



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:21 PM UTC

PDB ID : 8I08 / pdb_00008i08
Title : Crystal structure of Escherichia coli glyoxylate carboligase quadruple mutant
Authors : Kim, J.H.; Kim, J.S.
Deposited on : 2023-01-10
Resolution : 1.91 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

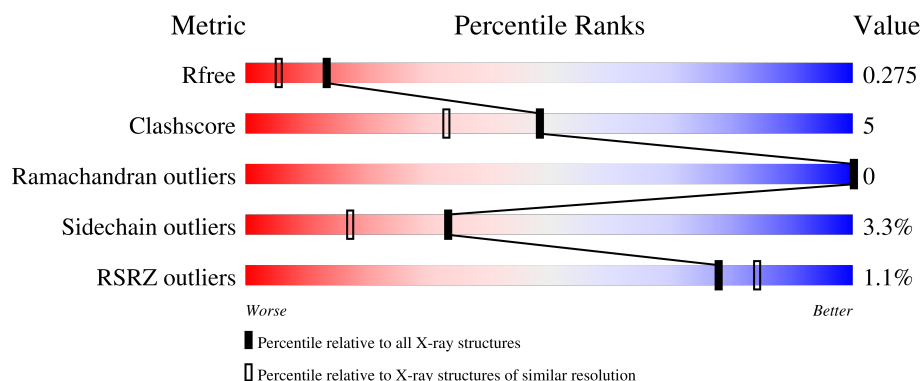
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	594	89% 10% .
1	B	594	87% 11% .
1	C	594	2% 87% 12% .
1	D	594	% 87% 12% .
1	E	594	% 82% 16% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	594	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '88%', and a small yellow segment at the end labeled '12%'.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31697 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 Glyoxylate carboligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4540	2877	791	836	36			
1	B	594	Total	C	N	O	S	0	0	0
			4539	2877	790	836	36			
1	C	594	Total	C	N	O	S	0	0	0
			4540	2877	791	836	36			
1	D	594	Total	C	N	O	S	0	0	0
			4540	2877	791	836	36			
1	E	594	Total	C	N	O	S	0	0	0
			4540	2877	791	836	36			
1	F	594	Total	C	N	O	S	0	0	0
			4540	2877	791	836	36			

There are 30 discrepancies between the modelled and reference sequences:

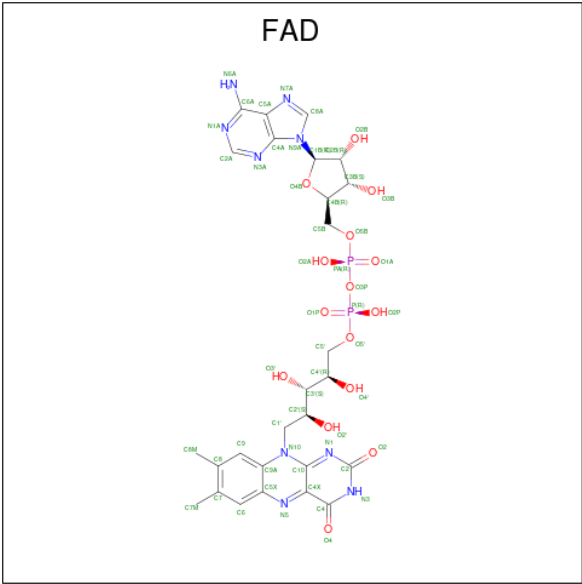
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P0AEP7
A	283	GLN	ASN	engineered mutation	UNP P0AEP7
A	478	MET	LEU	engineered mutation	UNP P0AEP7
A	484	MET	ARG	engineered mutation	UNP P0AEP7
A	488	LEU	MET	engineered mutation	UNP P0AEP7
B	0	GLY	-	expression tag	UNP P0AEP7
B	283	GLN	ASN	engineered mutation	UNP P0AEP7
B	478	MET	LEU	engineered mutation	UNP P0AEP7
B	484	MET	ARG	engineered mutation	UNP P0AEP7
B	488	LEU	MET	engineered mutation	UNP P0AEP7
C	0	GLY	-	expression tag	UNP P0AEP7
C	283	GLN	ASN	engineered mutation	UNP P0AEP7
C	478	MET	LEU	engineered mutation	UNP P0AEP7
C	484	MET	ARG	engineered mutation	UNP P0AEP7
C	488	LEU	MET	engineered mutation	UNP P0AEP7
D	0	GLY	-	expression tag	UNP P0AEP7
D	283	GLN	ASN	engineered mutation	UNP P0AEP7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	478	MET	LEU	engineered mutation	UNP P0AEP7
D	484	MET	ARG	engineered mutation	UNP P0AEP7
D	488	LEU	MET	engineered mutation	UNP P0AEP7
E	0	GLY	-	expression tag	UNP P0AEP7
E	283	GLN	ASN	engineered mutation	UNP P0AEP7
E	478	MET	LEU	engineered mutation	UNP P0AEP7
E	484	MET	ARG	engineered mutation	UNP P0AEP7
E	488	LEU	MET	engineered mutation	UNP P0AEP7
F	0	GLY	-	expression tag	UNP P0AEP7
F	283	GLN	ASN	engineered mutation	UNP P0AEP7
F	478	MET	LEU	engineered mutation	UNP P0AEP7
F	484	MET	ARG	engineered mutation	UNP P0AEP7
F	488	LEU	MET	engineered mutation	UNP P0AEP7

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



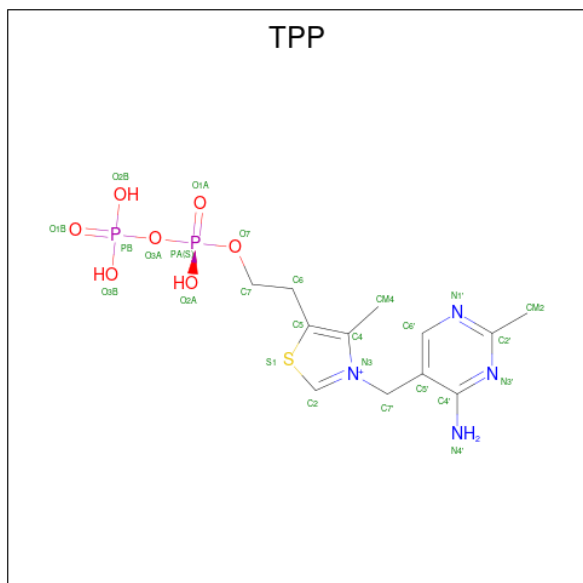
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).

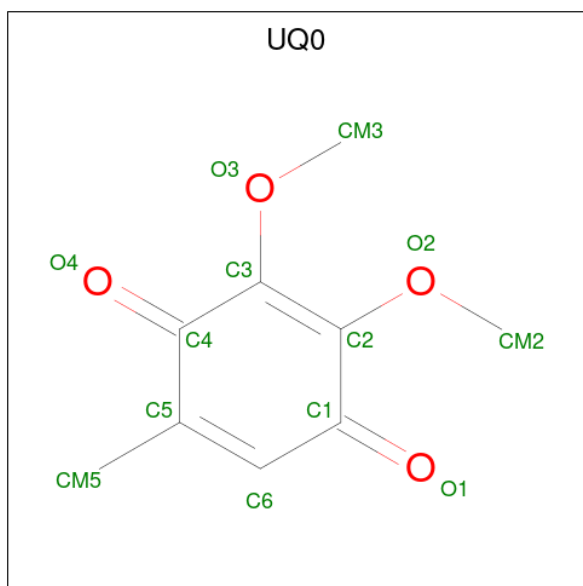


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2,3-DIMETHOXY-5-METHYL-1,4-BENZOQUINONE (CCD ID: UQ0) (formula: C₉H₁₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	9	4		
5	A	1	Total	C	O	0	0
			13	9	4		
5	B	1	Total	C	O	0	0
			13	9	4		
5	B	1	Total	C	O	0	0
			13	9	4		
5	C	1	Total	C	O	0	0
			13	9	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 13 9 4	0	0
5	D	1	Total C O 13 9 4	0	0
5	D	1	Total C O 13 9 4	0	0
5	E	1	Total C O 13 9 4	0	0
5	E	1	Total C O 13 9 4	0	0
5	F	1	Total C O 13 9 4	0	0
5	F	1	Total C O 13 9 4	0	0

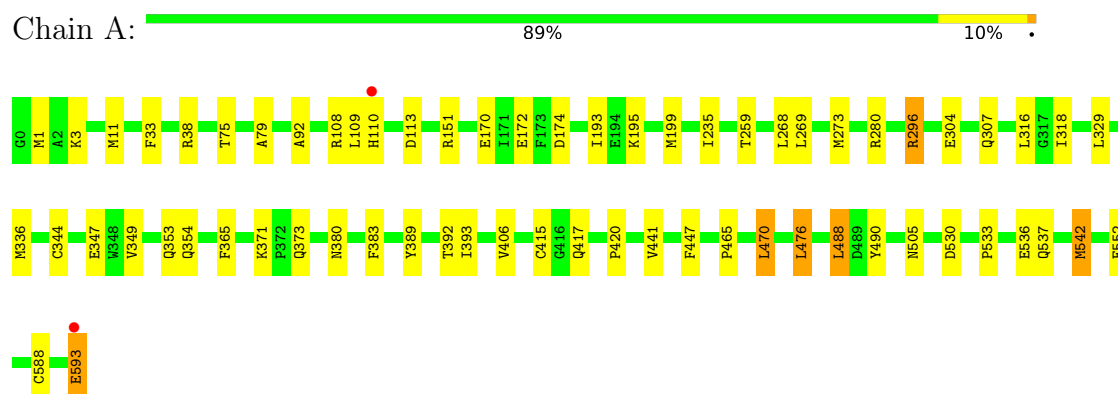
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	763	Total O 763 763	0	0
6	B	802	Total O 802 802	0	0
6	C	547	Total O 547 547	0	0
6	D	618	Total O 618 618	0	0
6	E	549	Total O 549 549	0	0
6	F	539	Total O 539 539	0	0

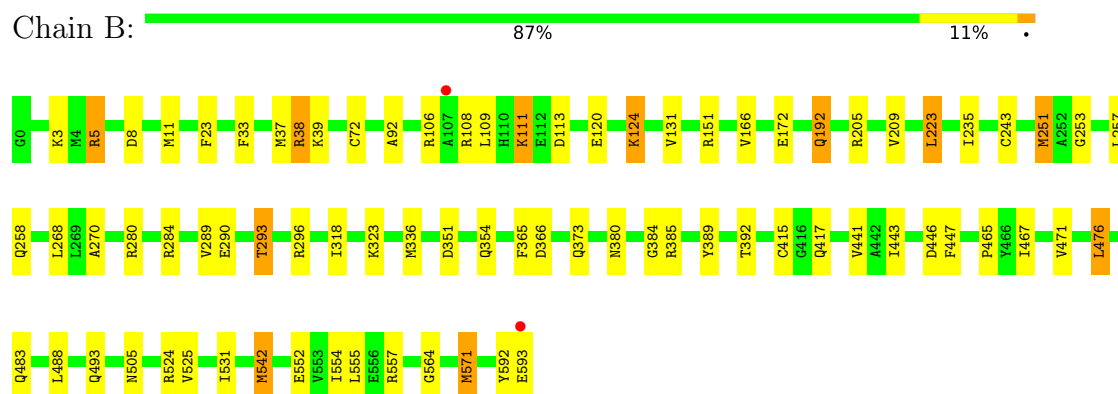
3 Residue-property plots

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

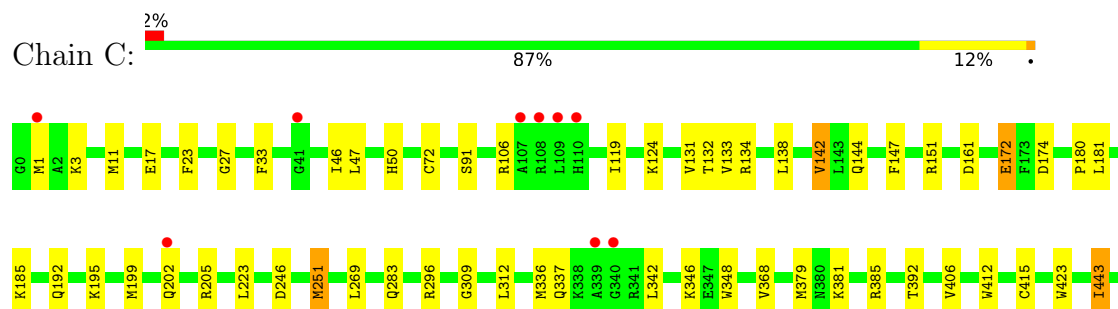
• Molecule 1: Glyoxylate carboligase



• Molecule 1: Glyoxylate carboligase

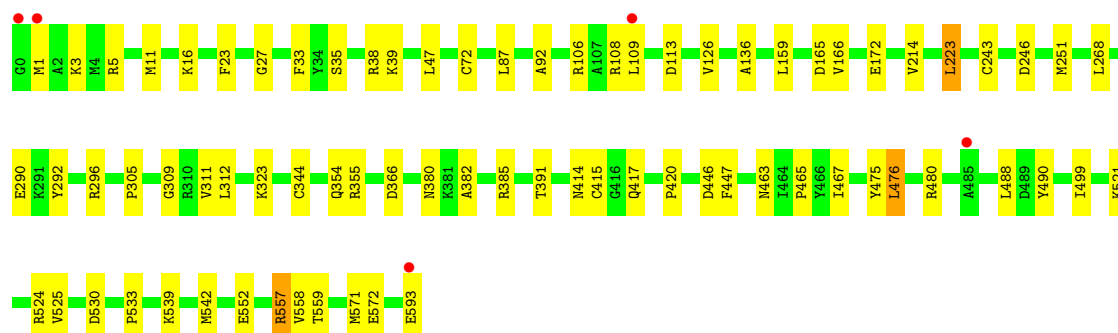
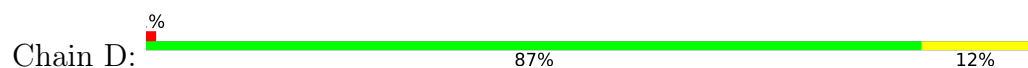


• Molecule 1: Glyoxylate carboligase

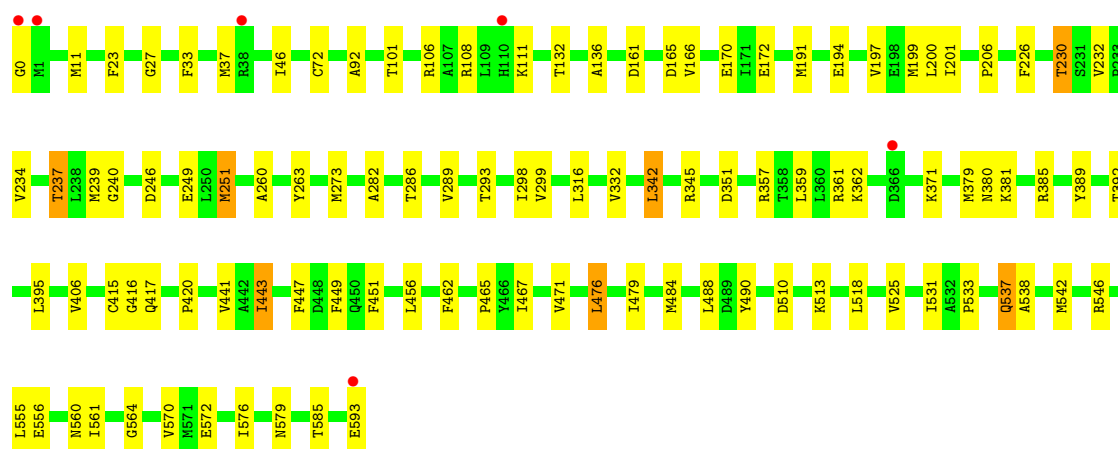
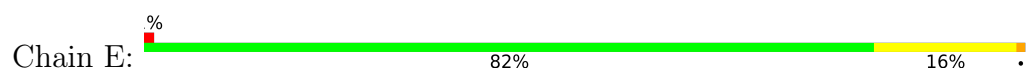




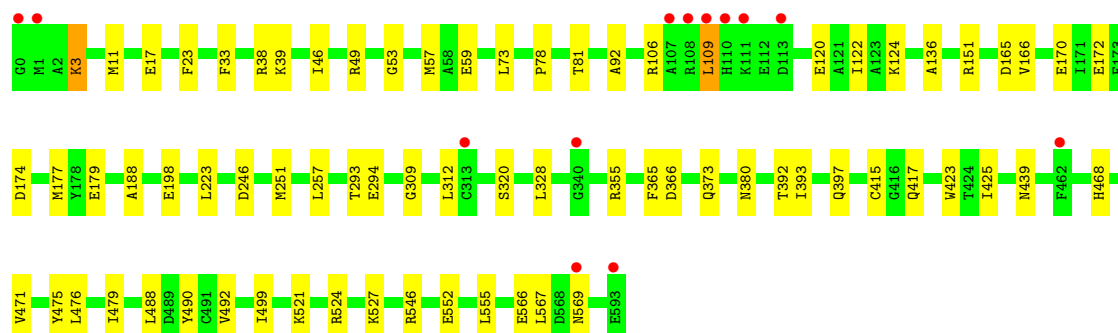
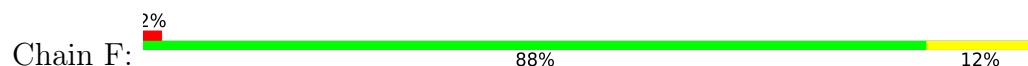
• Molecule 1: Glyoxylate carboligase



• Molecule 1: Glyoxylate carboligase



• Molecule 1: Glyoxylate carboligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.56Å 188.56Å 246.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 1.91 49.92 – 1.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.92-1.91) 99.4 (49.92-1.91)	Depositor EDS
R_{merge}	0.99	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.91Å)	Xtriage
Refinement program	PHENIX v2.0	Depositor
R, R_{free}	0.225 , 0.272 0.231 , 0.275	Depositor DCC
R_{free} test set	10000 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31697	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8869e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ0, TPP, FAD, MG

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	0.42	0/4632	0.64	3/6286 (0.0%)
1	B	0.41	0/4631	0.65	3/6285 (0.0%)
1	C	0.32	0/4632	0.53	0/6286
1	D	0.31	0/4632	0.51	0/6286
1	E	0.31	0/4632	0.53	2/6286 (0.0%)
1	F	0.29	0/4632	0.49	0/6286
All	All	0.35	0/27791	0.56	8/37715 (0.0%)

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
1	A	0	2
1	B	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	ARG	CA-C-N	-7.03	113.38	122.79
1	B	280	ARG	C-N-CA	-7.03	113.38	122.79
1	E	462	PHE	CA-C-N	-6.79	112.56	123.23
1	E	462	PHE	C-N-CA	-6.79	112.56	123.23
1	A	280	ARG	CA-C-N	-6.50	112.72	123.37

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	HIS	Peptide
1	A	296	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	592	TYR	Peptide
1	D	557	ARG	Sidechain

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	4540	0	4546	43	0
1	B	4539	0	4540	54	0
1	C	4540	0	4545	46	0
1	D	4540	0	4545	57	0
1	E	4540	0	4545	65	0
1	F	4540	0	4545	50	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	3	0
2	F	53	0	31	0	0
3	A	26	0	16	0	0
3	B	26	0	16	0	0
3	C	26	0	16	0	0
3	D	26	0	16	0	0
3	E	26	0	16	0	0
3	F	26	0	16	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	26	0	0	1	0
5	B	26	0	0	0	0
5	C	26	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	26	0	0	0	0
5	E	26	0	0	1	0
5	F	26	0	0	1	0
6	A	763	0	0	12	0
6	B	802	0	0	10	0
6	C	547	0	0	6	0
6	D	618	0	0	15	0
6	E	549	0	0	6	0
6	F	539	0	0	13	0
All	All	31697	0	27548	303	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.

The worst 5 of 303 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:A:199:MET:SD	6:A:1292:HOH:O	2.21	0.96
1:E:237:THR:HG22	1:E:240:GLY:H	1.34	0.91
1:B:467:ILE:HG13	1:B:542:MET:HE1	1.53	0.90
1:D:251:MET:SD	6:D:954:HOH:O	2.33	0.86
1:A:588:CYS:SG	5:A:705:UQ0:C6	2.64	0.86

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	592/594 (100%)	582 (98%)	10 (2%)	0	100	100
1	B	592/594 (100%)	583 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	592/594 (100%)	577 (98%)	15 (2%)	0	100	100
1	D	592/594 (100%)	578 (98%)	14 (2%)	0	100	100
1	E	592/594 (100%)	577 (98%)	15 (2%)	0	100	100
1	F	592/594 (100%)	581 (98%)	11 (2%)	0	100	100
All	All	3552/3564 (100%)	3478 (98%)	74 (2%)	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	475/475 (100%)	463 (98%)	12 (2%)	42	26
1	B	474/475 (100%)	457 (96%)	17 (4%)	31	15
1	C	475/475 (100%)	457 (96%)	18 (4%)	29	14
1	D	475/475 (100%)	463 (98%)	12 (2%)	42	26
1	E	475/475 (100%)	452 (95%)	23 (5%)	23	8
1	F	475/475 (100%)	463 (98%)	12 (2%)	42	26
All	All	2849/2850 (100%)	2755 (97%)	94 (3%)	33	17

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	488	LEU
1	E	289	VAL
1	E	37	MET
1	E	199	MET
1	E	351	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	354	GLN
1	F	202	GLN
1	F	544	GLN
1	F	411	HIS
1	C	115	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 10 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$
2	FAD	B	701	-	58,58,58	0.47	1 (1%)	85,89,89	0.62	1 (1%)
5	UQ0	E	601	-	13,13,13	3.42	8 (61%)	16,18,18	1.53	3 (18%)
5	UQ0	C	706	-	13,13,13	3.72	5 (38%)	16,18,18	1.31	2 (12%)
5	UQ0	F	601	-	13,13,13	3.36	7 (53%)	16,18,18	1.52	2 (12%)
3	TPP	E	603	4	26,27,27	0.65	1 (3%)	38,40,40	0.52	0
5	UQ0	A	706	-	13,13,13	3.70	5 (38%)	16,18,18	1.85	3 (18%)
5	UQ0	E	605	-	13,13,13	3.39	7 (53%)	16,18,18	0.99	1 (6%)
2	FAD	D	701	-	58,58,58	0.38	0	85,89,89	0.58	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	C	702	4	26,27,27	0.44	0	38,40,40	0.37	0
5	UQ0	D	704	-	13,13,13	3.48	6 (46%)	16,18,18	1.16	0
5	UQ0	F	605	-	13,13,13	3.52	7 (53%)	16,18,18	0.90	0
2	FAD	E	602	-	58,58,58	0.52	2 (3%)	85,89,89	0.52	0
2	FAD	A	701	-	58,58,58	0.63	2 (3%)	85,89,89	0.66	3 (3%)
5	UQ0	B	705	-	13,13,13	3.27	5 (38%)	16,18,18	1.88	6 (37%)
3	TPP	B	702	4	26,27,27	1.02	1 (3%)	38,40,40	0.61	2 (5%)
3	TPP	A	702	4	26,27,27	0.81	1 (3%)	38,40,40	0.52	0
2	FAD	F	602	-	58,58,58	0.35	0	85,89,89	0.52	0
2	FAD	C	701	-	58,58,58	0.60	1 (1%)	85,89,89	0.60	2 (2%)
5	UQ0	B	706	-	13,13,13	3.41	6 (46%)	16,18,18	1.74	3 (18%)
5	UQ0	C	704	-	13,13,13	3.39	5 (38%)	16,18,18	1.21	1 (6%)
3	TPP	F	603	4	26,27,27	0.66	0	38,40,40	0.52	0
3	TPP	D	702	4	26,27,27	0.72	1 (3%)	38,40,40	0.59	0
5	UQ0	D	706	-	13,13,13	3.63	6 (46%)	16,18,18	1.31	2 (12%)
5	UQ0	A	705	-	13,13,13	3.02	6 (46%)	16,18,18	2.94	5 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	701	-	-	5/34/50/50	0/6/6/6
5	UQ0	E	601	-	-	0/4/24/24	0/1/1/1
5	UQ0	C	706	-	-	0/4/24/24	0/1/1/1
5	UQ0	F	601	-	-	0/4/24/24	0/1/1/1
3	TPP	E	603	4	-	4/17/17/17	0/2/2/2
5	UQ0	A	706	-	-	1/4/24/24	0/1/1/1
5	UQ0	E	605	-	-	0/4/24/24	0/1/1/1
2	FAD	D	701	-	-	8/34/50/50	0/6/6/6
3	TPP	C	702	4	-	2/17/17/17	0/2/2/2
5	UQ0	D	704	-	-	1/4/24/24	0/1/1/1
5	UQ0	F	605	-	-	0/4/24/24	0/1/1/1
2	FAD	E	602	-	-	11/34/50/50	0/6/6/6
2	FAD	A	701	-	-	6/34/50/50	0/6/6/6
5	UQ0	B	705	-	-	1/4/24/24	0/1/1/1
3	TPP	B	702	4	-	2/17/17/17	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	A	702	4	-	1/17/17/17	0/2/2/2
2	FAD	F	602	-	-	11/34/50/50	0/6/6/6
2	FAD	C	701	-	-	8/34/50/50	0/6/6/6
5	UQ0	B	706	-	-	0/4/24/24	0/1/1/1
5	UQ0	C	704	-	-	0/4/24/24	0/1/1/1
3	TPP	F	603	4	-	2/17/17/17	0/2/2/2
3	TPP	D	702	4	-	1/17/17/17	0/2/2/2
5	UQ0	D	706	-	-	0/4/24/24	0/1/1/1
5	UQ0	A	705	-	-	0/4/24/24	0/1/1/1

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	UQ0	C6-C5	10.04	1.55	1.35
5	C	706	UQ0	C6-C5	9.88	1.55	1.35
5	D	706	UQ0	C6-C5	9.48	1.54	1.35
5	D	704	UQ0	C6-C5	9.24	1.53	1.35
5	F	605	UQ0	C6-C5	9.14	1.53	1.35

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	705	UQ0	CM5-C5-C4	9.42	123.89	117.41
5	A	706	UQ0	C6-C5-C4	4.89	123.66	119.56
5	F	601	UQ0	C6-C5-C4	4.50	123.33	119.56
5	A	705	UQ0	C6-C5-C4	-4.09	116.13	119.56
5	B	706	UQ0	C6-C5-C4	4.06	122.95	119.56

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

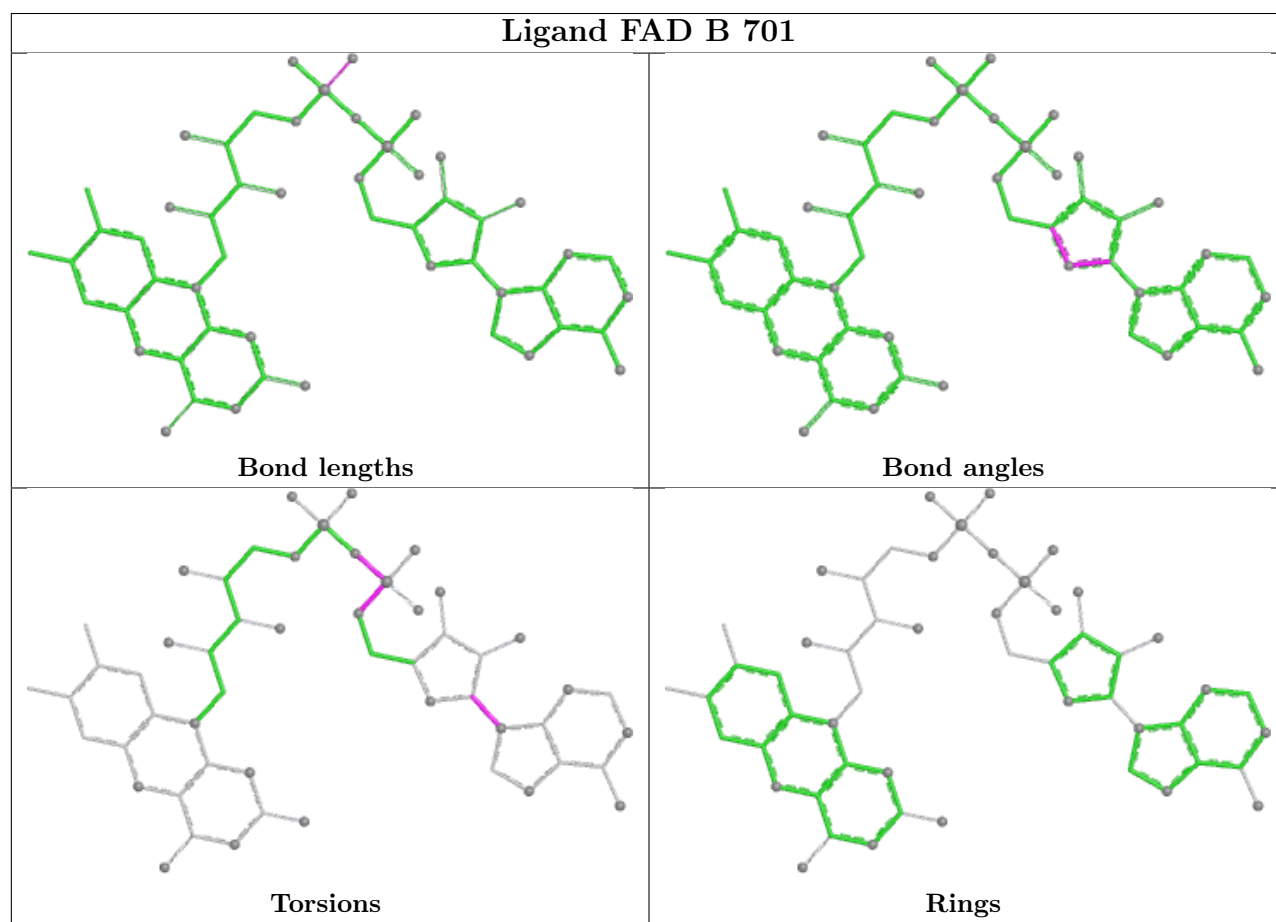
Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5'-O5'-P-O1P
2	C	701	FAD	C5'-O5'-P-O3P
2	D	701	FAD	C5B-O5B-PA-O1A

There are no ring outliers.

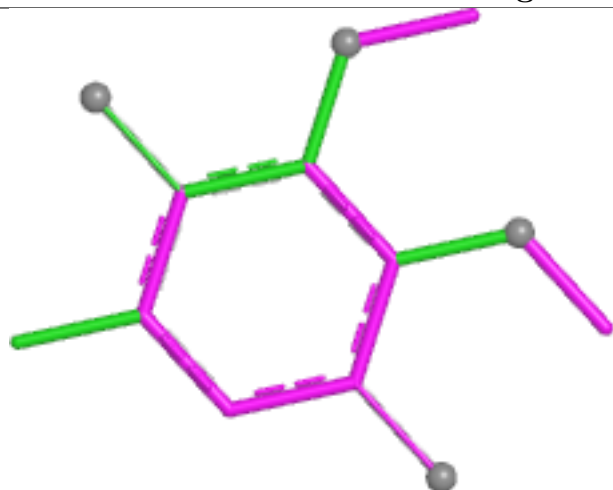
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	601	UQ0	1	0
5	F	601	UQ0	1	0
2	E	602	FAD	3	0
2	A	701	FAD	1	0
5	A	705	UQ0	1	0

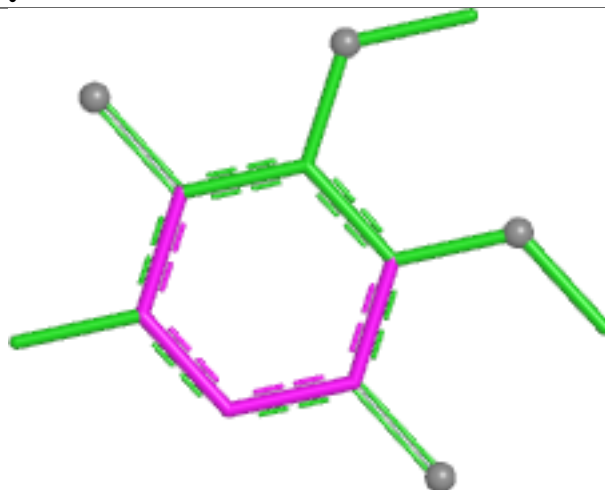
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



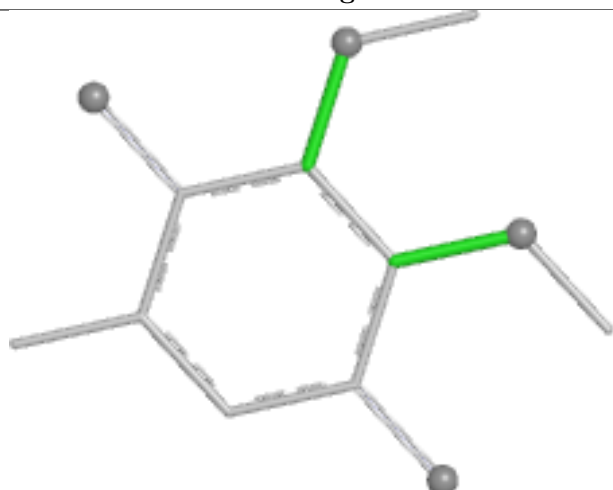
Ligand UQ0 E 601



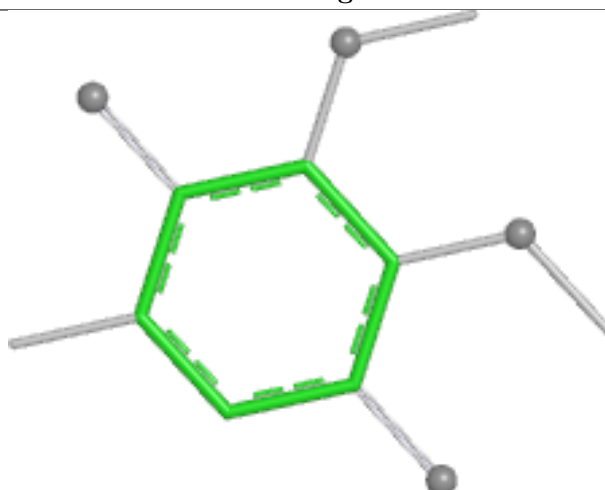
Bond lengths



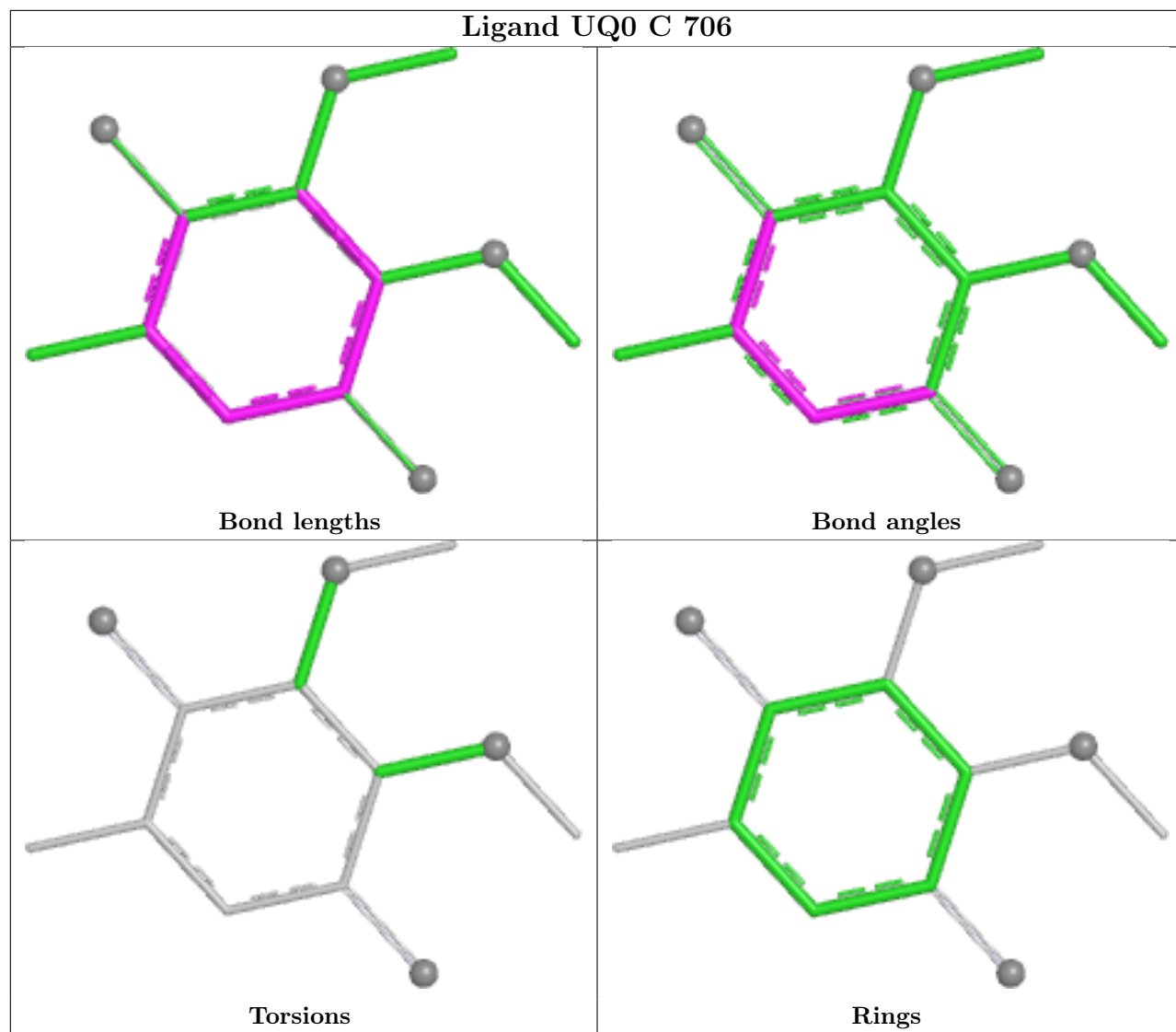
Bond angles



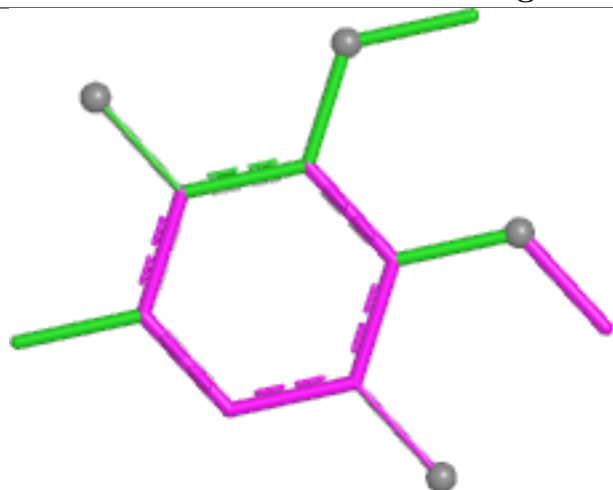
Torsions



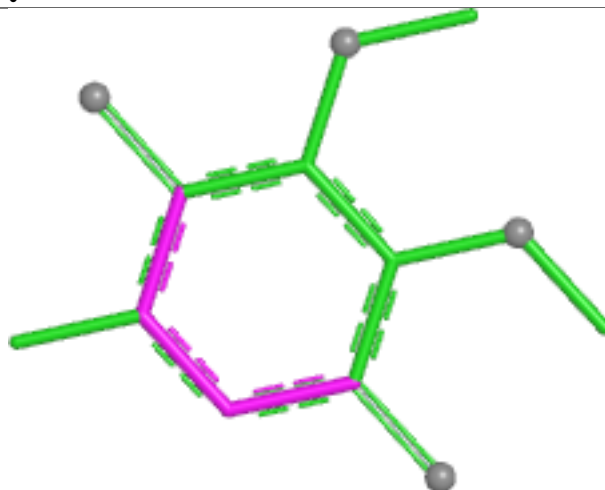
Rings



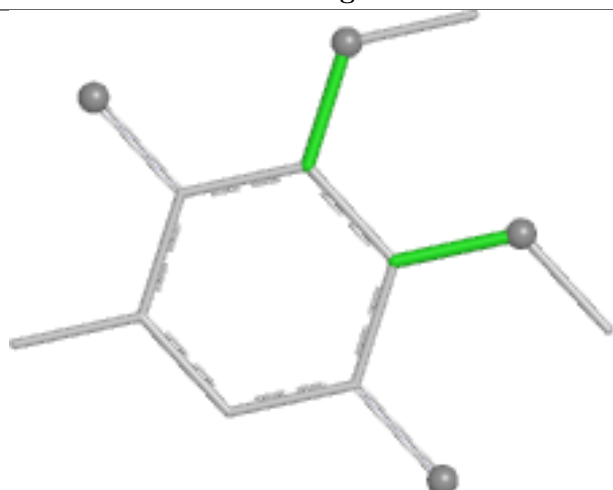
Ligand UQ0 F 601



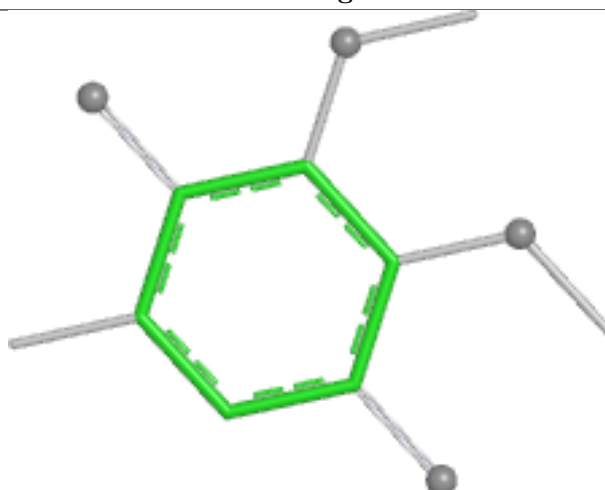
Bond lengths



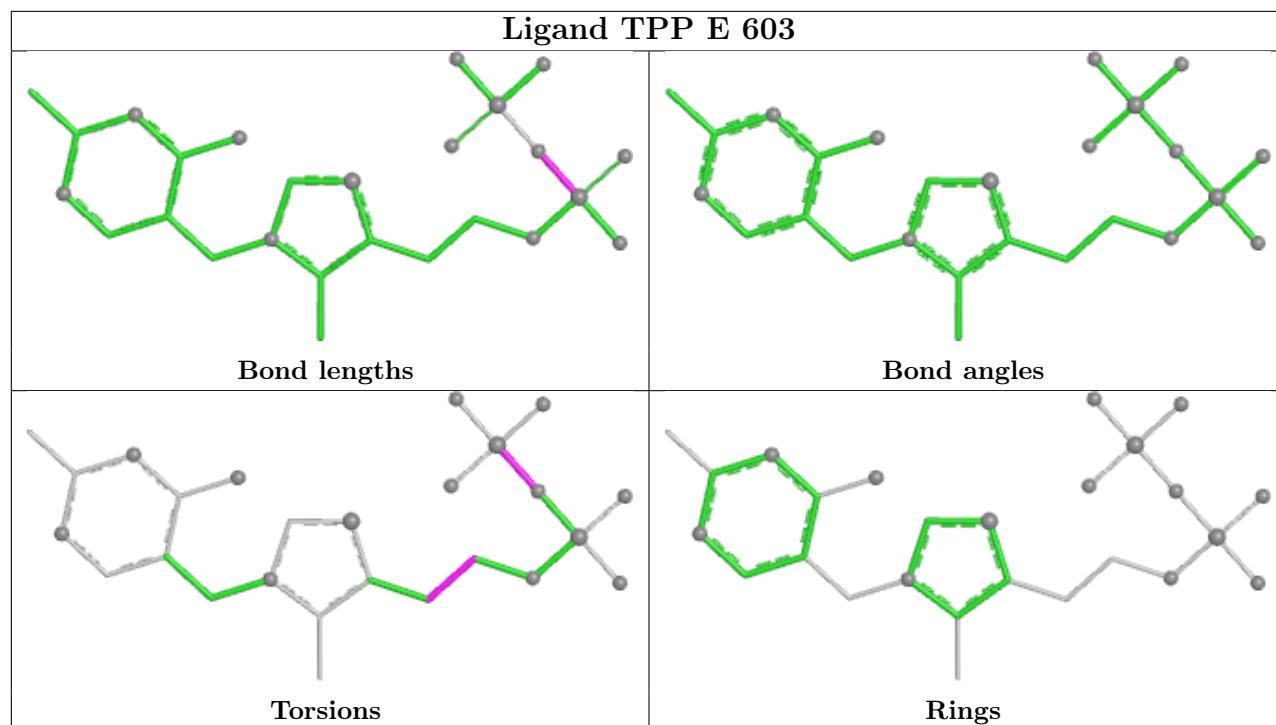
Bond angles

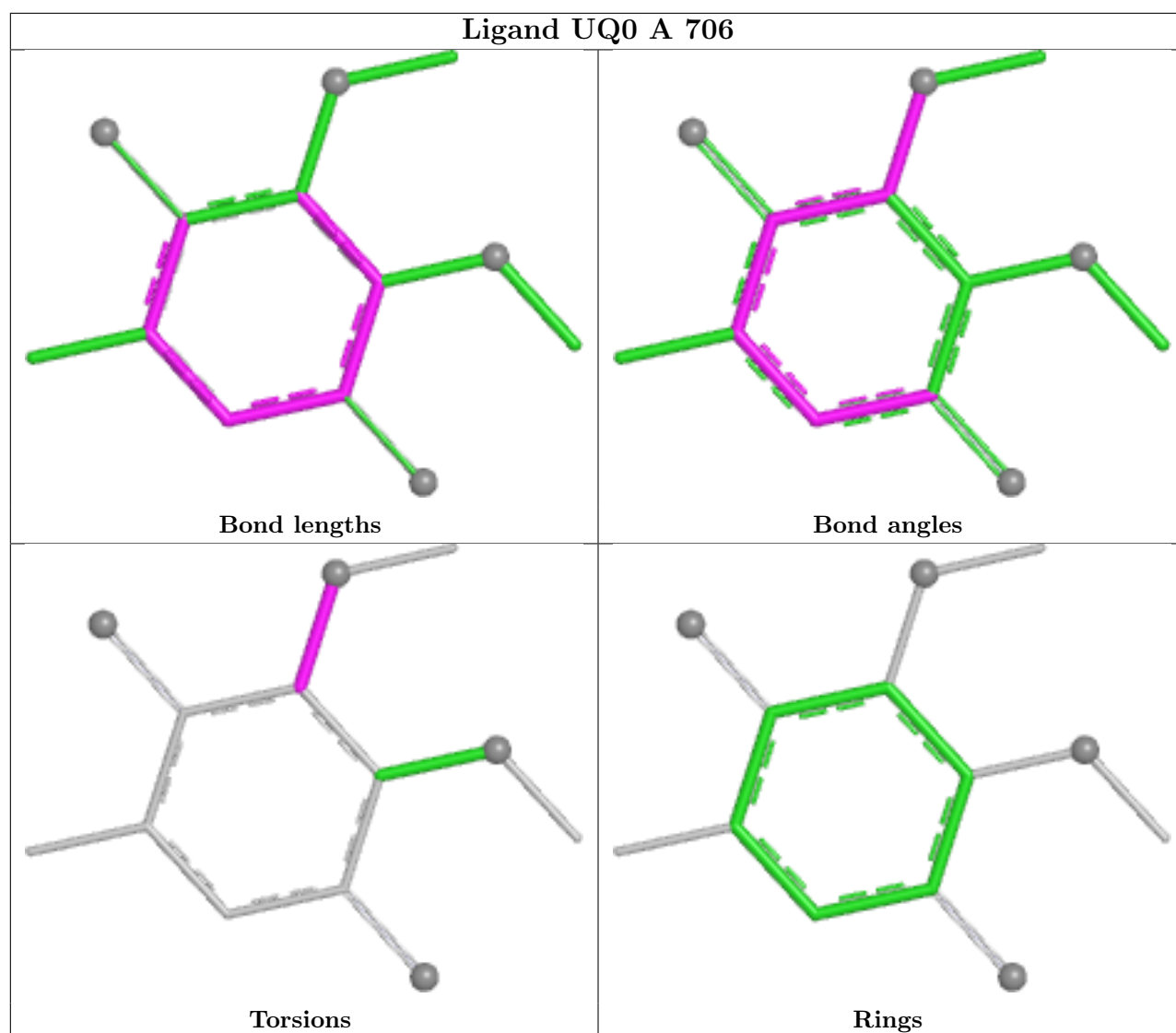


Torsions

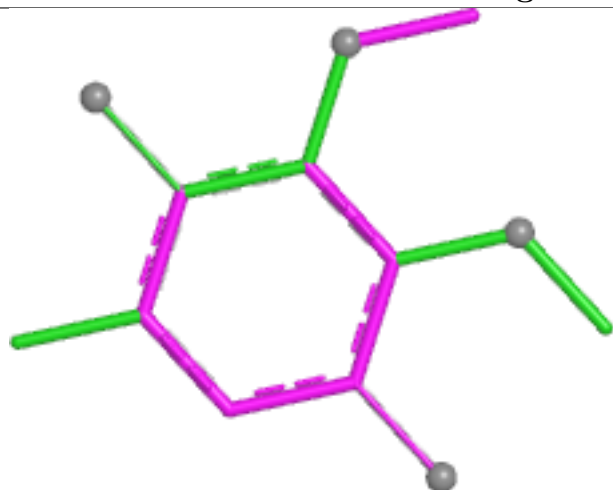


Rings

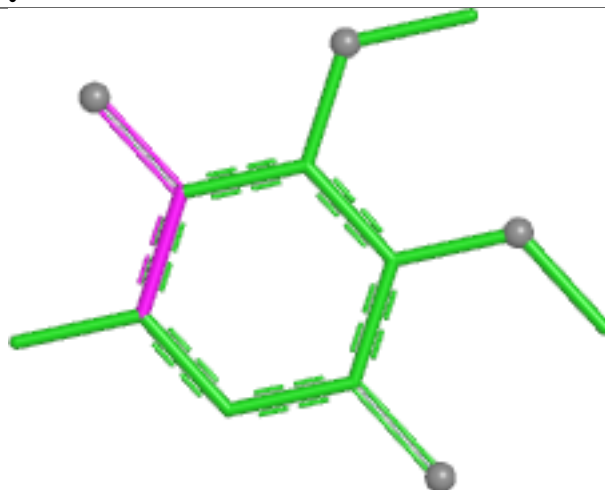




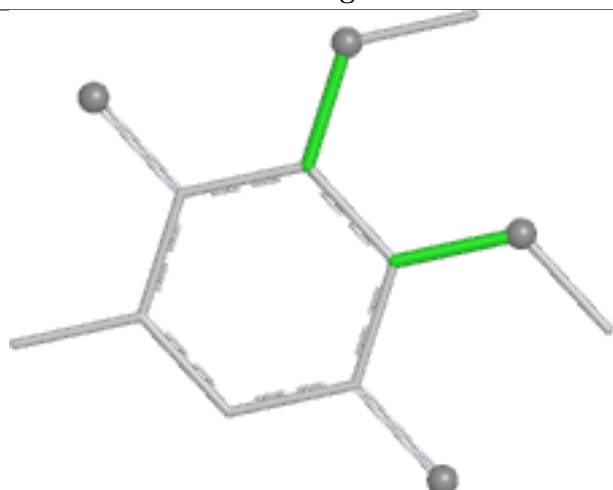
Ligand UQ0 E 605



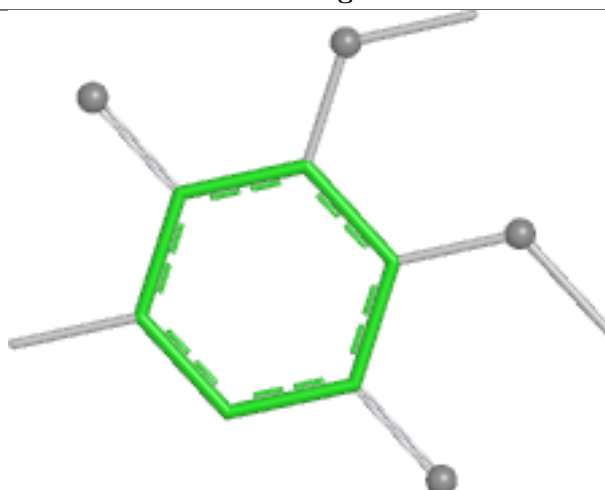
Bond lengths



Bond angles

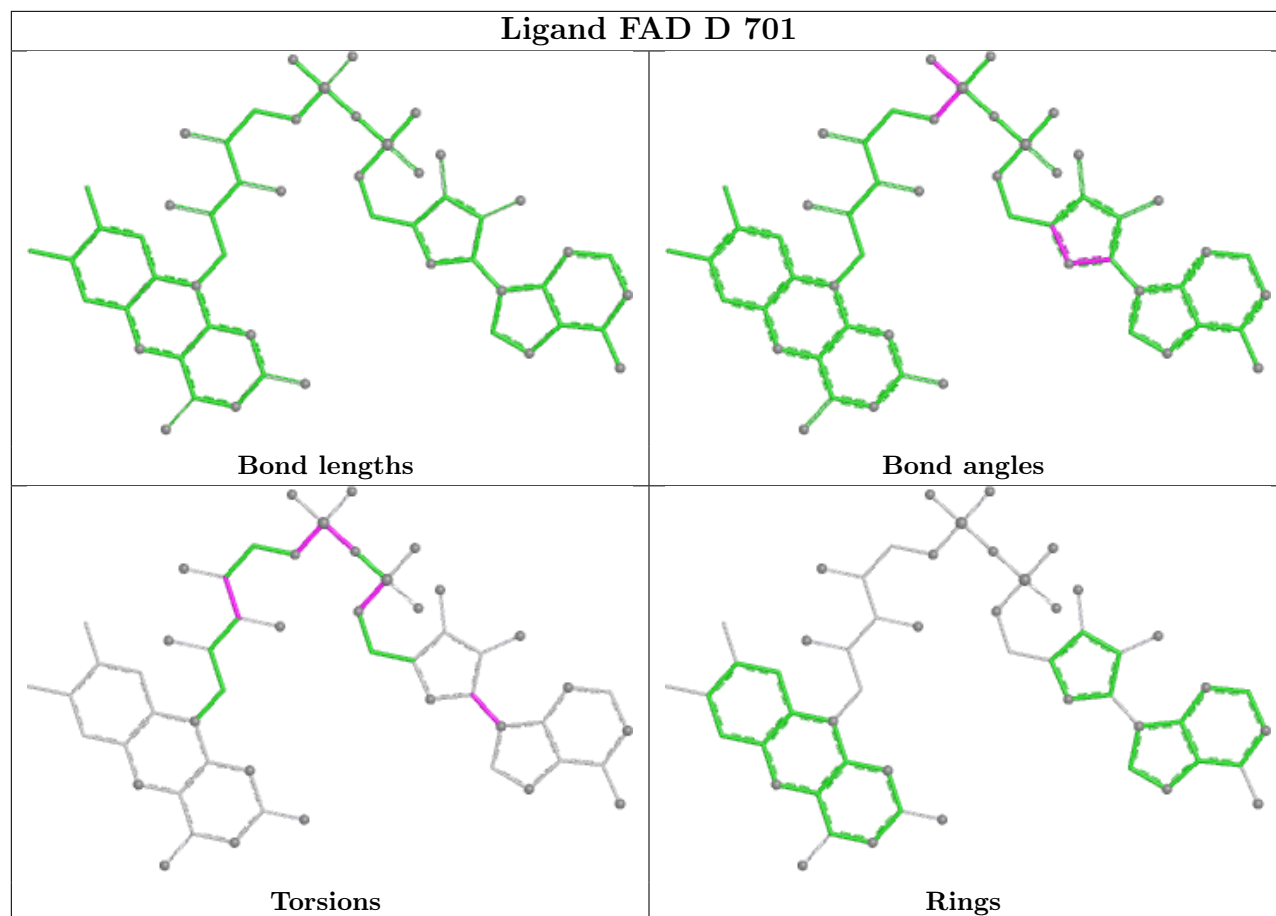


Torsions

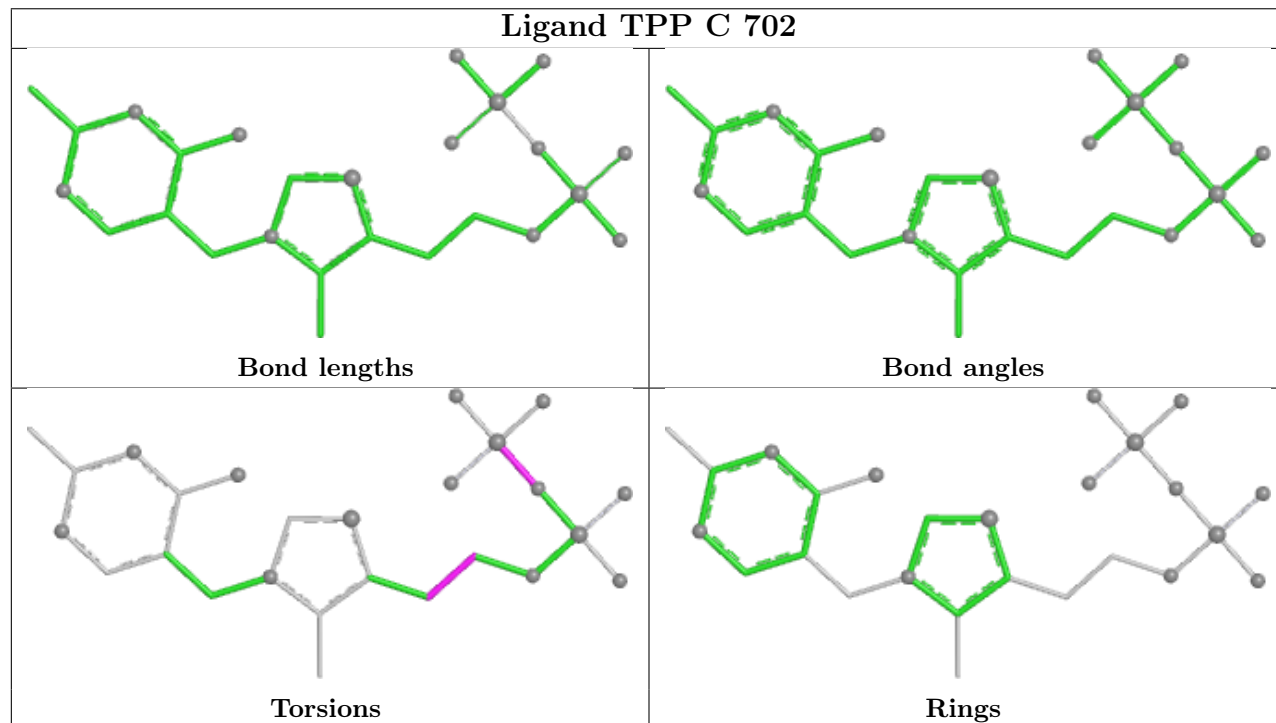


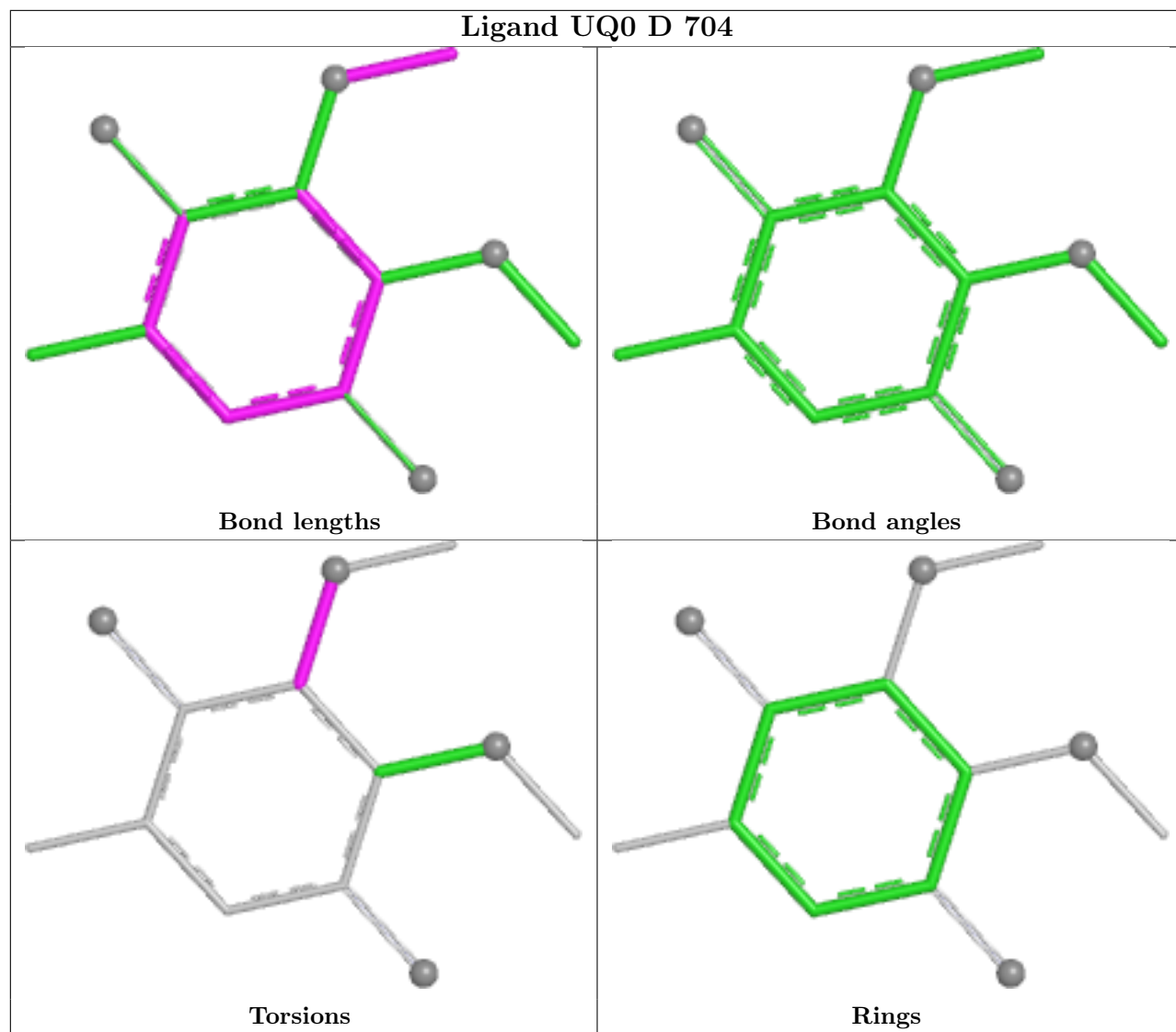
Rings

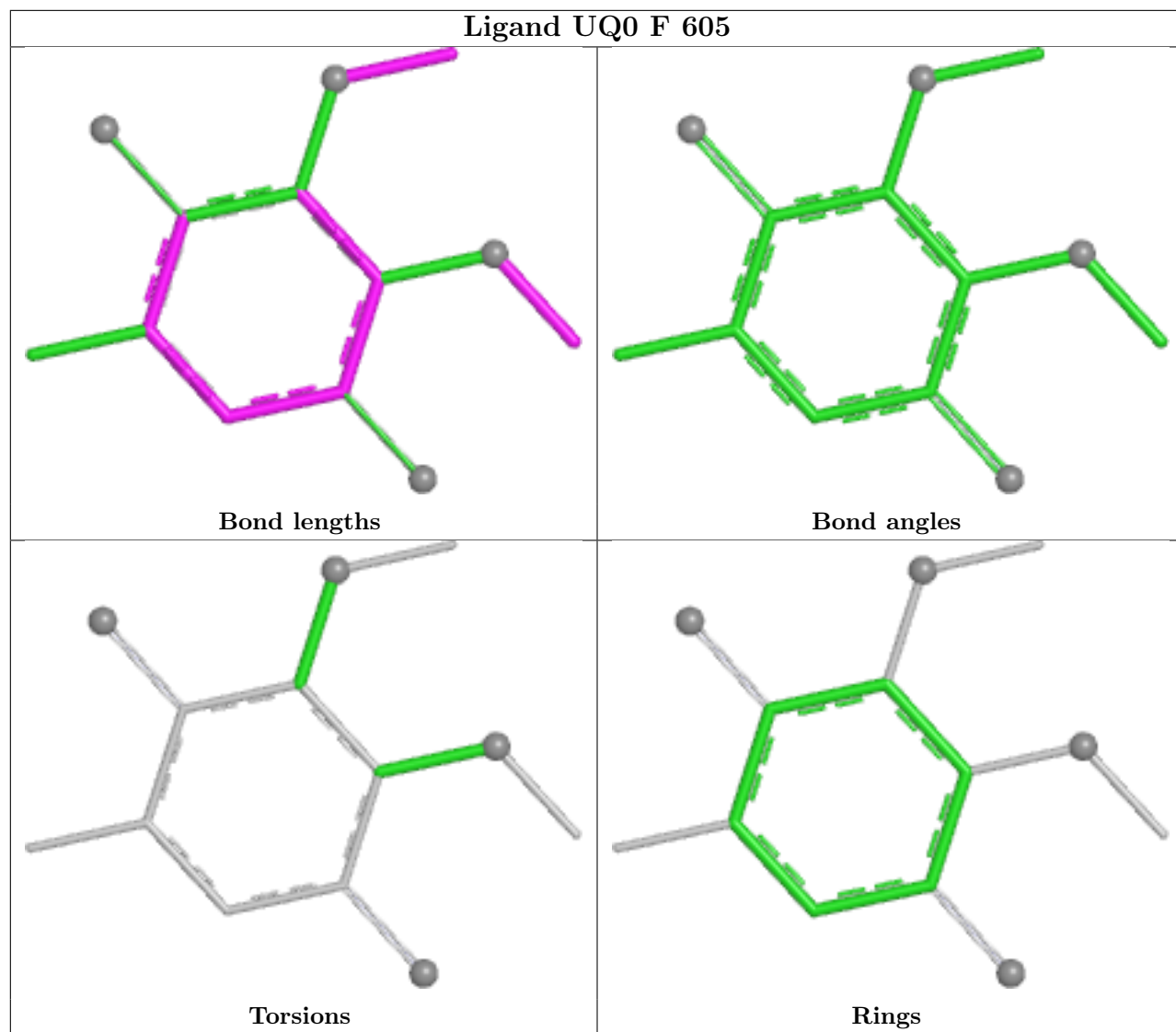
Ligand FAD D 701

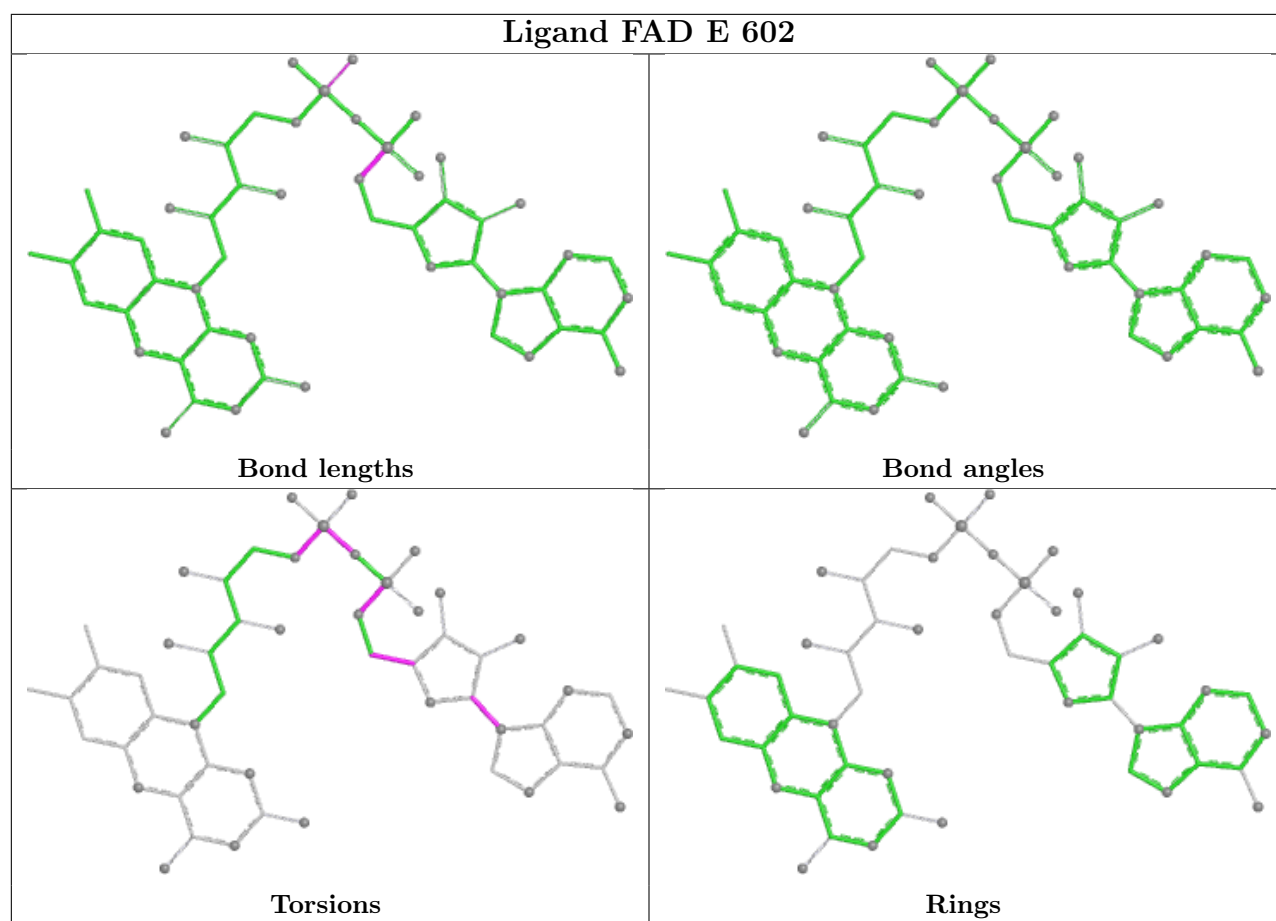


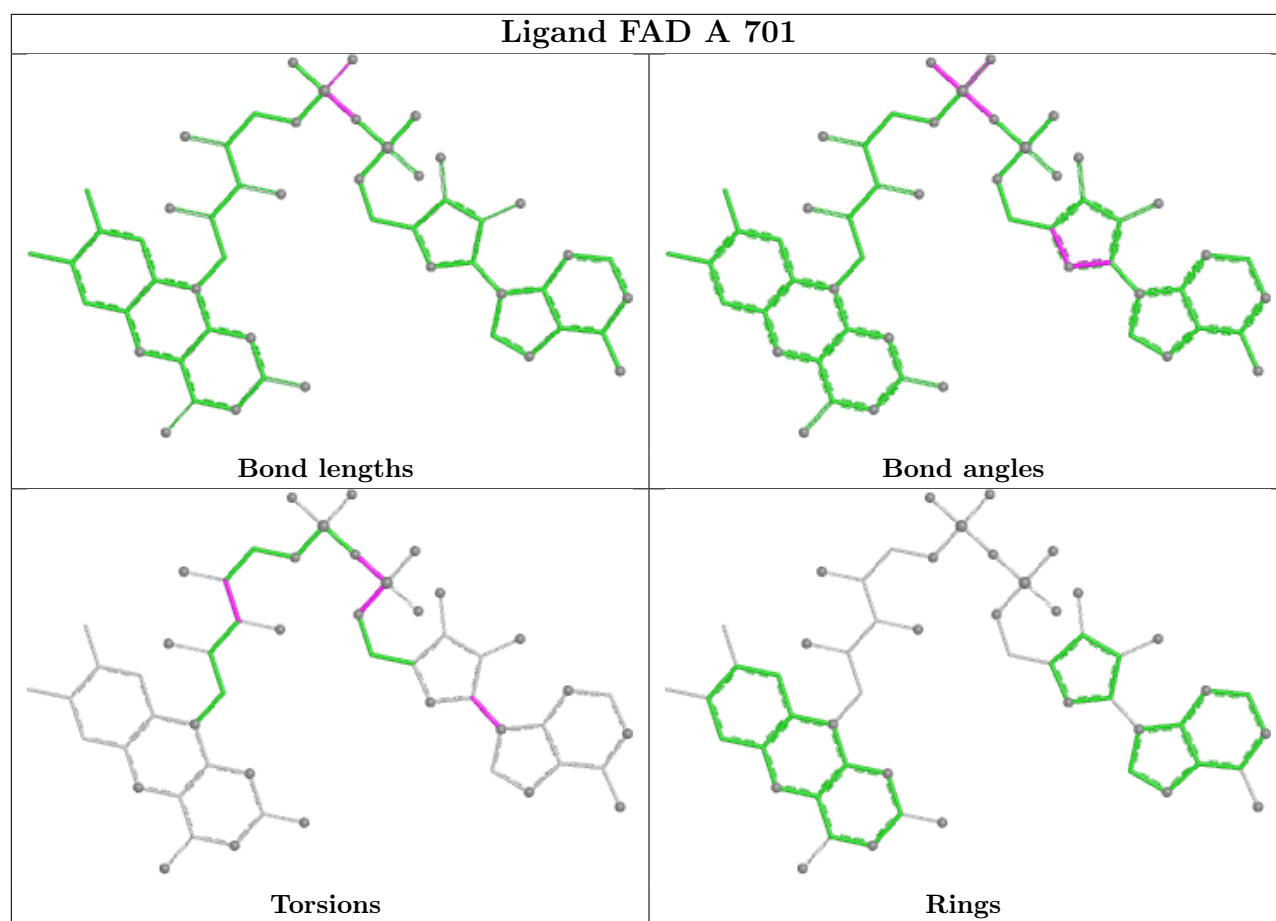
Ligand TPP C 702

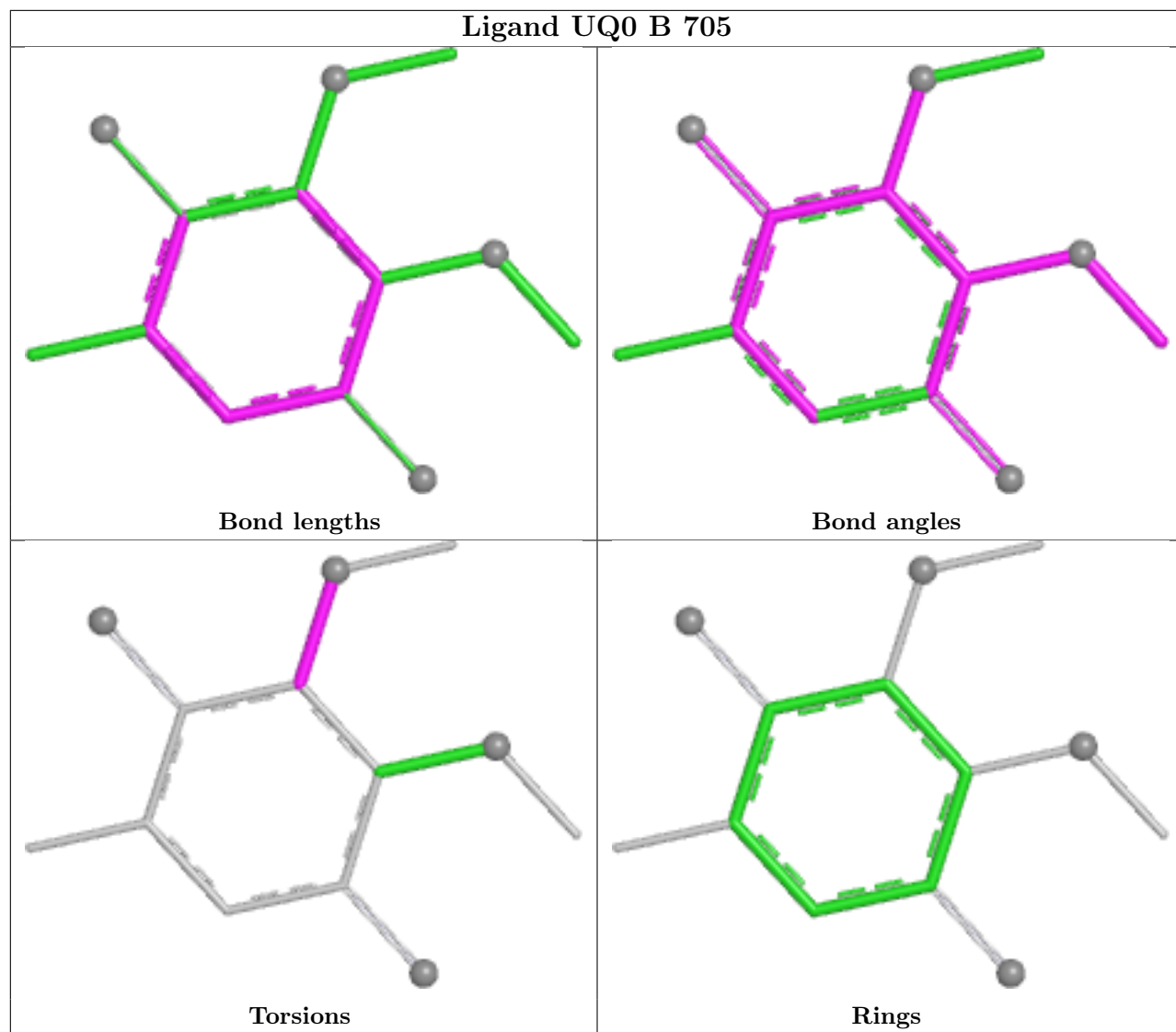




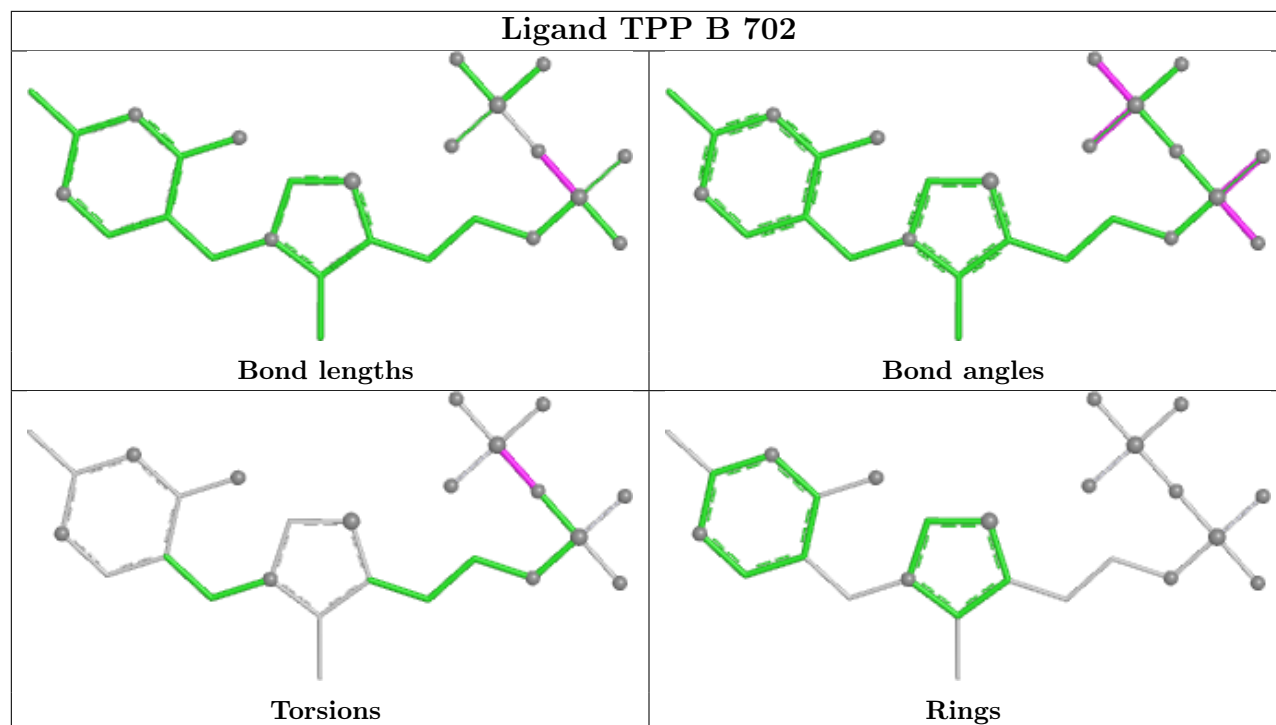




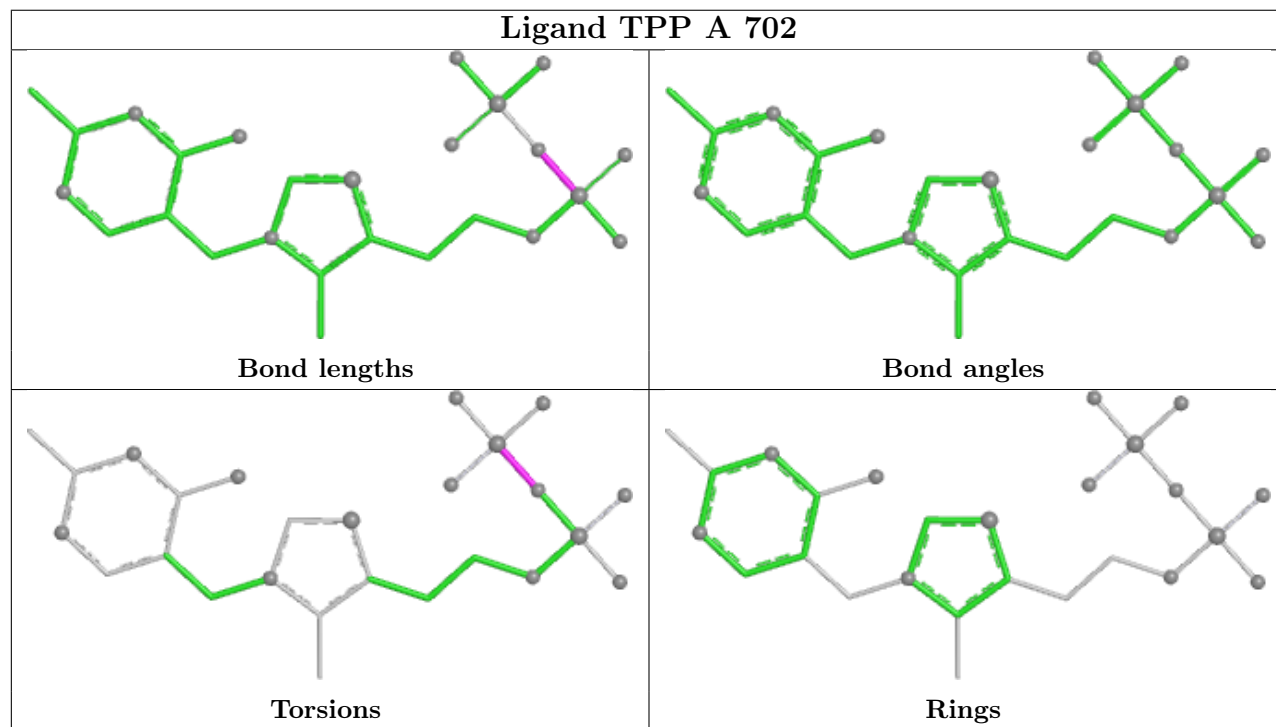


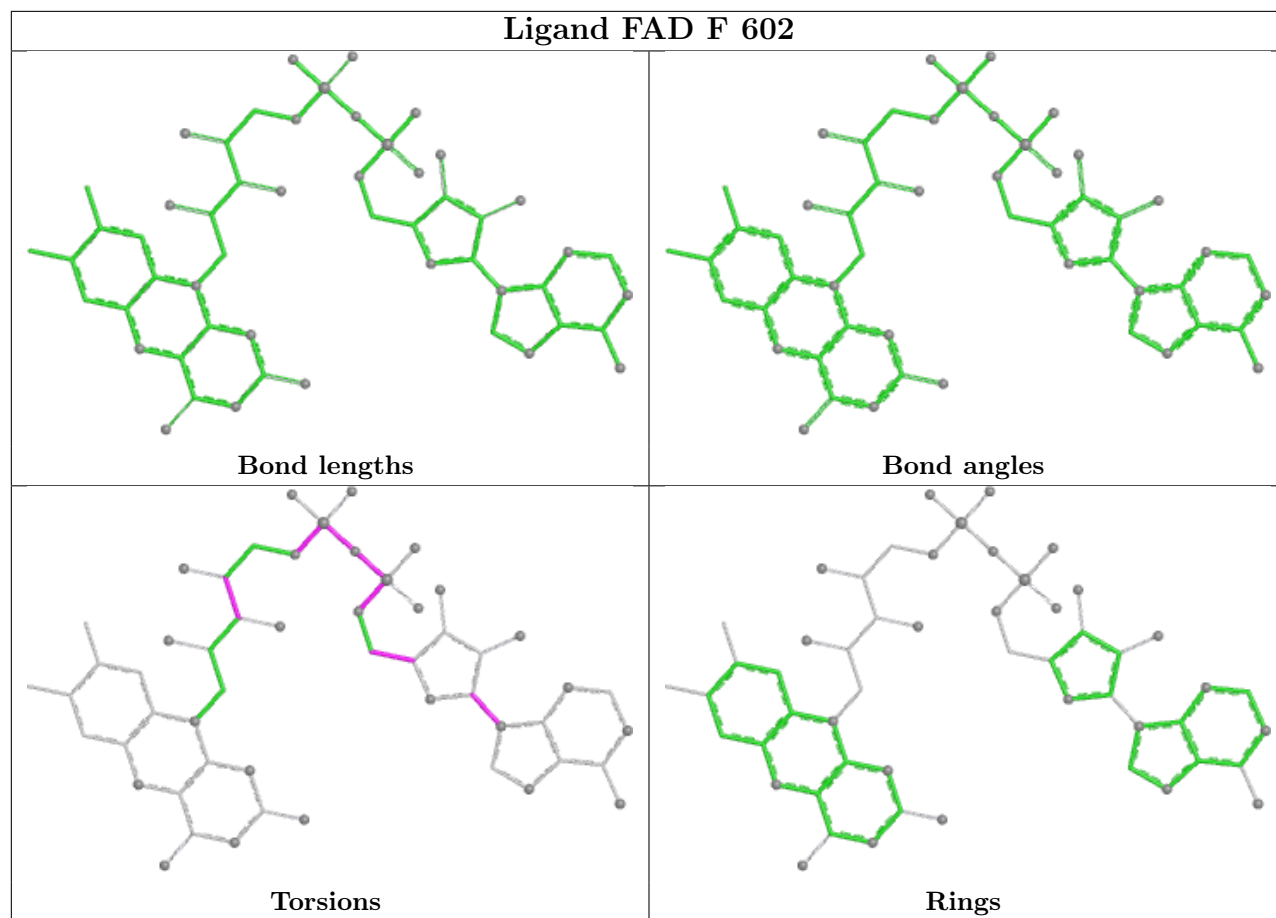


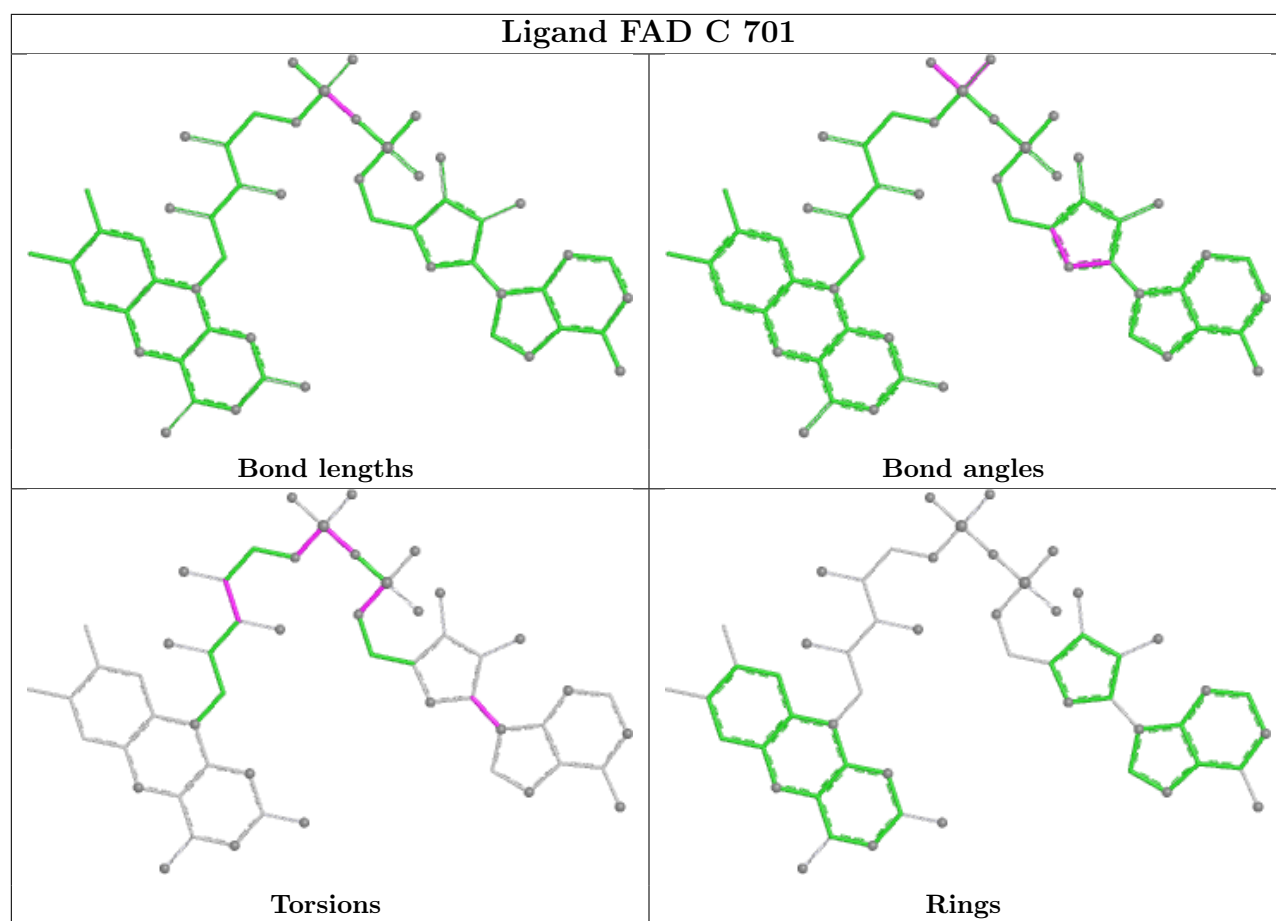
Ligand TPP B 702

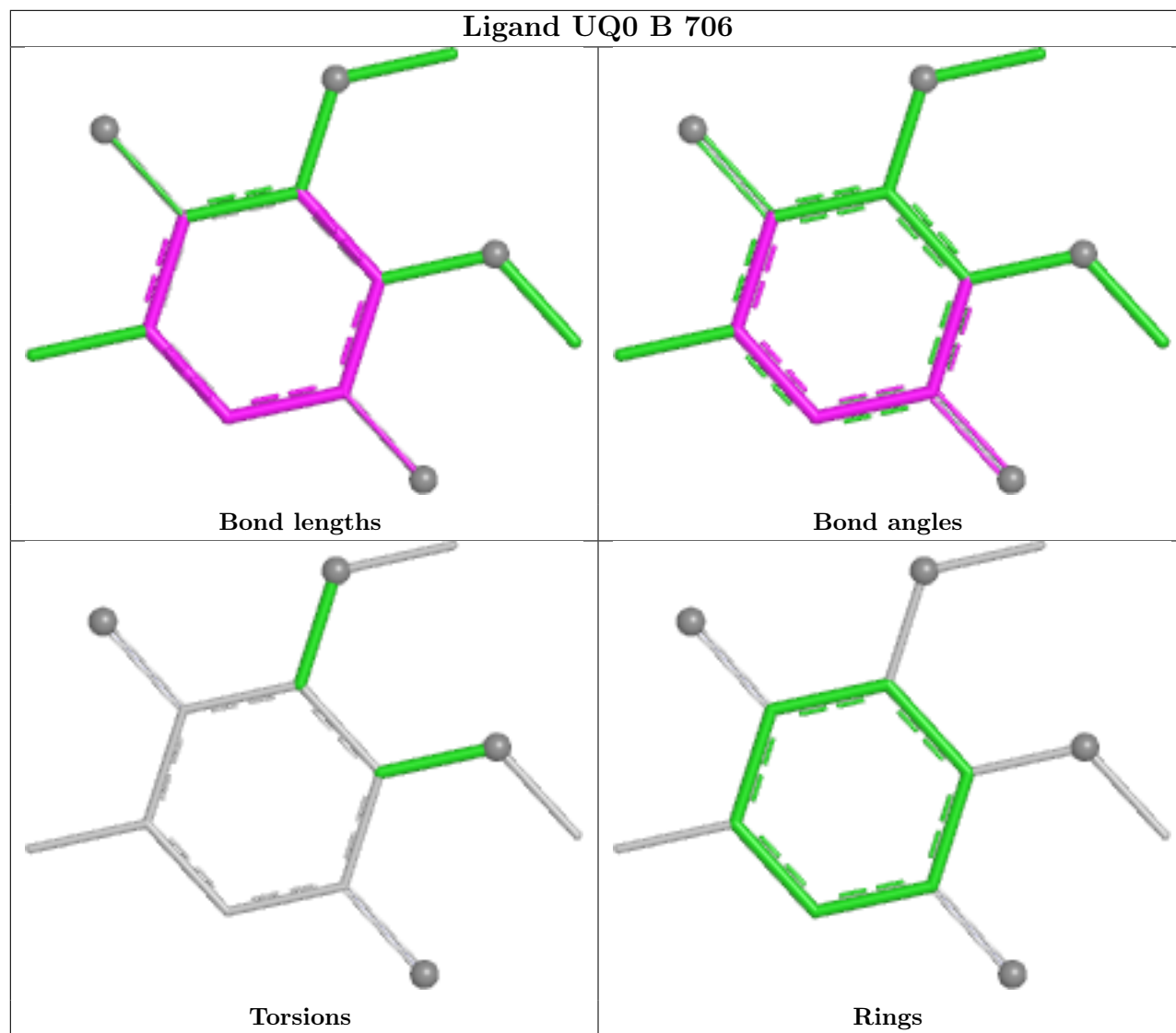


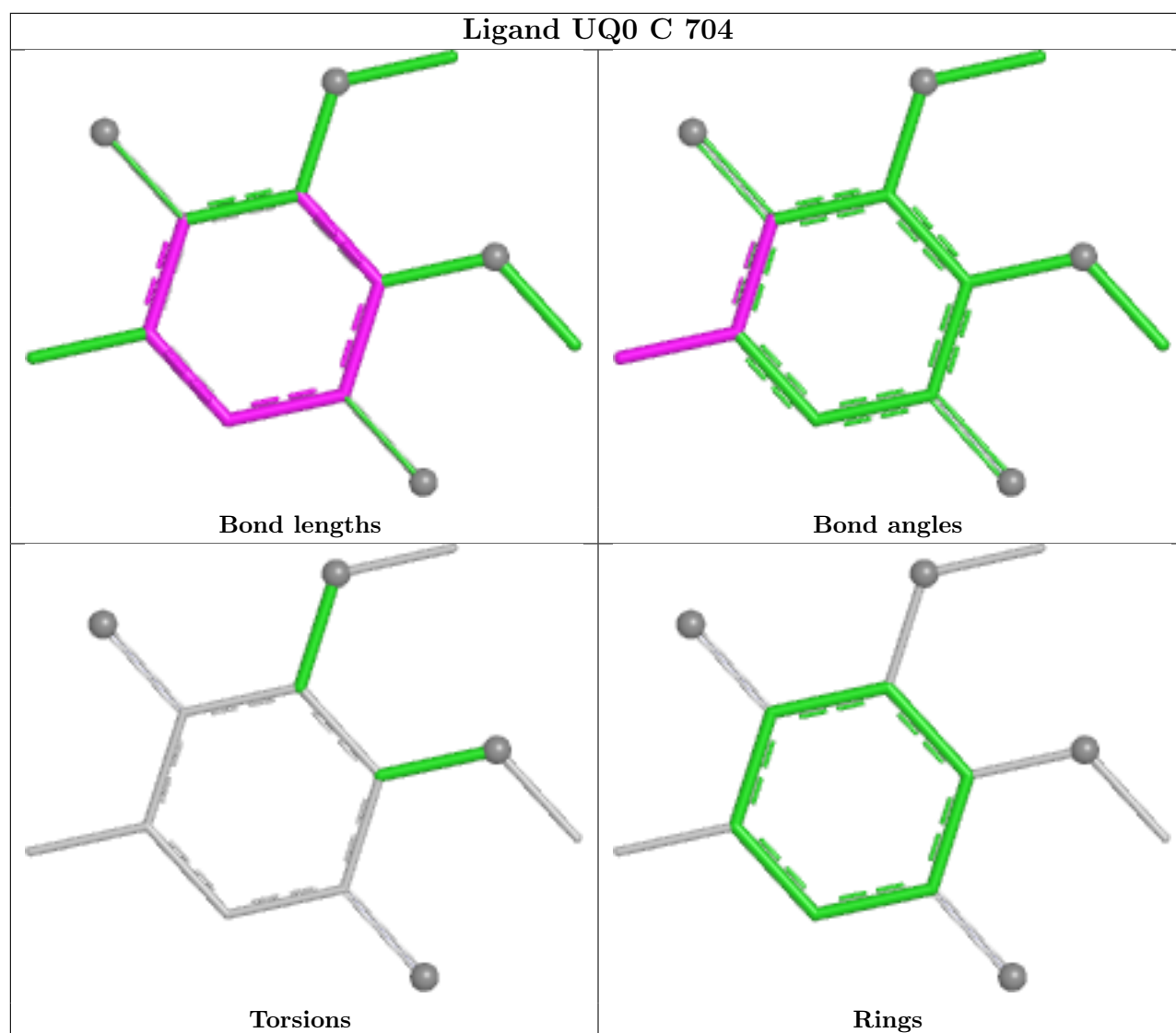
Ligand TPP A 702



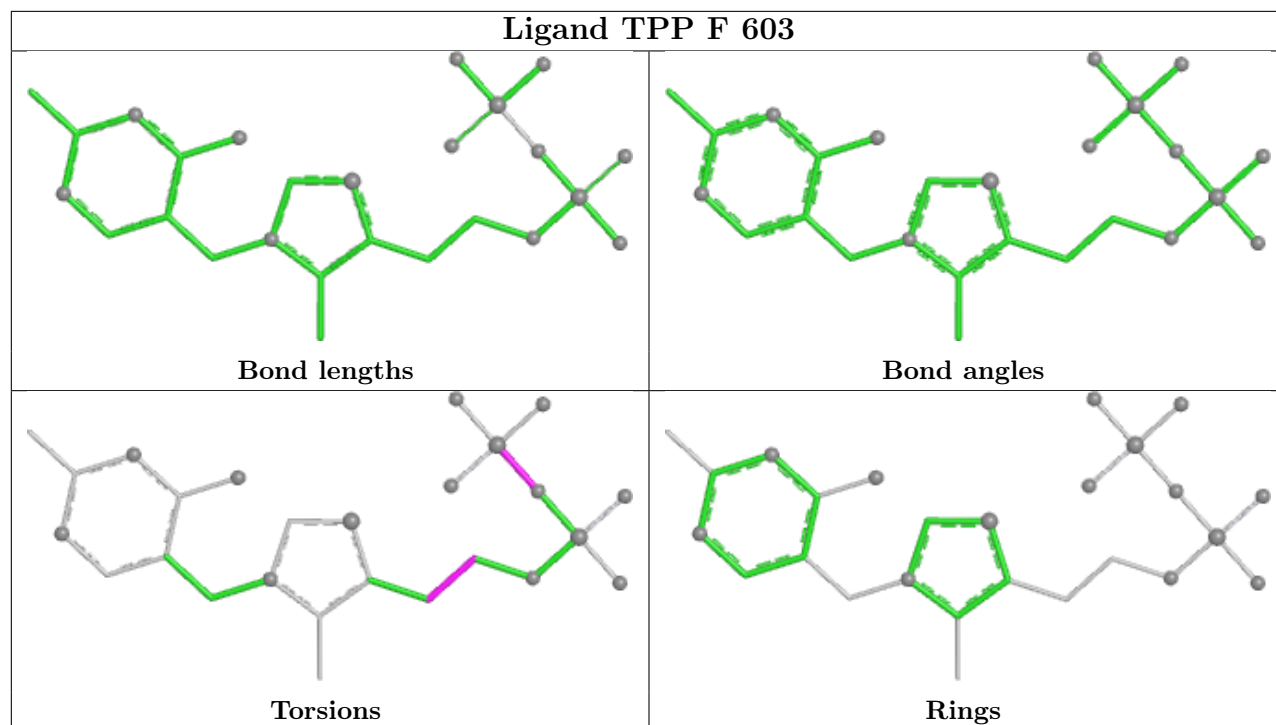




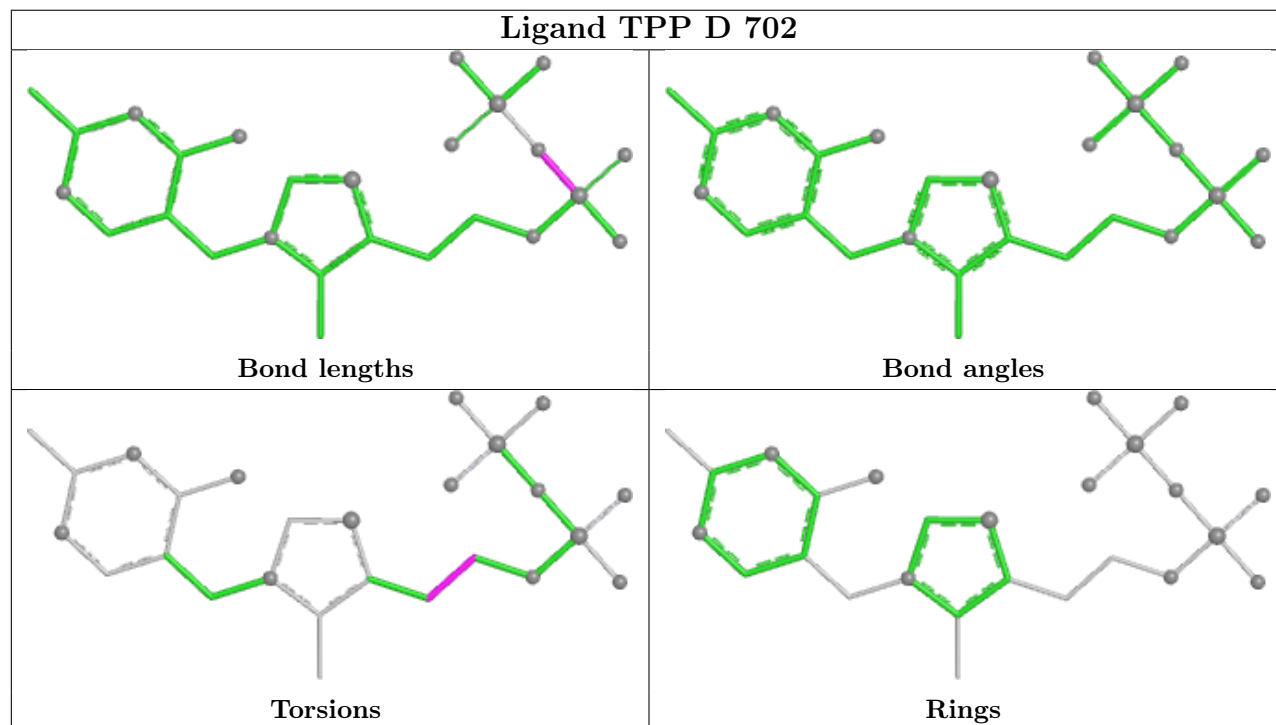


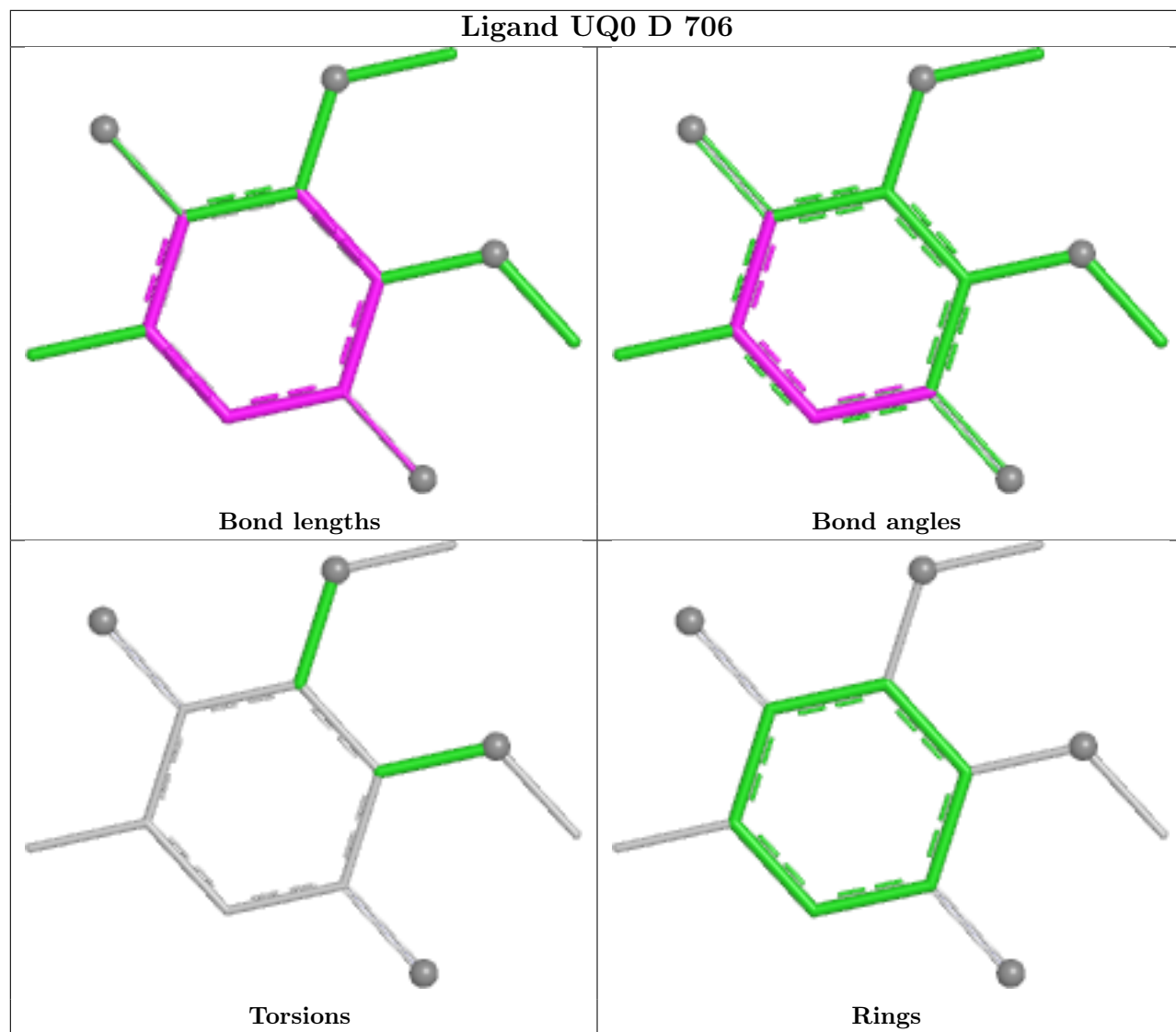


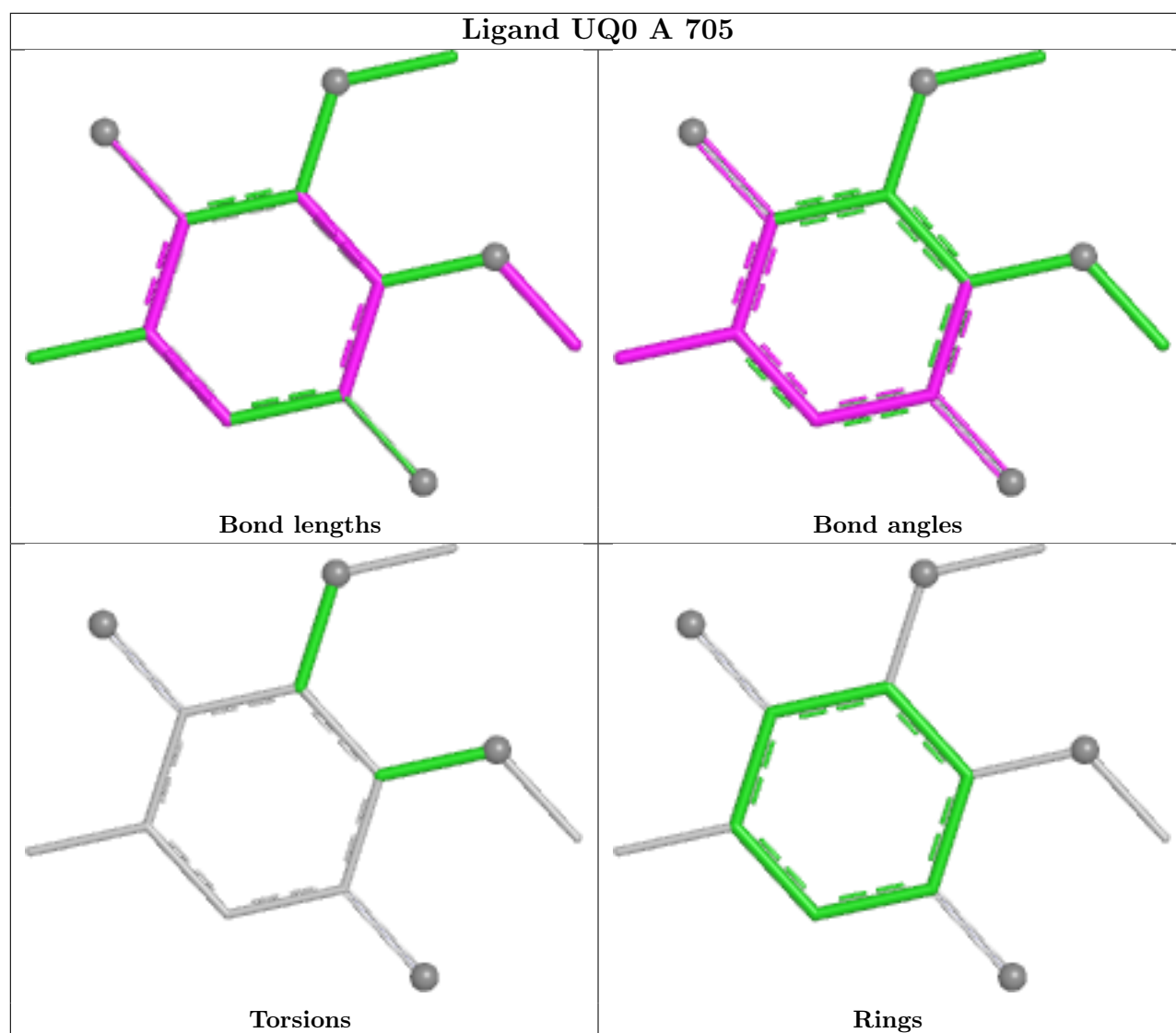
Ligand TPP F 603



Ligand TPP D 702







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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/594 (100%)	-0.73	2 (0%) 90 93	11, 17, 33, 60	0
1	B	594/594 (100%)	-0.68	2 (0%) 90 93	11, 18, 36, 71	0
1	C	594/594 (100%)	-0.14	10 (1%) 69 75	23, 31, 50, 86	0
1	D	594/594 (100%)	-0.12	5 (0%) 82 88	21, 31, 53, 78	0
1	E	594/594 (100%)	0.05	6 (1%) 79 85	23, 35, 55, 75	0
1	F	594/594 (100%)	0.13	13 (2%) 62 69	23, 35, 56, 84	0
All	All	3564/3564 (100%)	-0.25	38 (1%) 78 84	11, 29, 50, 86	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	0	GLY	3.7
1	D	0	GLY	3.5
1	D	593	GLU	3.4
1	E	1	MET	3.3
1	C	109	LEU	3.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

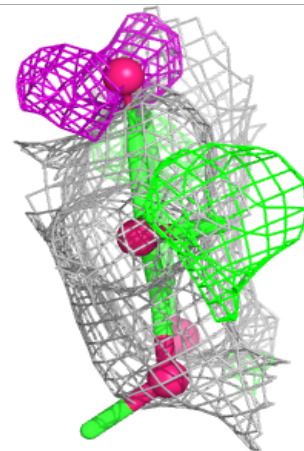
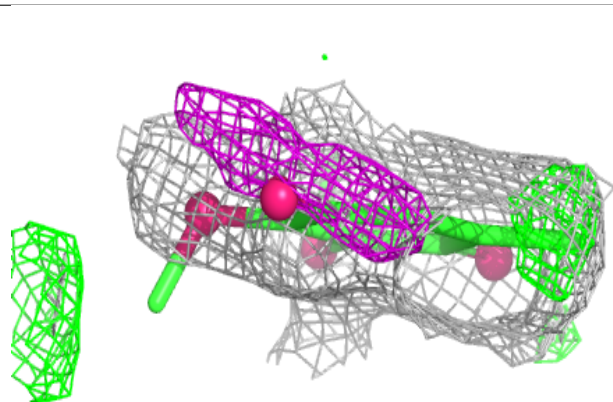
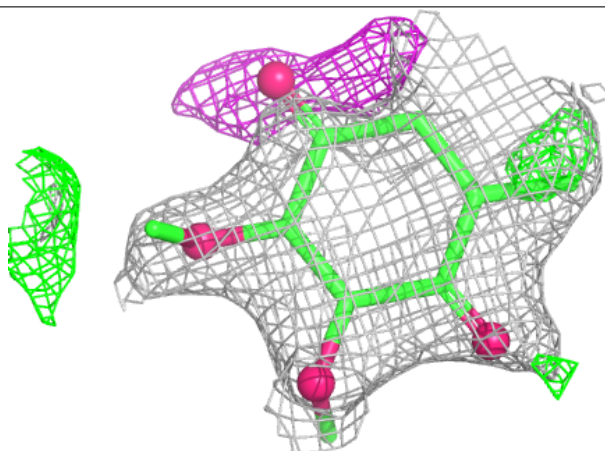
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	UQ0	E	601	13/13	0.76	0.19	59,67,74,77	0
5	UQ0	F	601	13/13	0.78	0.17	57,65,72,75	0
5	UQ0	C	706	13/13	0.80	0.17	47,55,62,63	0
5	UQ0	E	605	13/13	0.81	0.17	73,80,83,85	0
5	UQ0	D	706	13/13	0.84	0.14	55,59,62,62	0
5	UQ0	C	704	13/13	0.84	0.17	66,70,72,72	0
5	UQ0	A	705	13/13	0.87	0.11	26,33,36,36	0
5	UQ0	B	706	13/13	0.89	0.10	20,28,39,40	0
5	UQ0	A	706	13/13	0.90	0.11	18,25,34,43	0
5	UQ0	D	704	13/13	0.90	0.12	43,48,55,59	0
5	UQ0	F	605	13/13	0.90	0.13	44,47,56,58	0
5	UQ0	B	705	13/13	0.94	0.09	23,27,36,40	0
2	FAD	E	602	53/53	0.96	0.07	29,32,36,37	0
2	FAD	B	701	53/53	0.97	0.05	11,14,20,27	0
2	FAD	F	602	53/53	0.97	0.06	24,30,37,39	0
3	TPP	F	603	26/26	0.97	0.06	27,31,35,36	0
2	FAD	C	701	53/53	0.97	0.06	22,26,30,31	0
2	FAD	D	701	53/53	0.97	0.06	20,28,31,35	0
4	MG	D	705	1/1	0.98	0.07	26,26,26,26	0
4	MG	F	604	1/1	0.98	0.05	29,29,29,29	0
3	TPP	C	702	26/26	0.98	0.05	21,26,29,32	0
3	TPP	D	702	26/26	0.98	0.06	23,29,30,32	0
3	TPP	E	603	26/26	0.98	0.05	26,30,32,36	0
2	FAD	A	701	53/53	0.98	0.04	11,13,16,22	0
4	MG	C	705	1/1	0.98	0.04	27,27,27,27	0
4	MG	D	703	1/1	0.99	0.02	24,24,24,24	0
3	TPP	B	702	26/26	0.99	0.04	11,14,18,20	0
4	MG	E	604	1/1	0.99	0.02	27,27,27,27	0
4	MG	A	703	1/1	0.99	0.01	12,12,12,12	0
4	MG	A	704	1/1	0.99	0.04	11,11,11,11	1
4	MG	B	703	1/1	0.99	0.03	12,12,12,12	0
4	MG	C	703	1/1	0.99	0.02	24,24,24,24	0
3	TPP	A	702	26/26	0.99	0.04	10,12,18,26	0
4	MG	B	704	1/1	1.00	0.05	11,11,11,11	1

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.

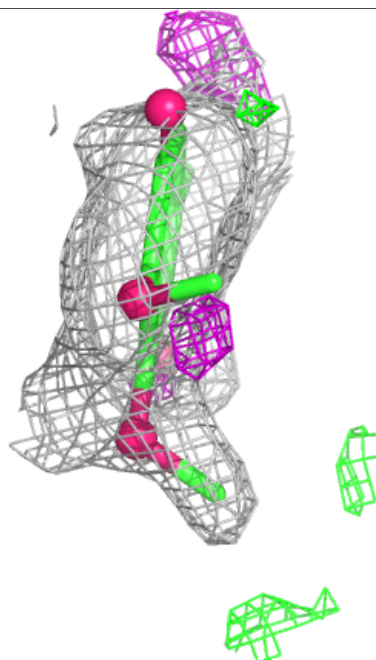
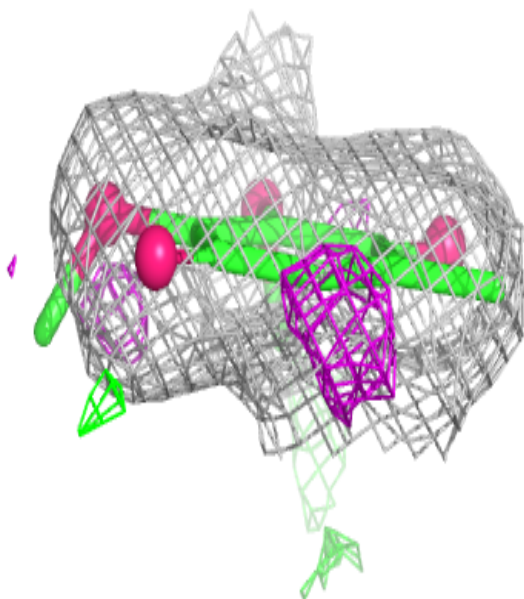
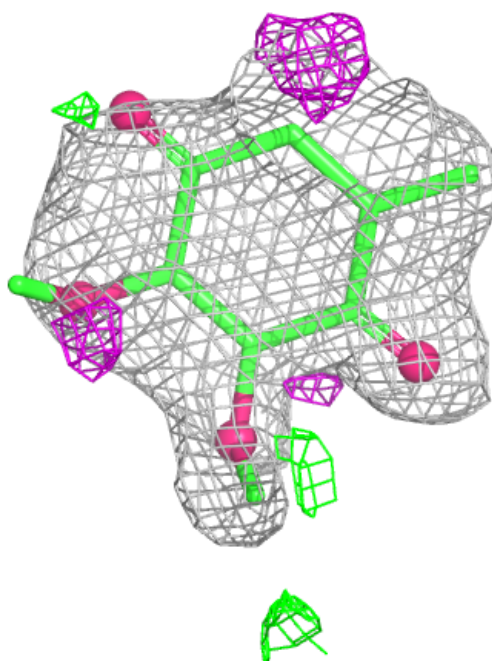
Electron density around UQ0 E 601:

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



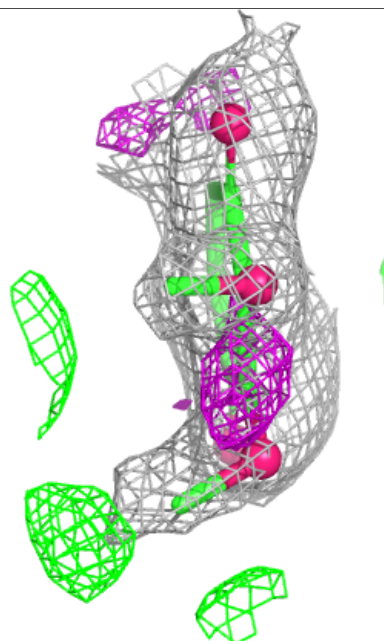
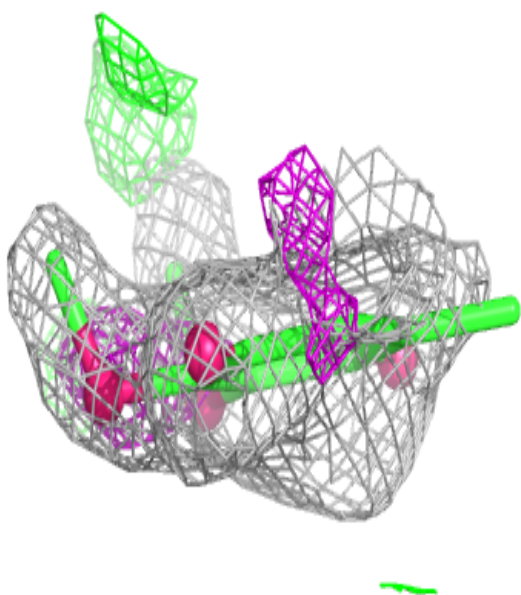
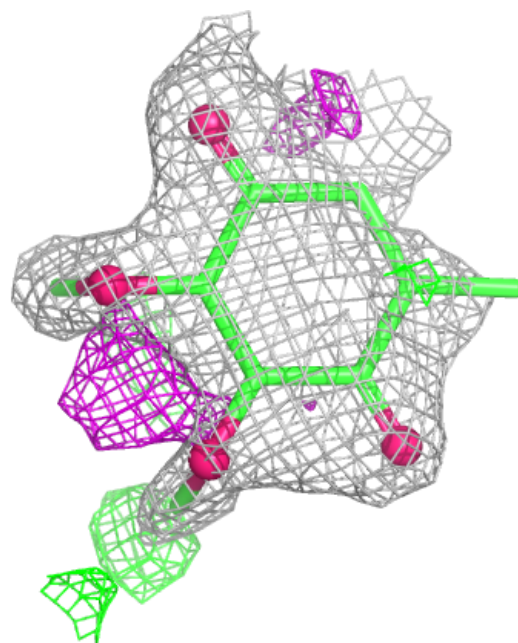
Electron density around UQ0 F 601:

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



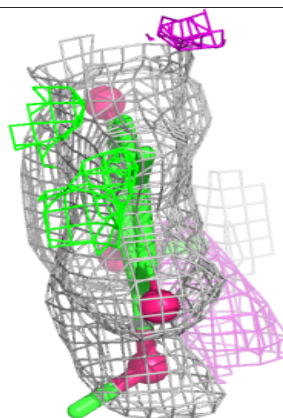
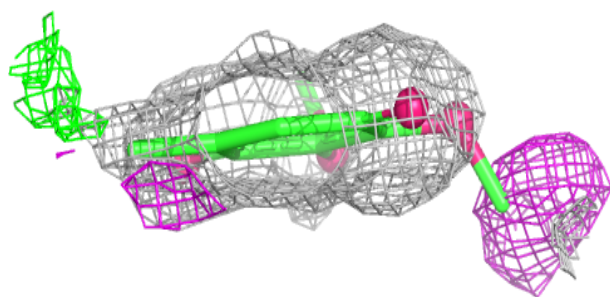
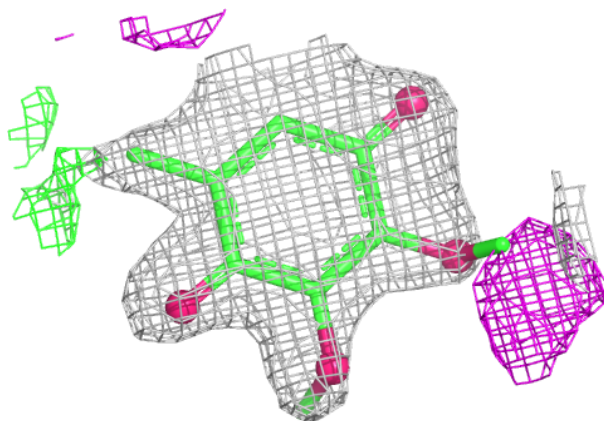
Electron density around UQ0 C 706:

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



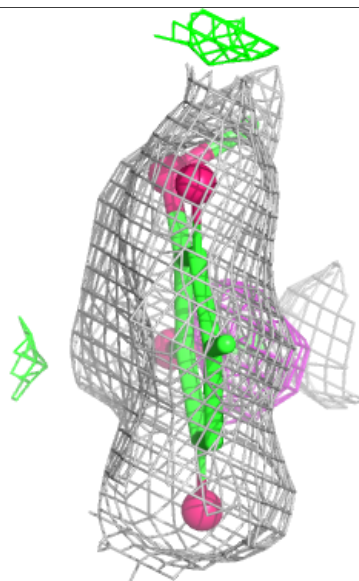
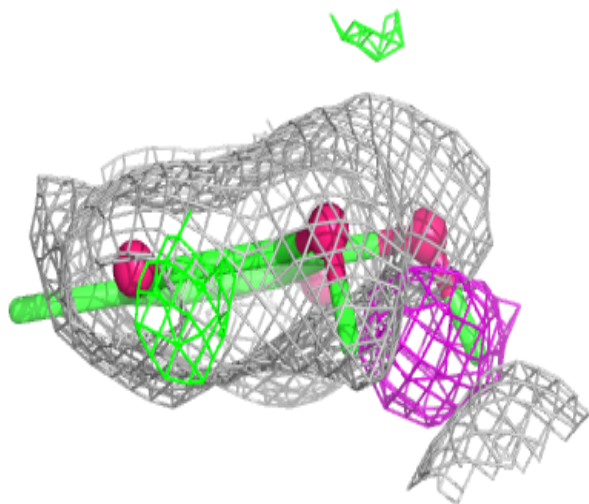
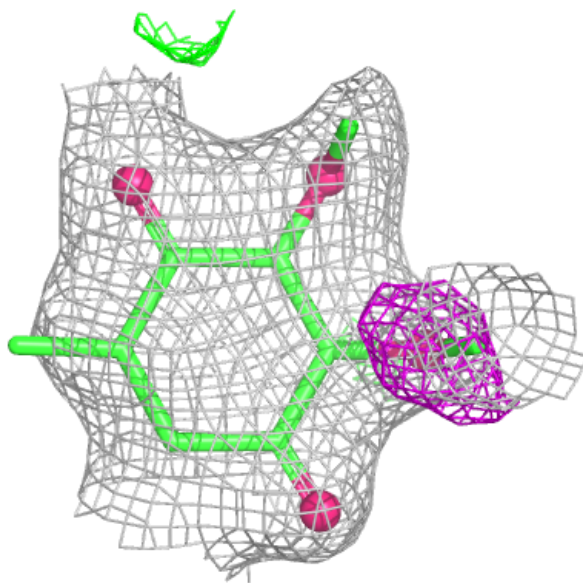
Electron density around UQ0 E 605:

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



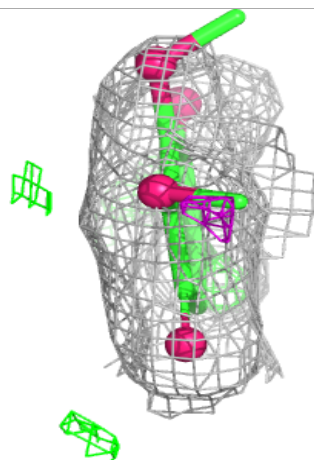
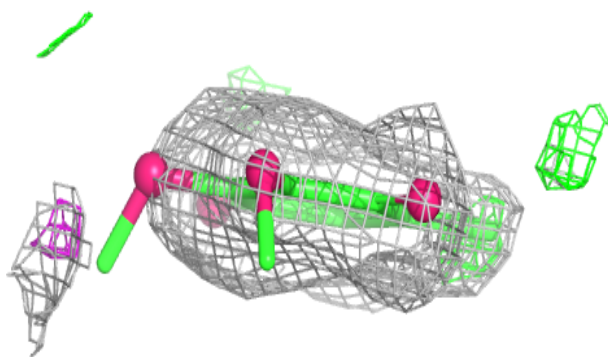
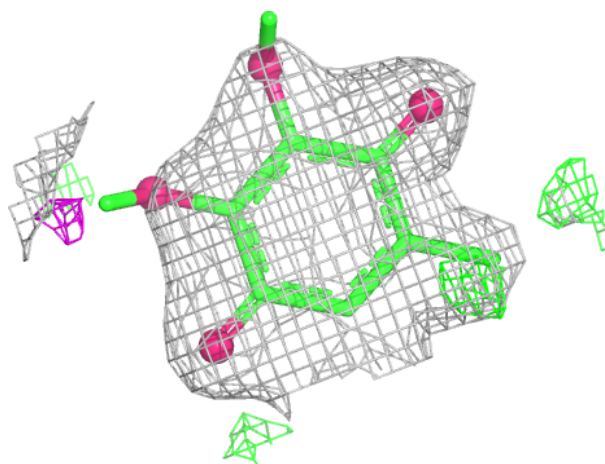
Electron density around UQ0 D 706:

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



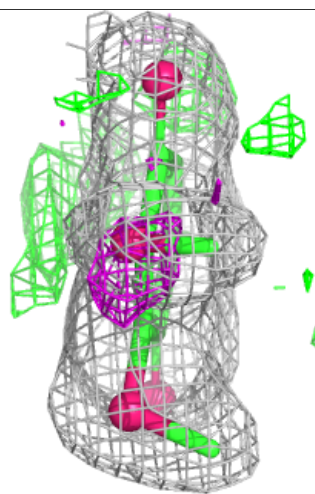
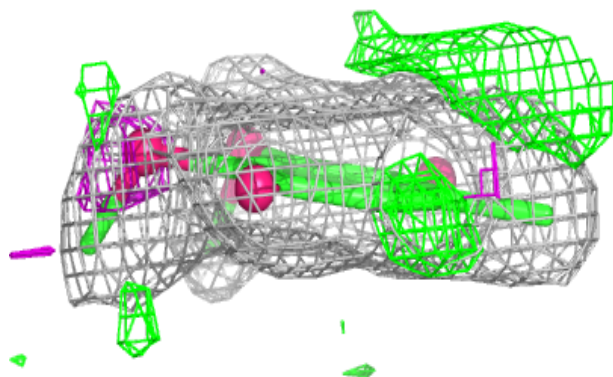
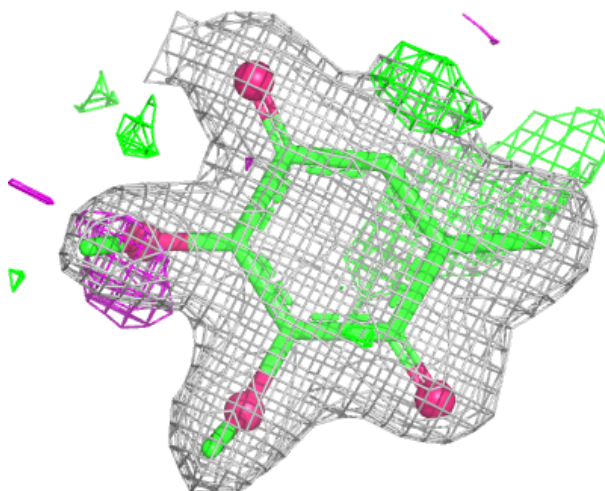
Electron density around UQ0 C 704:

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



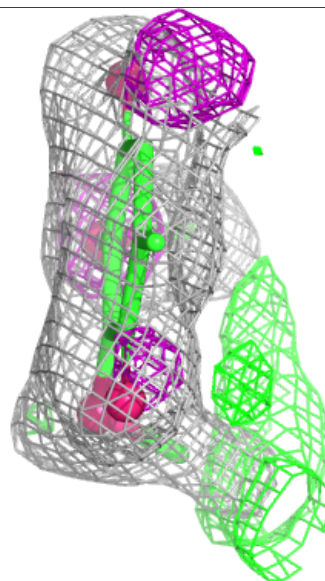
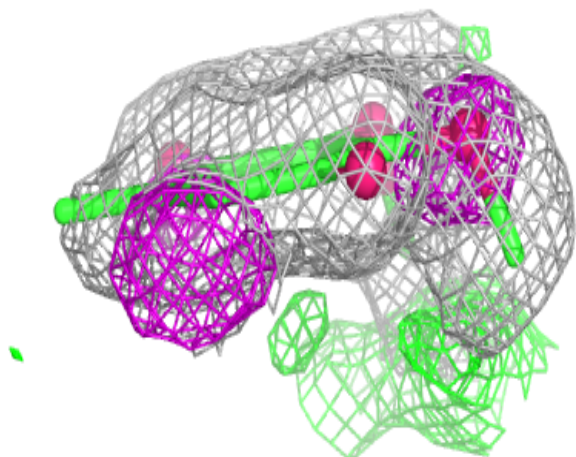
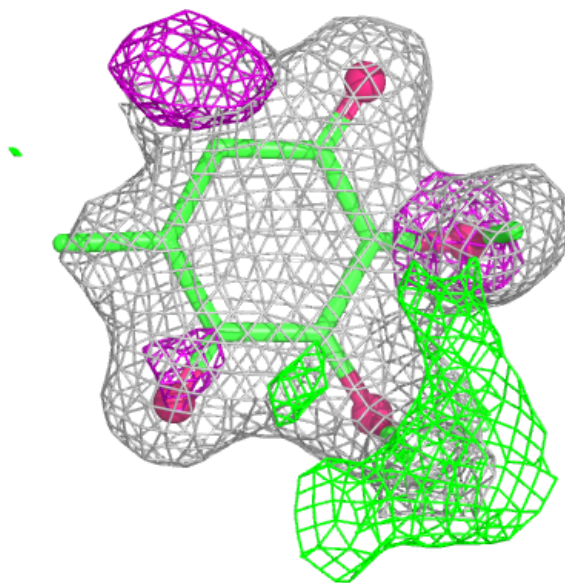
Electron density around UQ0 A 705:

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



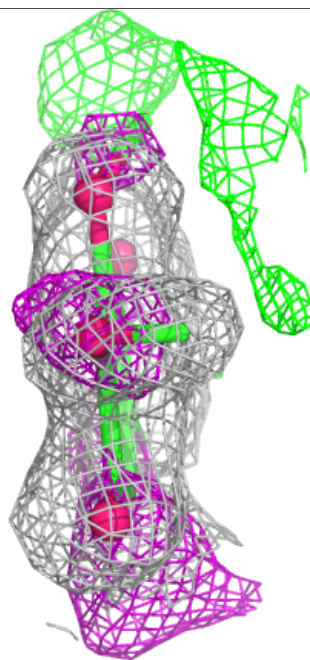
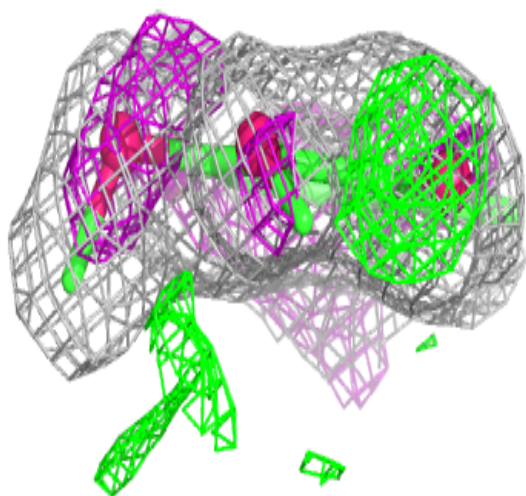
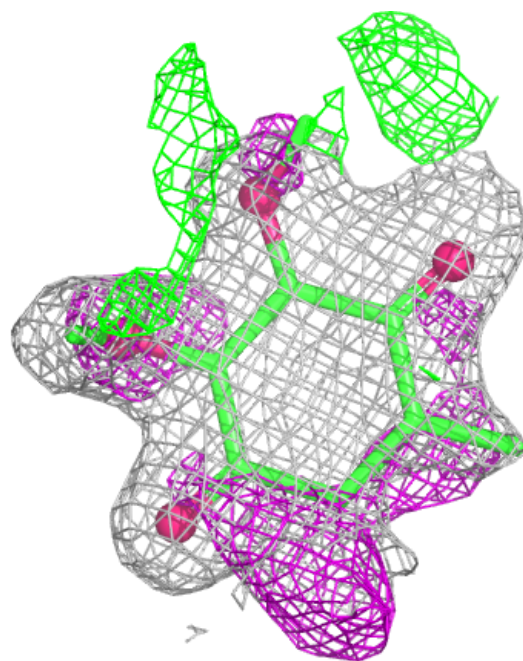
Electron density around UQ0 B 706:

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



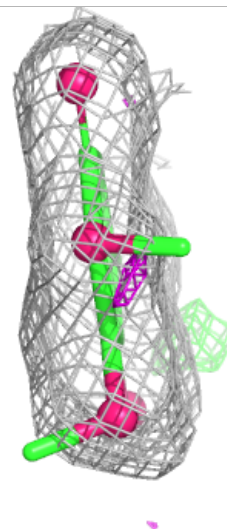
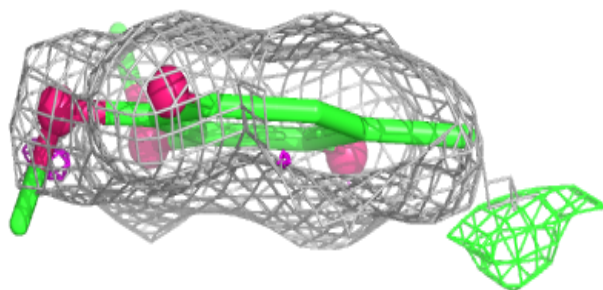
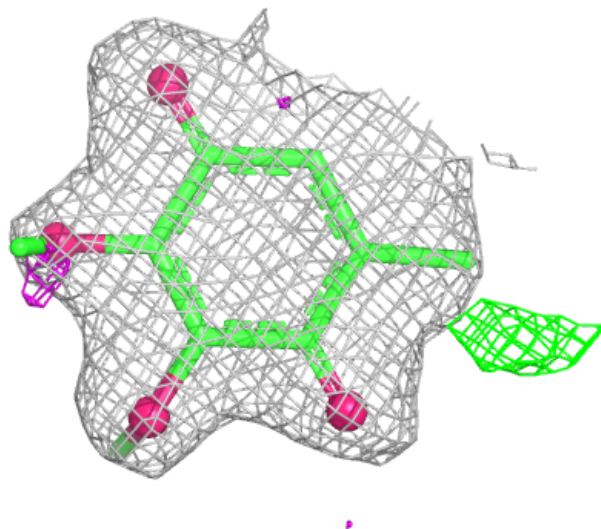
Electron density around UQ0 A 706:

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



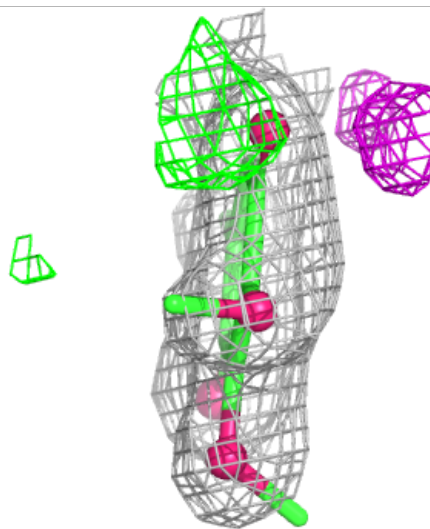
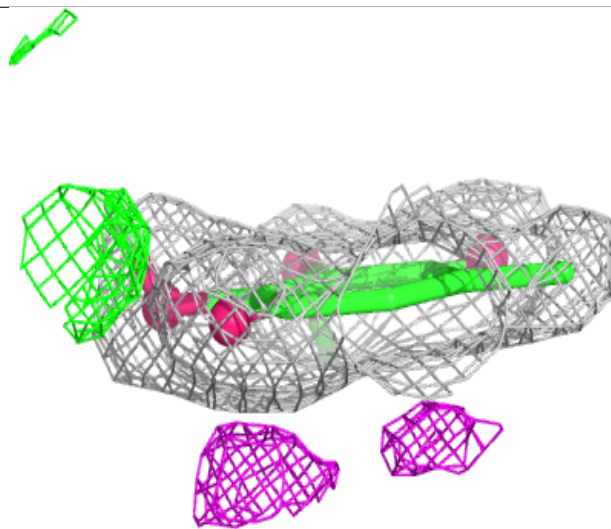
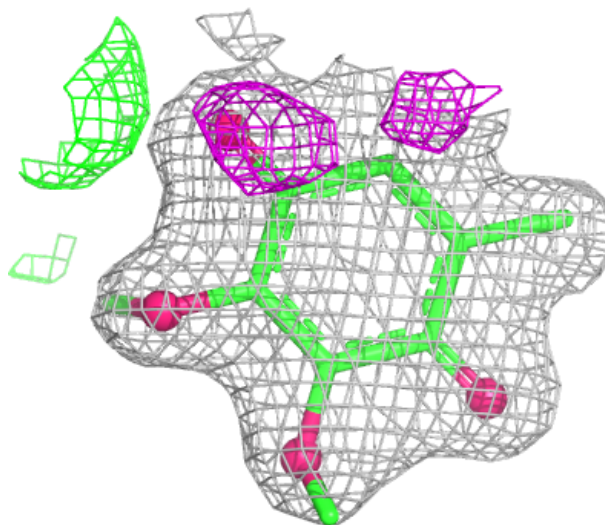
Electron density around UQ0 D 704:

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



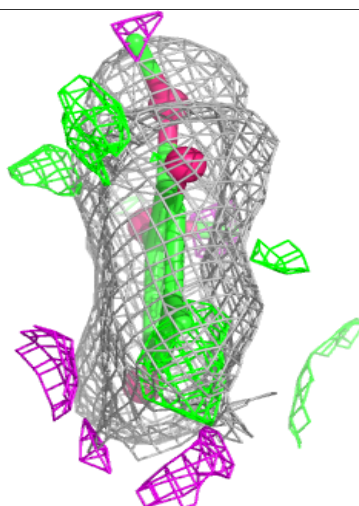
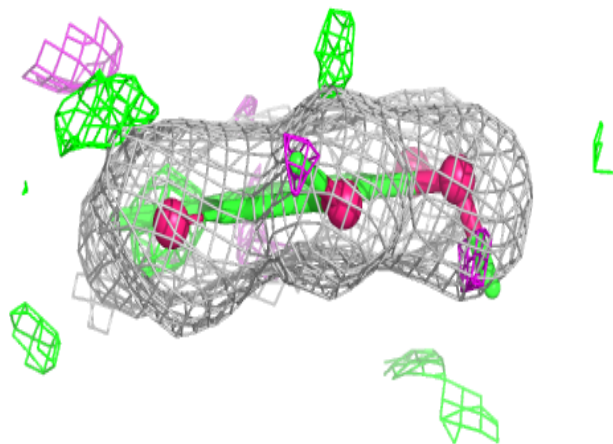
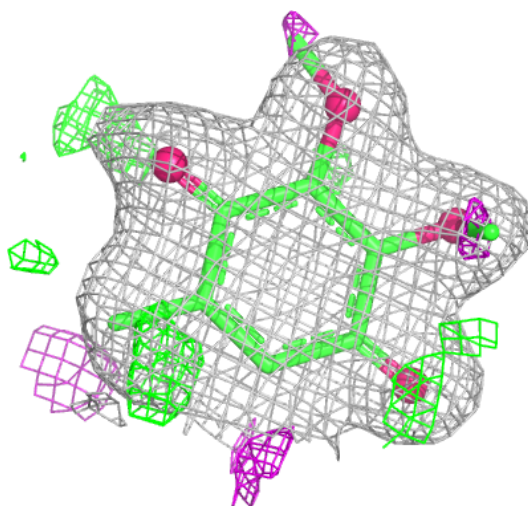
Electron density around UQ0 F 605:

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



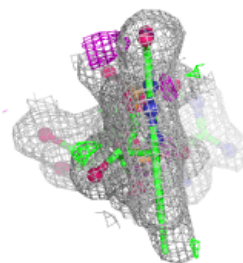
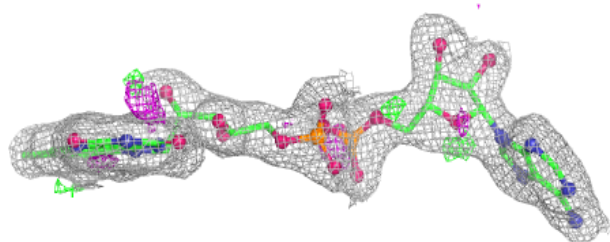
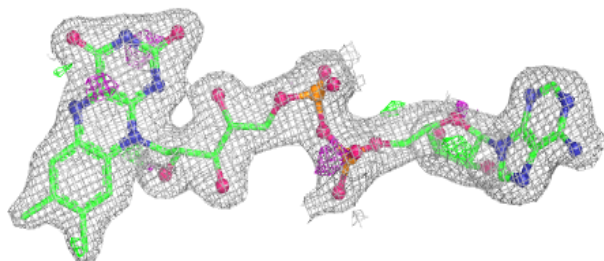
Electron density around UQ0 B 705:

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

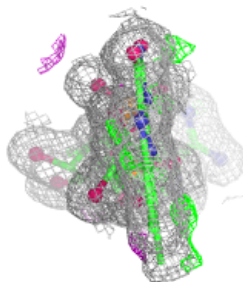
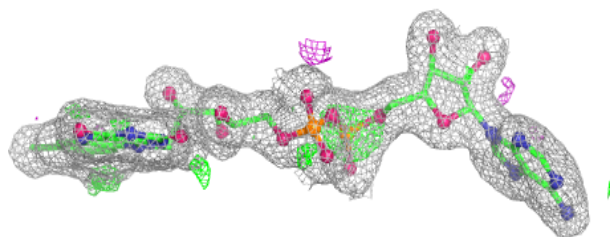
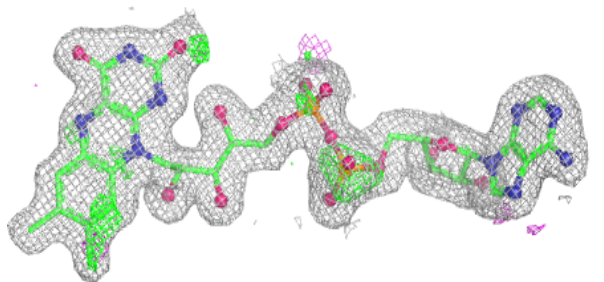


Electron density around FAD E 602:

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

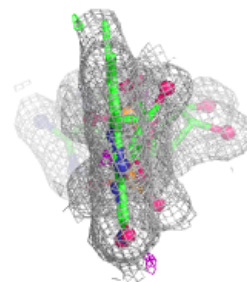
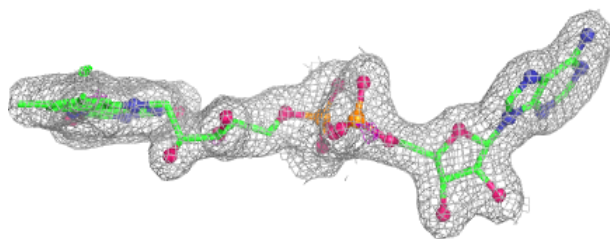
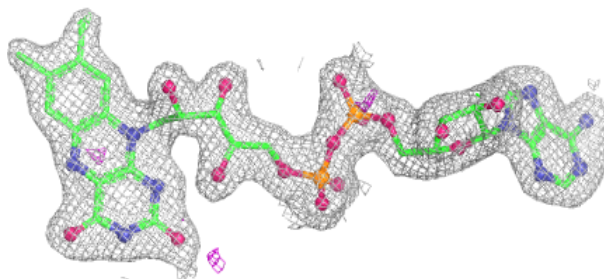
**Electron density around FAD B 701:**

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

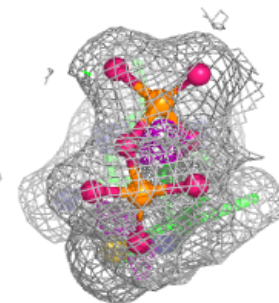
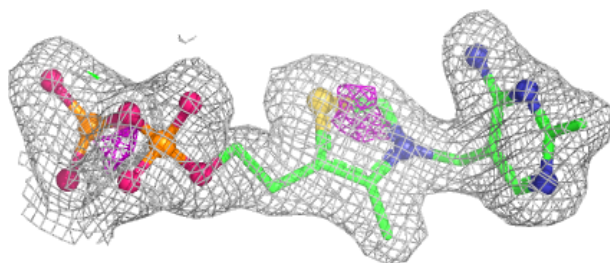
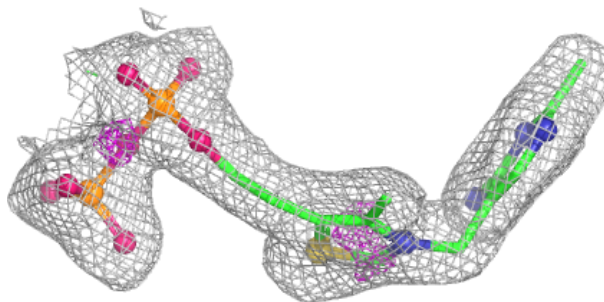


Electron density around FAD F 602:

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

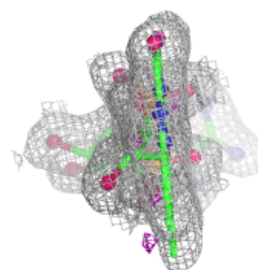
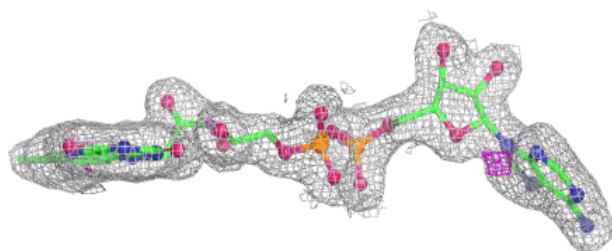
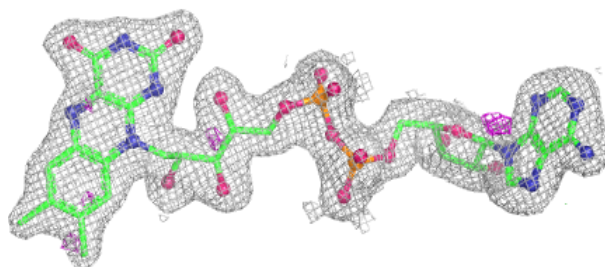
**Electron density around TPP F 603:**

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

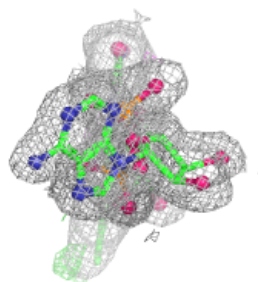
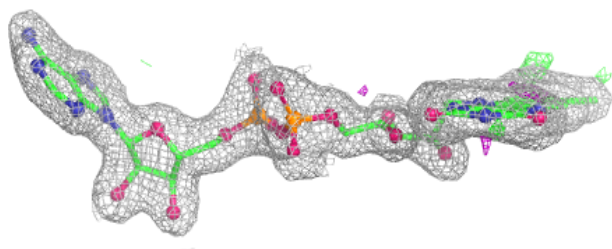
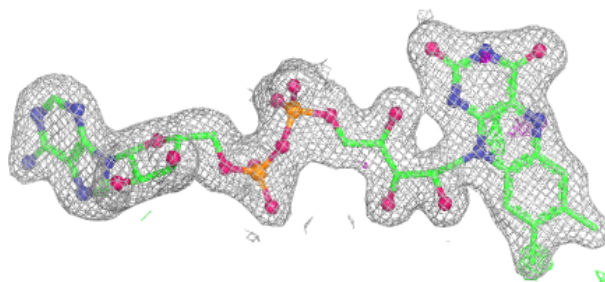


Electron density around FAD C 701:

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

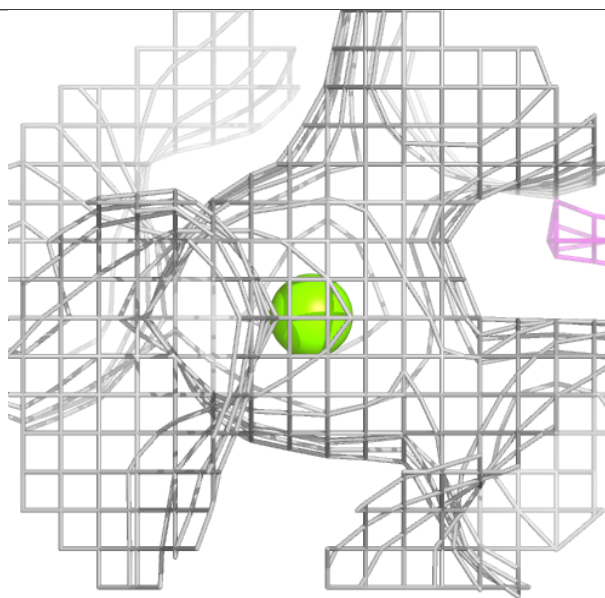
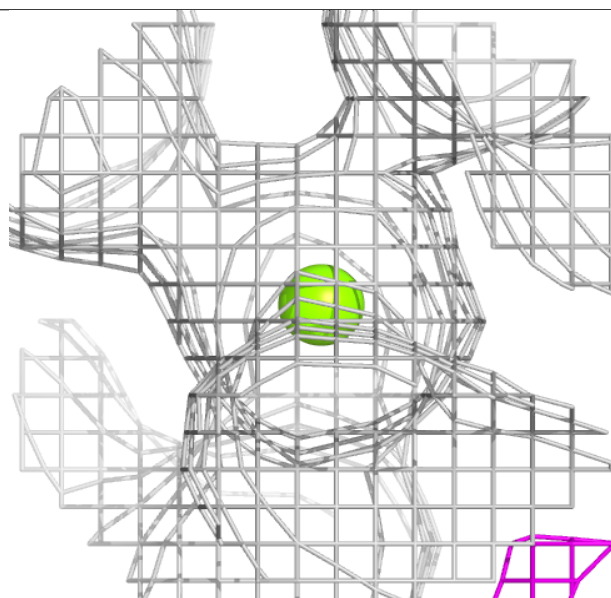
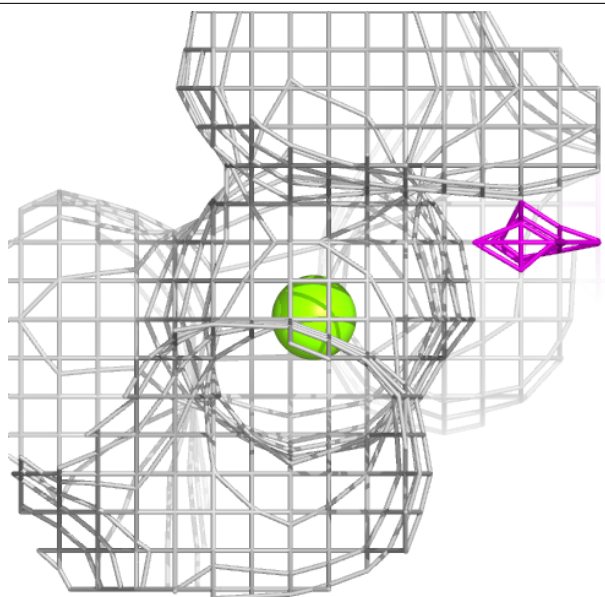
**Electron density around FAD D 701:**

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



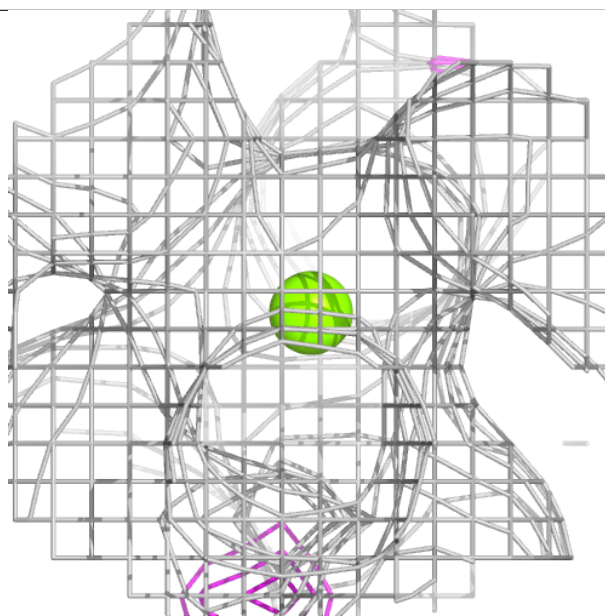
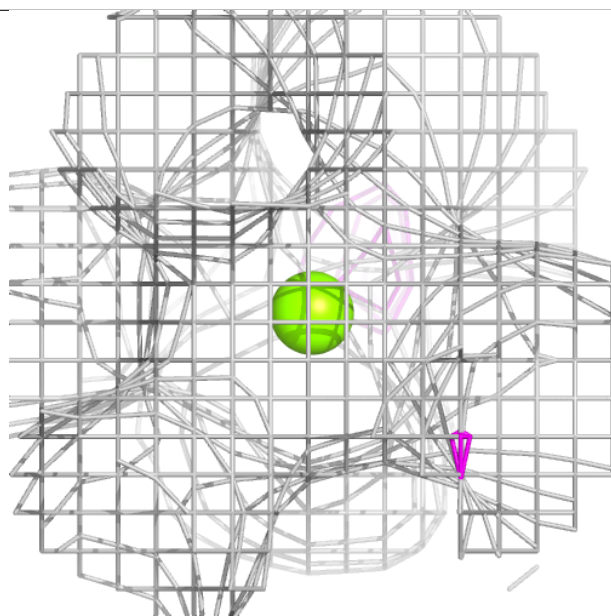
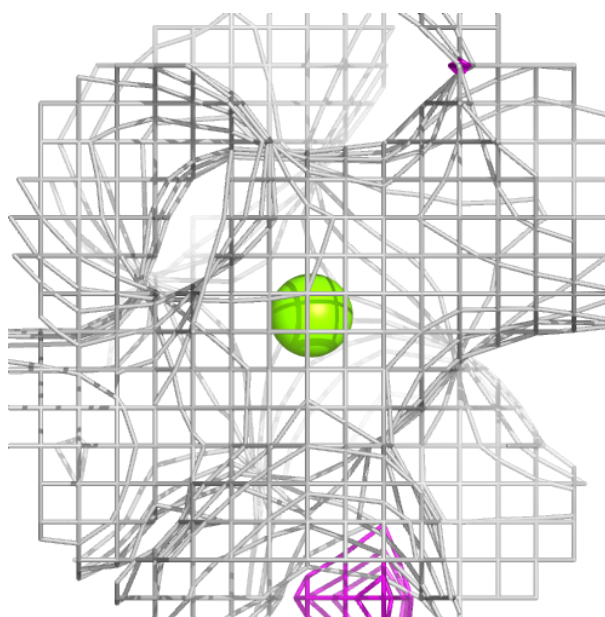
Electron density around MG D 705:

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



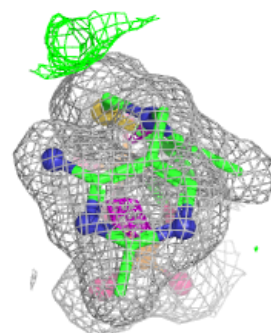
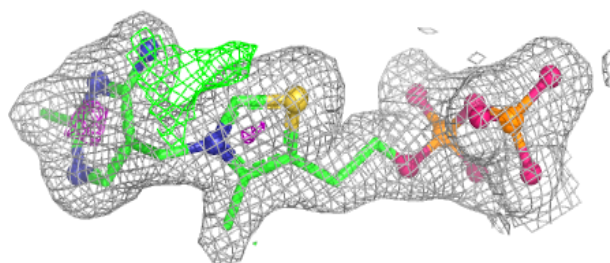
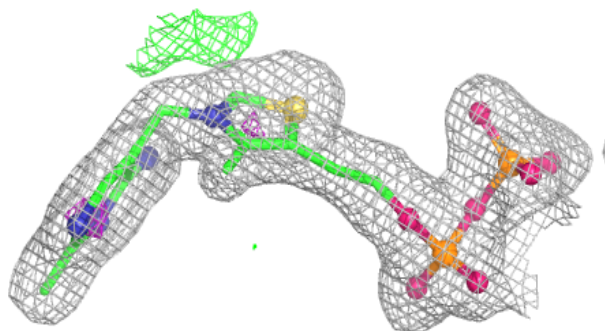
Electron density around MG F 604:

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

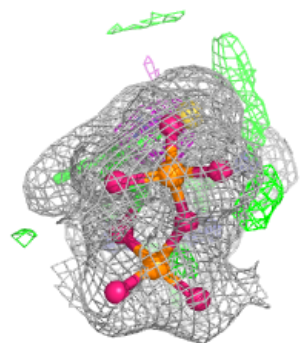
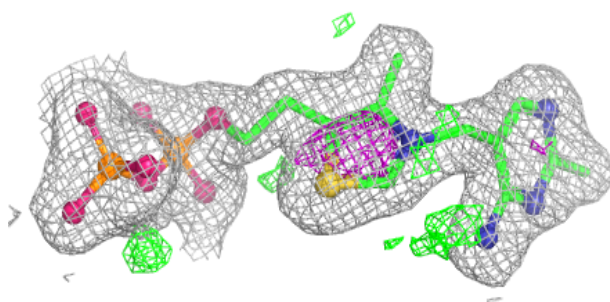
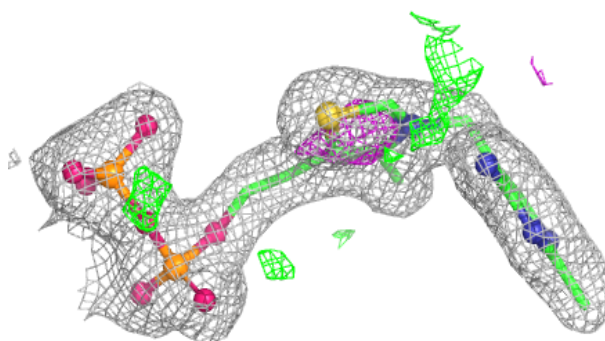


Electron density around TPP C 702:

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

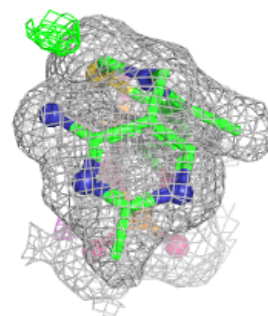
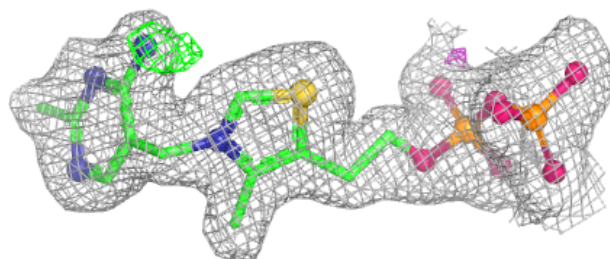
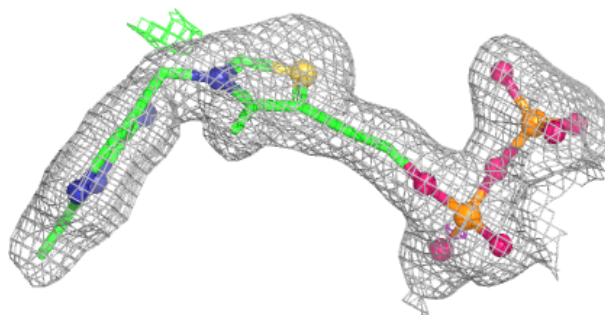
**Electron density around TPP D 702:**

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

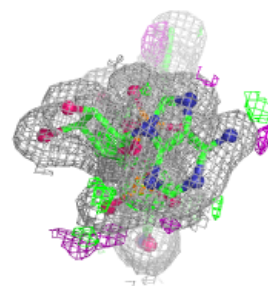
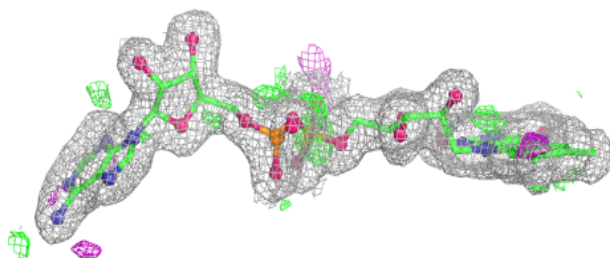
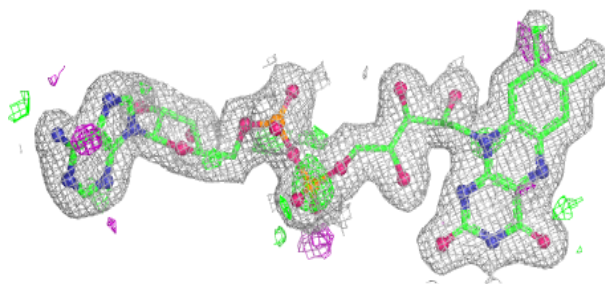


Electron density around TPP E 603:

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

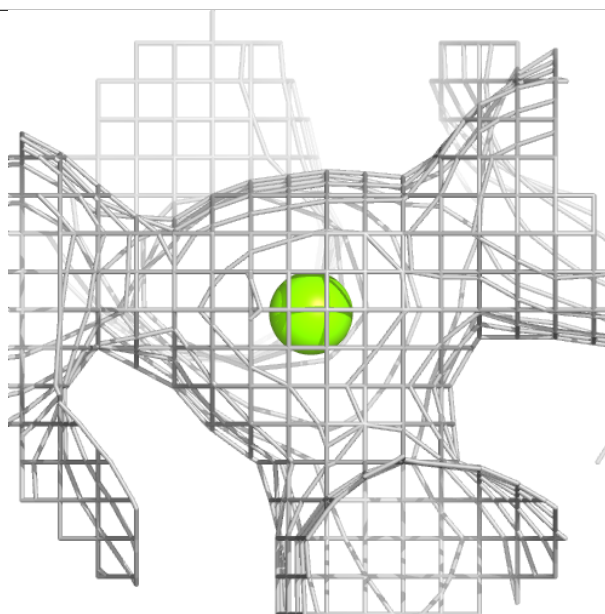
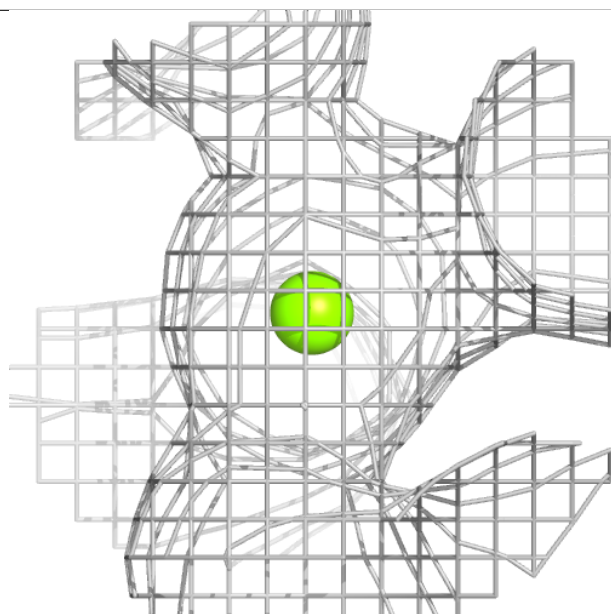
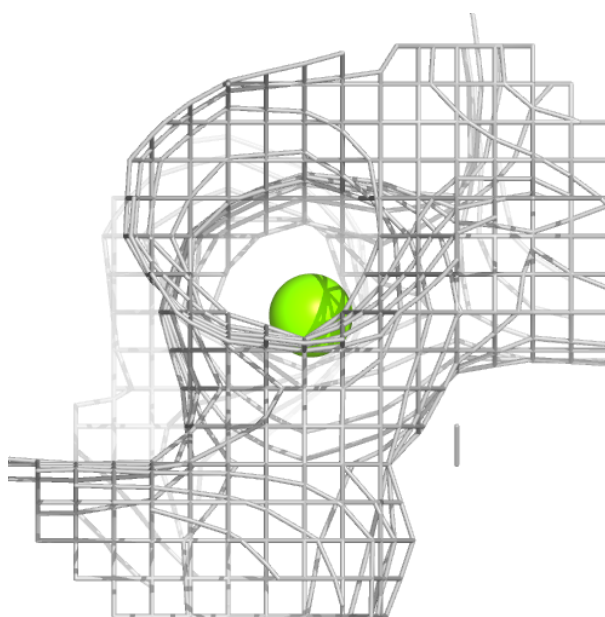
**Electron density around FAD A 701:**

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



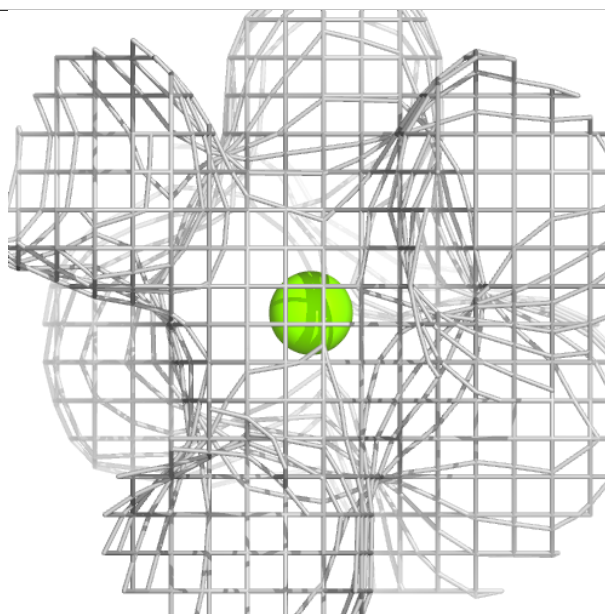
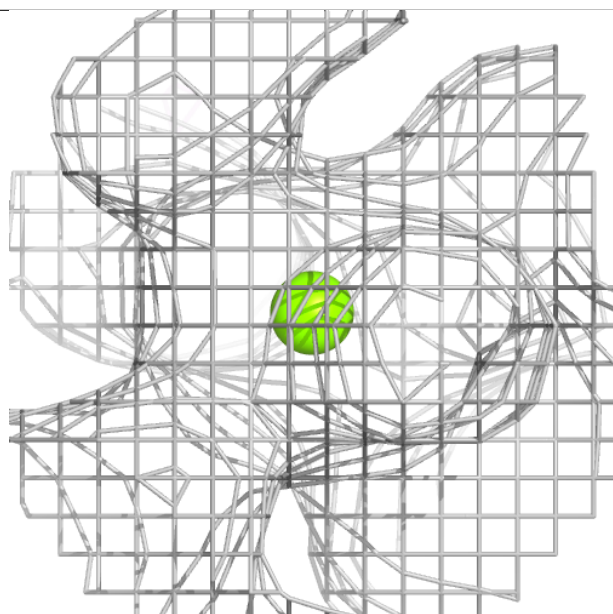
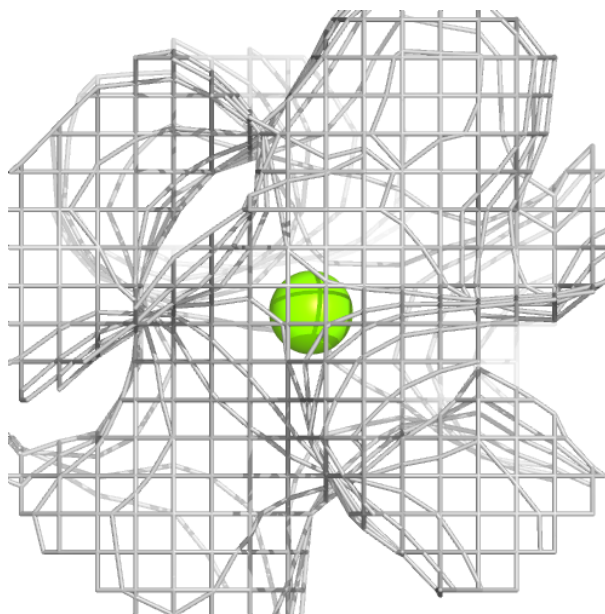
Electron density around MG C 705:

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



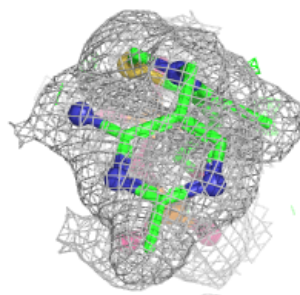
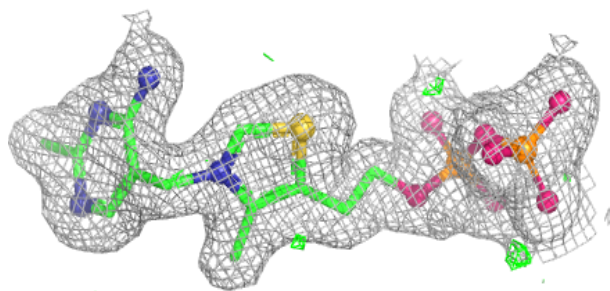
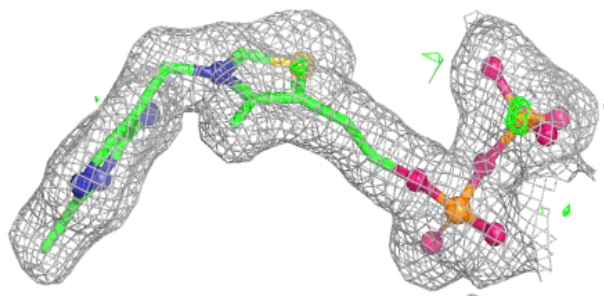
Electron density around MG D 703:

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



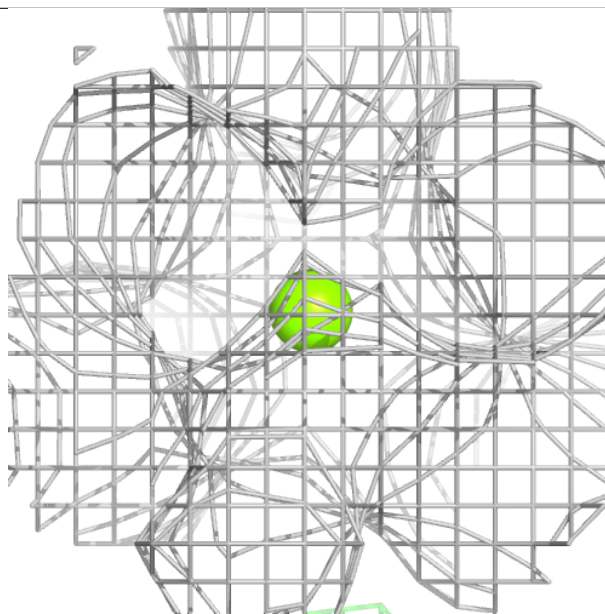
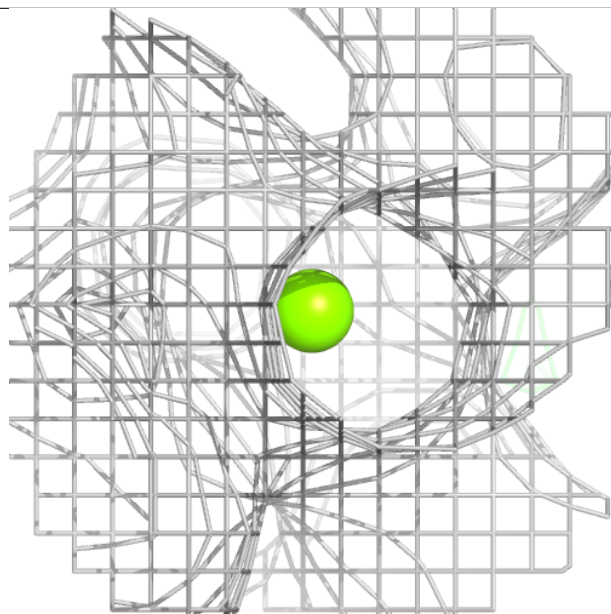
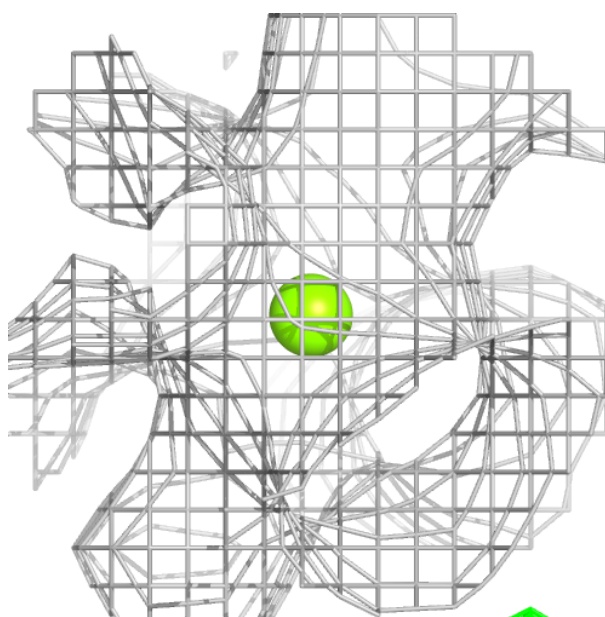
Electron density around TPP B 702:

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



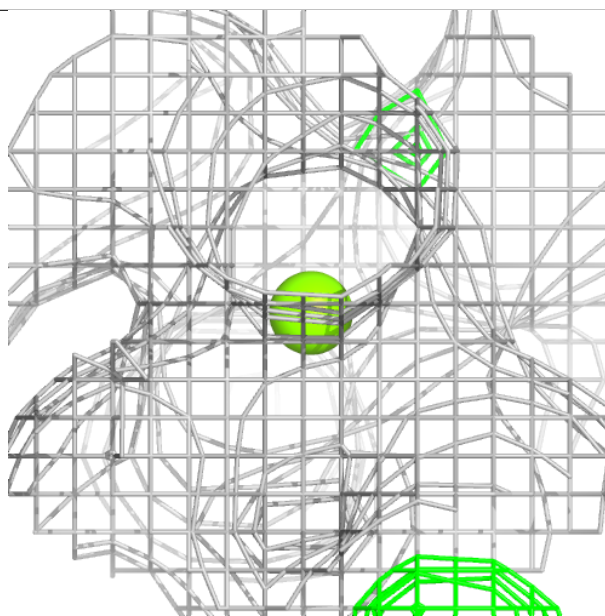
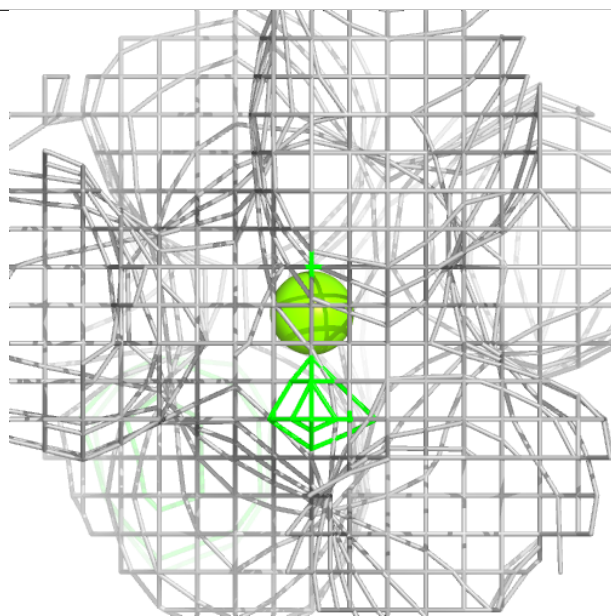
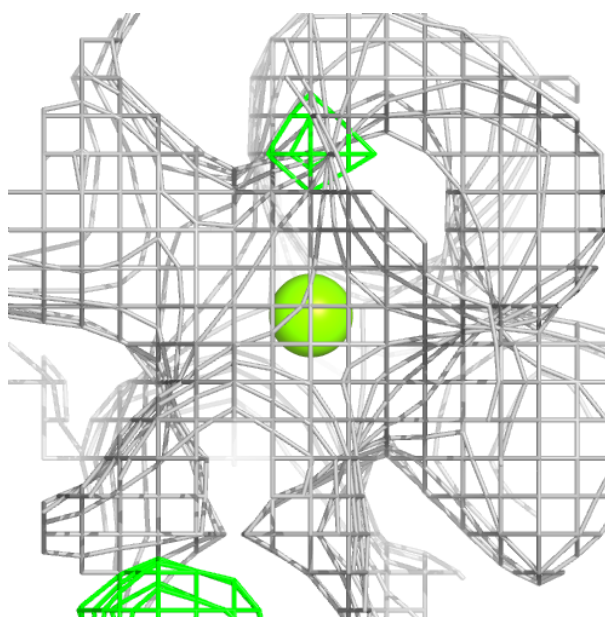
Electron density around MG E 604:

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



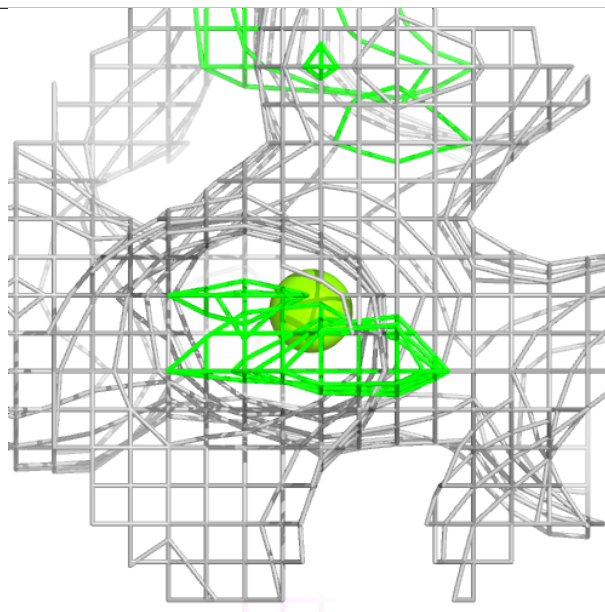
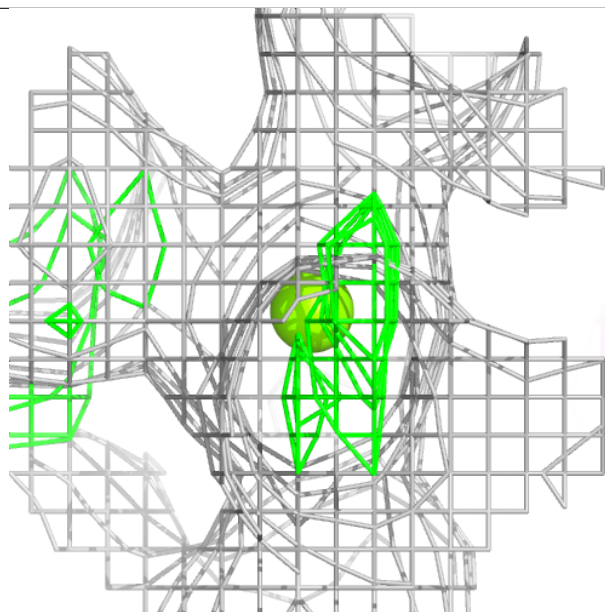
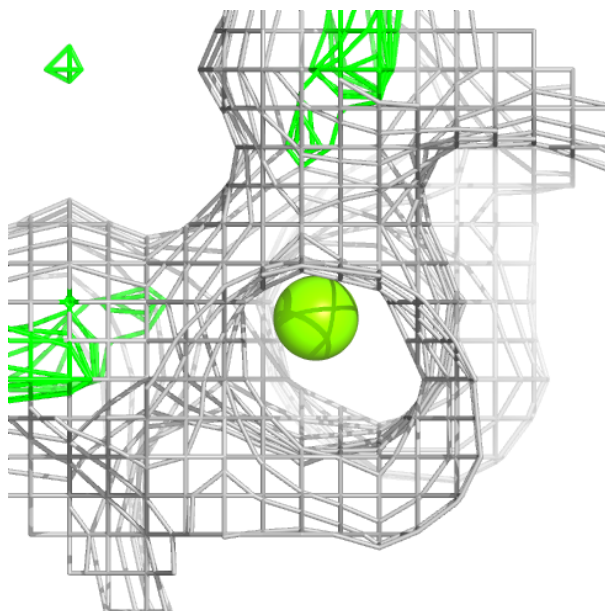
Electron density around MG A 703:

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



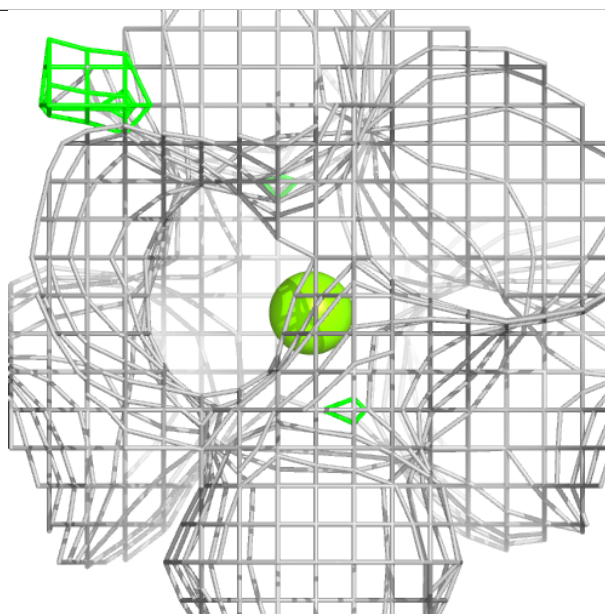
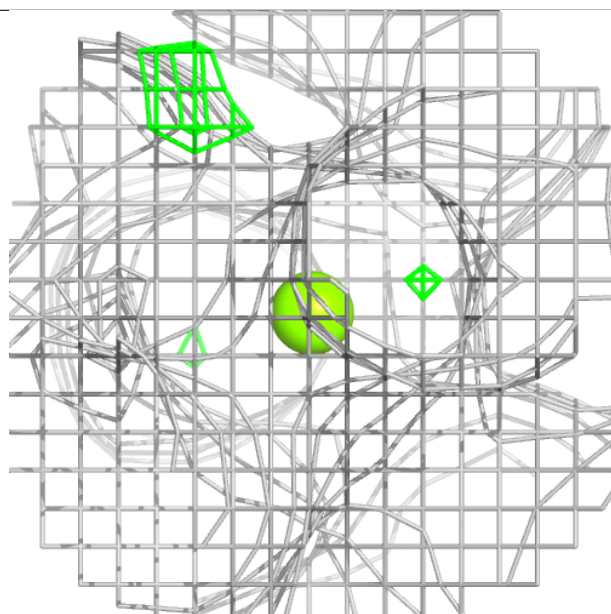
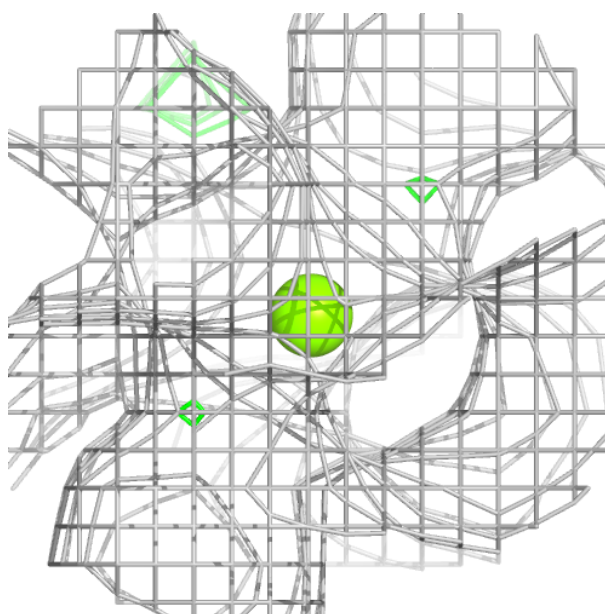
Electron density around MG A 704:

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



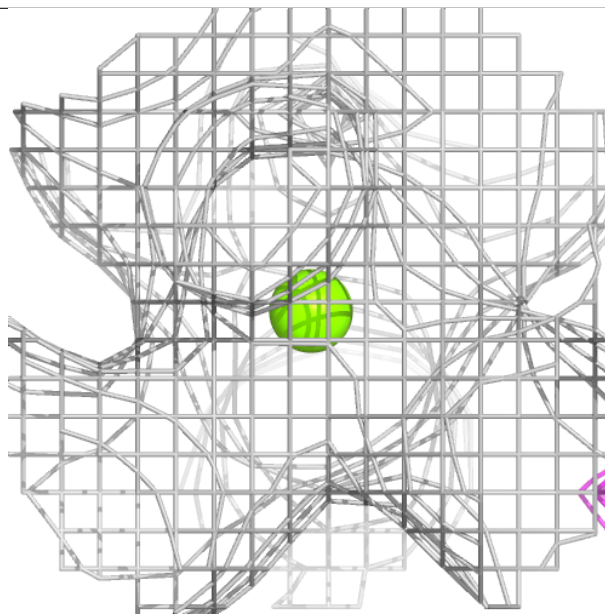
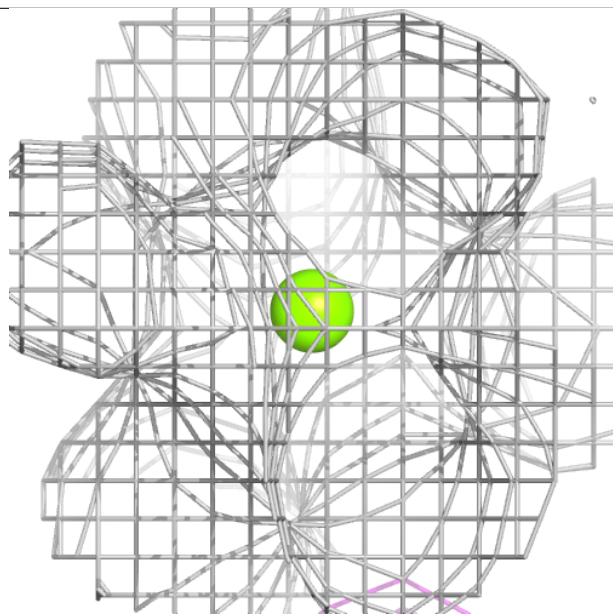
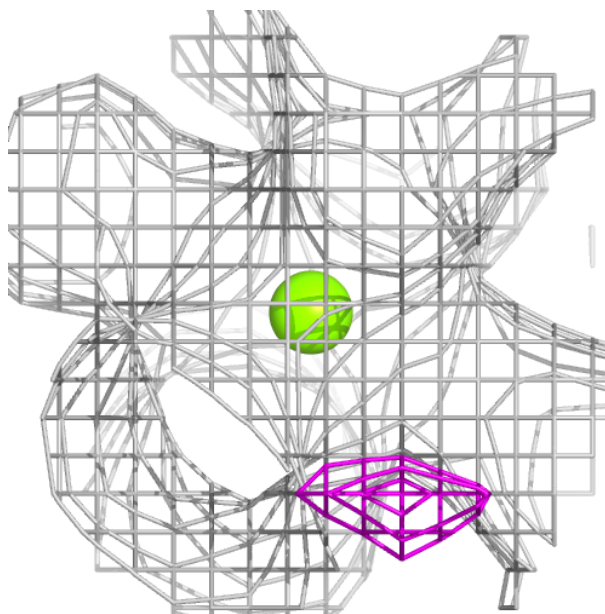
Electron density around MG B 703:

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



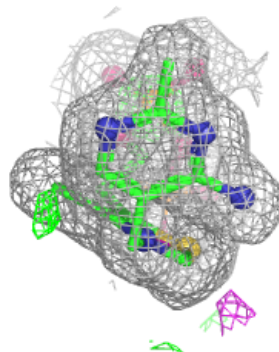
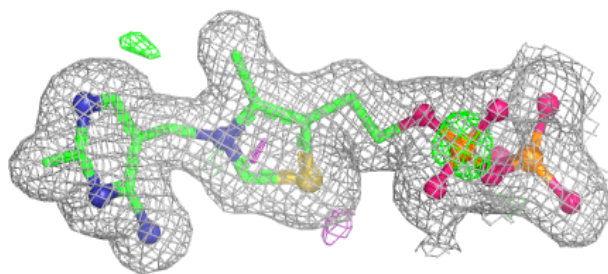
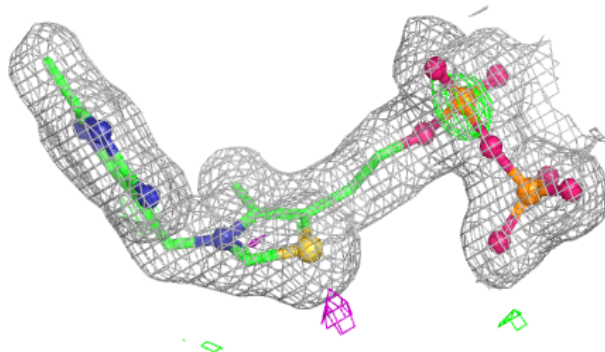
Electron density around MG C 703:

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



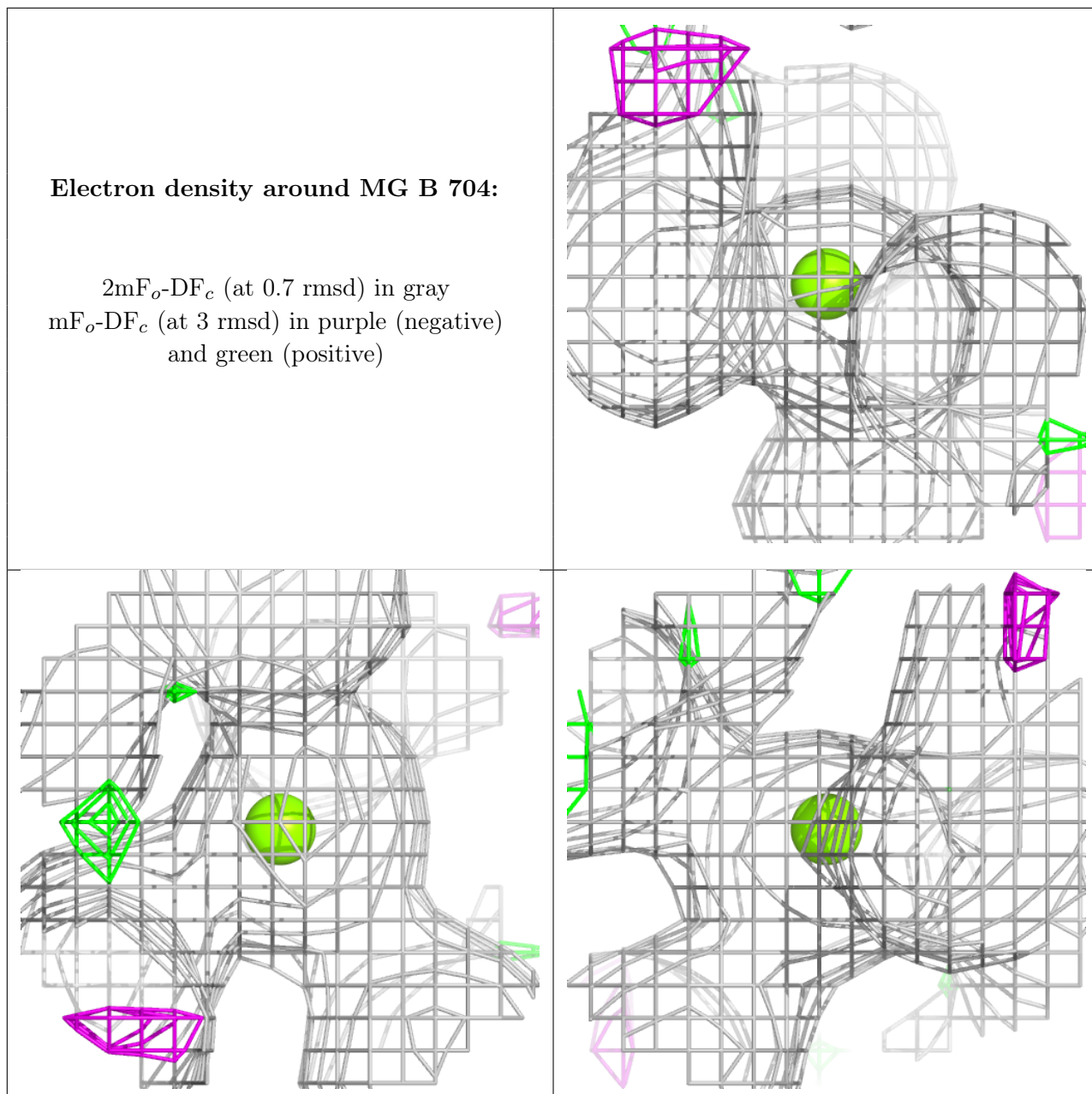
Electron density around TPP A 702:

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



Electron density around MG B 704:

$2mF_o-DF_c$ (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.