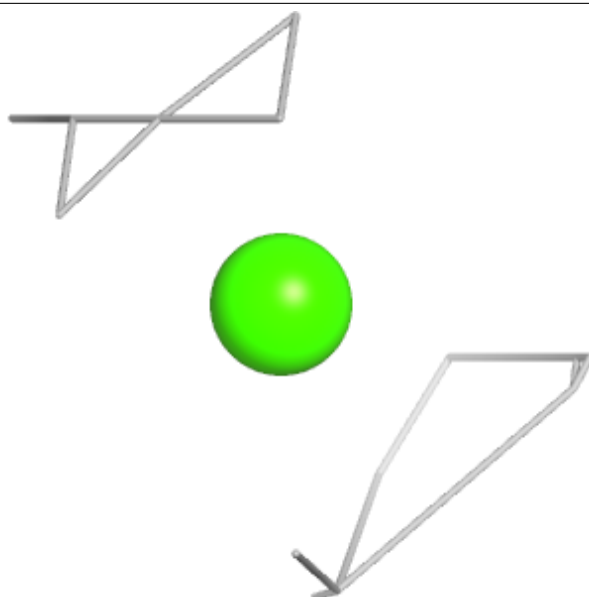
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

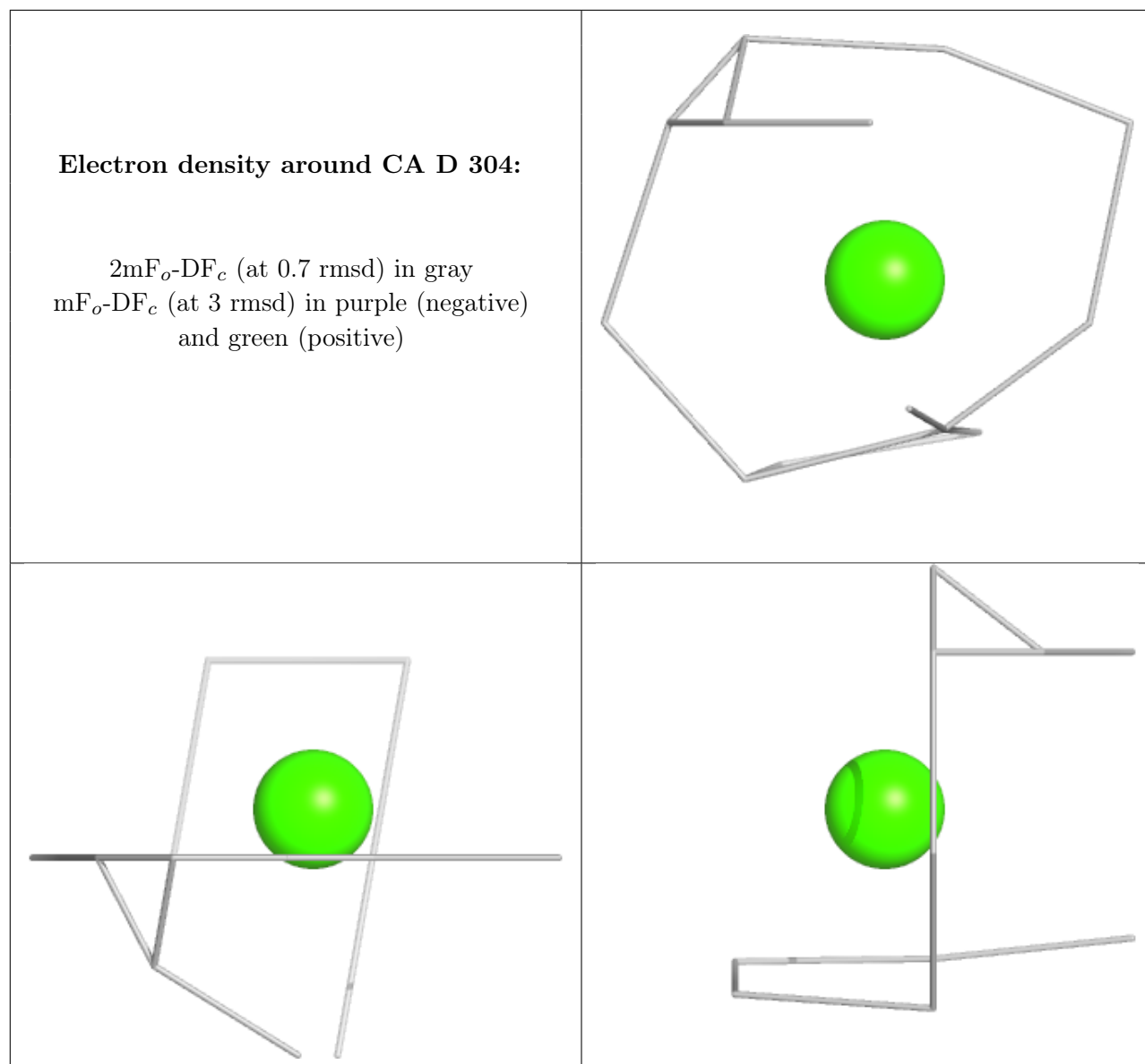




**Electron density around CA B 410:**

$2mF_o-DF_c$  (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.