



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:28 AM UTC

PDB ID : 8I01 / pdb_00008i01
Title : Crystal structure of Escherichia coli glyoxylate carboligase
Authors : Kim, J.H.; Kim, J.S.
Deposited on : 2023-01-10
Resolution : 2.15 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

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

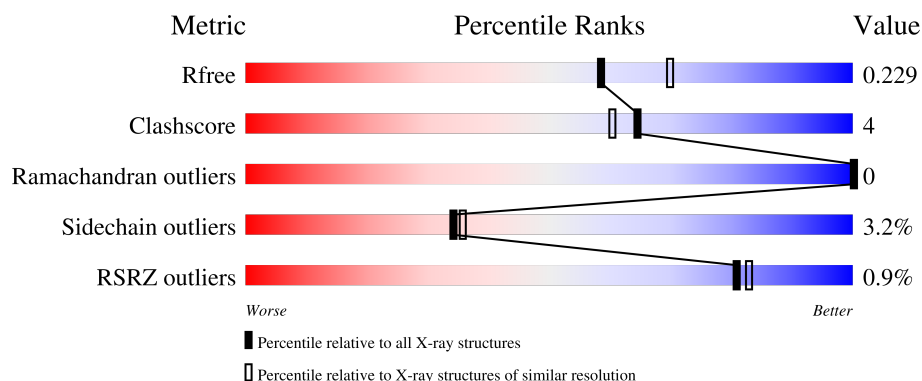
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	 91% 8%
1	B	594	 90% 9%
1	C	594	 90% 8%
1	D	594	 91% 8%
1	E	594	 87% 11%

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Mol	Chain	Length	Quality of chain
1	F	594	2% 91% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30468 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.

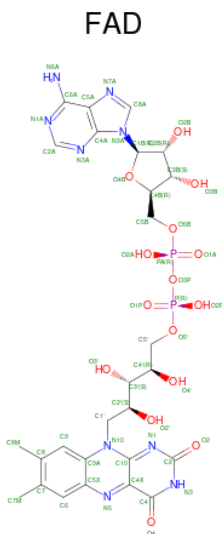
- Molecule 1 is a protein called Glyoxylate carboligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4542	2878	794	836	34			
1	B	594	Total	C	N	O	S	0	0	0
			4541	2878	793	836	34			
1	C	593	Total	C	N	O	S	0	0	0
			4538	2876	793	835	34			
1	D	594	Total	C	N	O	S	0	0	0
			4542	2878	794	836	34			
1	E	593	Total	C	N	O	S	0	0	0
			4538	2876	793	835	34			
1	F	594	Total	C	N	O	S	0	0	0
			4542	2878	794	836	34			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P0AEP7
A	488	LEU	MET	engineered mutation	UNP P0AEP7
B	0	GLY	-	expression tag	UNP P0AEP7
B	488	LEU	MET	engineered mutation	UNP P0AEP7
C	0	GLY	-	expression tag	UNP P0AEP7
C	488	LEU	MET	engineered mutation	UNP P0AEP7
D	0	GLY	-	expression tag	UNP P0AEP7
D	488	LEU	MET	engineered mutation	UNP P0AEP7
E	0	GLY	-	expression tag	UNP P0AEP7
E	488	LEU	MET	engineered mutation	UNP P0AEP7
F	0	GLY	-	expression tag	UNP P0AEP7
F	488	LEU	MET	engineered mutation	UNP P0AEP7

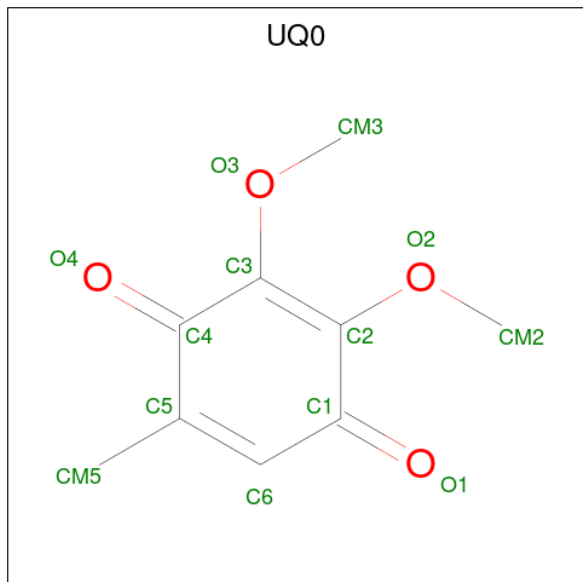
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $\text{C}_{12}\text{H}_{19}\text{N}_4\text{O}_7\text{P}_2\text{S}$) (labeled as "Ligand of Interest" by depositor).

- Molecule 5 is 2,3-DIMETHOXY-5-METHYL-1,4-BENZOQUINONE (CCD ID: UQ0) (formula: $C_9H_{10}O_4$) (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		
5	C	1	Total	C	O	0	0
			13	9	4		
5	C	1	Total	C	O	0	0
			13	9	4		
5	D	1	Total	C	O	0	0
			13	9	4		
5	D	1	Total	C	O	0	0
			13	9	4		
5	D	1	Total	C	O	0	0
			13	9	4		
5	E	1	Total	C	O	0	0
			13	9	4		
5	F	1	Total	C	O	0	0
			13	9	4		

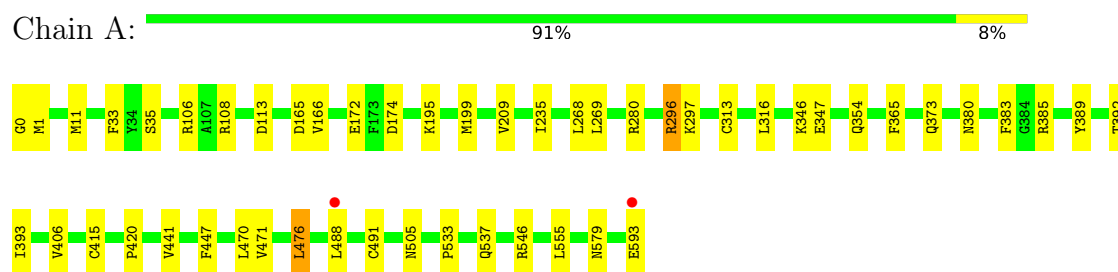
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	531	Total 531	O 531	0	0
6	B	486	Total 486	O 486	0	0
6	C	402	Total 402	O 402	0	0
6	D	400	Total 400	O 400	0	0
6	E	396	Total 396	O 396	0	0
6	F	370	Total 370	O 370	0	0

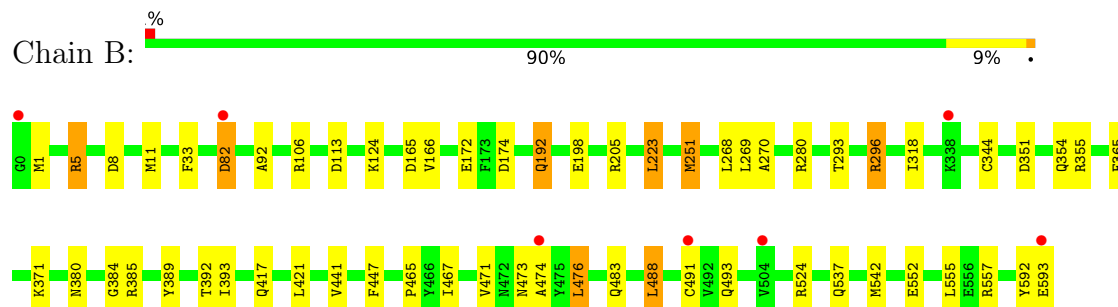
3 Residue-property plots [i](#)

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.

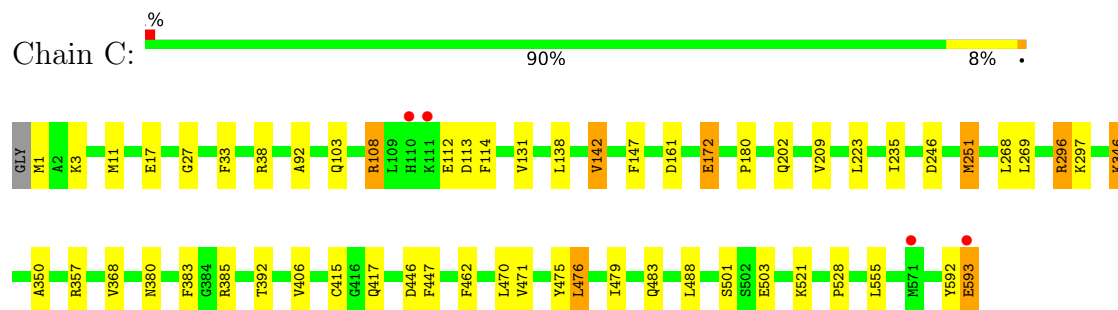
• Molecule 1: Glyoxylate carboligase



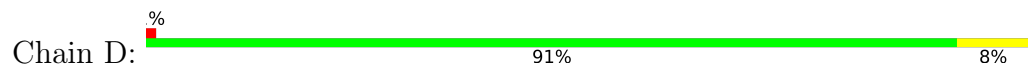
• Molecule 1: Glyoxylate carboligase

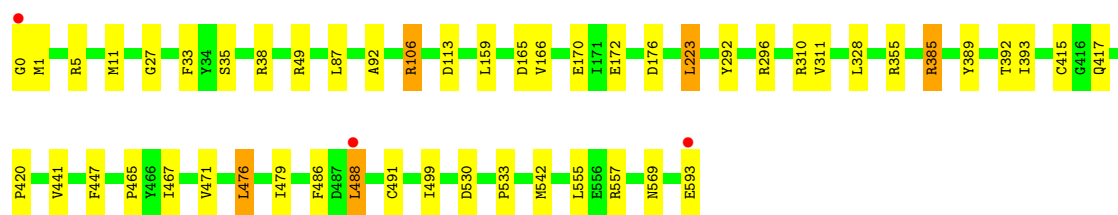


• Molecule 1: Glyoxylate carboligase

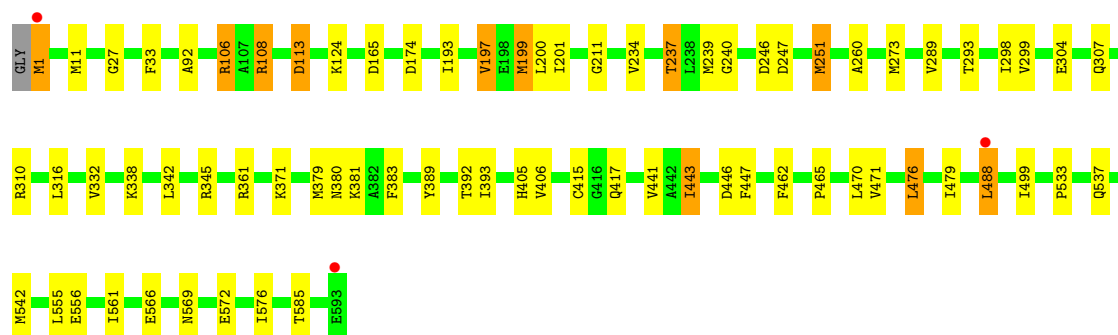
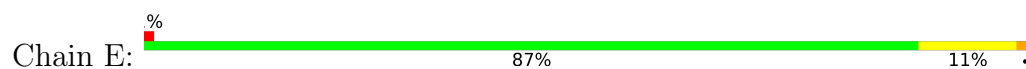


• Molecule 1: Glyoxylate carboligase

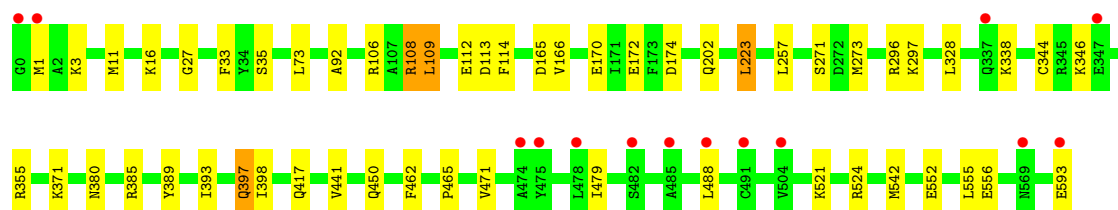




● Molecule 1: Glyoxylate carboligase



● 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	189.62Å 189.62Å 248.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.15 48.58 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.58-2.15) 99.7 (48.58-2.15)	Depositor EDS
R_{merge}	0.99	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.16Å)	Xtrriage
Refinement program	PHENIX v2.0	Depositor
R, R_{free}	0.191 , 0.231 0.191 , 0.229	Depositor DCC
R_{free} test set	9738 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.146	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	30468	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.55 % 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 5.9354e-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: TPP, MG, UQ0, FAD

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	0.40	0/4634	0.63	4/6290 (0.1%)
1	B	0.43	1/4633 (0.0%)	0.62	3/6289 (0.0%)
1	C	0.36	0/4630	0.56	2/6285 (0.0%)
1	D	0.35	0/4634	0.54	0/6290
1	E	0.36	0/4630	0.57	2/6285 (0.0%)
1	F	0.34	0/4634	0.53	2/6290 (0.0%)
All	All	0.38	1/27795 (0.0%)	0.58	13/37729 (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	1
1	B	0	2
1	C	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	ASP	CG-OD2	8.36	1.41	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	LEU	CA-CB-CG	8.75	146.93	116.30
1	B	280	ARG	CA-C-N	-8.52	109.40	123.37
1	B	280	ARG	C-N-CA	-8.52	109.40	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	CA-C-N	-8.15	110.00	123.37
1	A	280	ARG	C-N-CA	-8.15	110.00	123.37
1	E	462	PHE	CA-C-N	-5.72	114.43	123.12
1	E	462	PHE	C-N-CA	-5.72	114.43	123.12
1	A	280	ARG	N-CA-C	-5.68	101.51	109.69
1	B	280	ARG	N-CA-C	-5.40	101.23	109.65
1	C	462	PHE	CA-C-N	-5.35	114.86	122.41
1	C	462	PHE	C-N-CA	-5.35	114.86	122.41
1	F	462	PHE	CA-C-N	-5.34	114.86	122.77
1	F	462	PHE	C-N-CA	-5.34	114.86	122.77

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	592	TYR	Peptide
1	C	296	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	4542	0	4550	28	0
1	B	4541	0	4545	40	1
1	C	4538	0	4547	34	0
1	D	4542	0	4550	33	0
1	E	4538	0	4547	50	0
1	F	4542	0	4550	40	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	2	0
2	E	53	0	31	3	0
2	F	53	0	31	1	0
3	A	26	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	16	1	1
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	1	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
5	A	26	0	0	1	2
5	B	26	0	0	2	2
5	C	39	0	0	2	0
5	D	39	0	0	1	0
5	E	13	0	0	0	0
5	F	13	0	0	0	0
6	A	531	0	0	7	1
6	B	486	0	0	9	1
6	C	402	0	0	5	0
6	D	400	0	0	2	0
6	E	396	0	0	5	0
6	F	370	0	0	8	0
All	All	30468	0	27571	214	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (214) 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:D:292:TYR:O	1:D:296:ARG:NH1	2.03	0.91
1:B:384:GLY:HA2	1:B:593:GLU:HG2	1.59	0.85
1:E:361:ARG:HD3	1:E:572:GLU:OE2	1.77	0.85
1:F:393:ILE:HA	1:F:397:GLN:HG2	1.61	0.83
1:B:467:ILE:HG13	1:B:542:MET:HE1	1.62	0.82
1:E:237:THR:HG22	1:E:240:GLY:H	1.46	0.80
1:E:1:MET:N	6:E:802:HOH:O	2.14	0.79
1:D:557:ARG:NH2	6:D:801:HOH:O	2.16	0.78
1:D:385:ARG:H	1:D:593:GLU:HG3	1.51	0.74
1:A:385:ARG:H	1:A:593:GLU:HG3	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:PHE:O	6:A:801:HOH:O	2.07	0.72
1:A:106:ARG:HD2	1:A:166:VAL:HG23	1.70	0.72
1:B:380:ASN:O	6:B:801:HOH:O	2.07	0.72
1:D:35:SER:HA	1:F:488:LEU:HD21	1.71	0.71
1:F:106:ARG:HA	1:F:109:LEU:HD22	1.73	0.71
1:B:205:ARG:NH1	1:B:270:ALA:O	2.23	0.71
1:E:237:THR:HG21	2:E:701:FAD:O2P	1.90	0.71
1:C:17:GLU:HG2	1:C:147:PHE:CG	2.26	0.70
5:C:705:UQ0:O4	6:C:802:HOH:O	2.10	0.69
1:A:108:ARG:NH2	6:A:804:HOH:O	2.25	0.69
1:C:383:PHE:O	6:C:801:HOH:O	2.10	0.69
1:D:355:ARG:NH2	6:D:803:HOH:O	2.25	0.69
1:B:5:ARG:HD3	1:B:8:ASP:OD2	1.93	0.68
1:F:355:ARG:NH2	6:F:802:HOH:O	2.27	0.68
1:B:106:ARG:HD2	1:B:166:VAL:HG23	1.76	0.68
1:F:471:VAL:HB	1:F:555:LEU:HD11	1.76	0.66
1:E:200:LEU:HA	1:E:273:MET:HE1	1.78	0.66
1:A:380:ASN:O	6:A:801:HOH:O	2.13	0.65
1:C:17:GLU:HG2	1:C:147:PHE:CD2	2.32	0.64
1:B:192:GLN:HG2	1:B:318:ILE:HG12	1.79	0.64
1:E:383:PHE:O	6:E:801:HOH:O	2.14	0.64
1:B:524:ARG:HD3	1:B:552:GLU:OE1	1.97	0.64
1:A:579:ASN:ND2	6:A:808:HOH:O	2.30	0.63
1:F:106:ARG:HD3	1:F:165:ASP:OD2	1.99	0.63
1:B:557:ARG:NE	6:B:805:HOH:O	2.27	0.63
1:D:471:VAL:HB	1:D:555:LEU:HD11	1.81	0.63
1:C:38:ARG:HD3	1:E:488:LEU:HD22	1.82	0.62
1:A:313:CYS:SG	6:B:819:HOH:O	2.43	0.61
1:B:537:GLN:HG2	6:B:1247:HOH:O	2.01	0.61
1:C:380:ASN:O	6:C:801:HOH:O	2.16	0.60
1:E:108:ARG:NH1	1:E:113:ASP:OD1	2.32	0.60
1:D:467:ILE:HG13	1:D:542:MET:HE1	1.83	0.60
1:C:471:VAL:HB	1:C:555:LEU:HD11	1.84	0.59
1:B:106:ARG:HD3	1:B:165:ASP:OD2	2.03	0.59
1:F:344:CYS:SG	6:F:1115:HOH:O	2.57	0.59
1:A:195:LYS:HE3	1:A:199:MET:HE2	1.84	0.58
1:E:371:LYS:HE3	1:E:556:GLU:OE2	2.03	0.58
1:E:237:THR:HG22	1:E:240:GLY:N	2.16	0.58
1:E:572:GLU:HG2	1:E:576:ILE:HG22	1.84	0.58
1:E:11:MET:HE1	1:E:33:PHE:CZ	2.37	0.58
1:F:273:MET:HE3	1:F:297:LYS:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:HE3	1:C:172:GLU:OE2	2.04	0.57
1:A:11:MET:HE1	1:A:33:PHE:CZ	2.39	0.57
1:B:465:PRO:HB2	1:B:542:MET:HG3	1.86	0.57
1:F:393:ILE:CA	1:F:397:GLN:HG2	2.31	0.57
1:E:260:ALA:O	1:E:361:ARG:NH2	2.38	0.57
1:A:491:CYS:HA	5:A:706:UQ0:O1	2.05	0.57
1:A:385:ARG:HB2	1:A:593:GLU:HB2	1.85	0.57
1:F:106:ARG:HD2	1:F:166:VAL:HG23	1.86	0.56
1:E:379:MET:HE1	1:E:443:ILE:HG12	1.87	0.56
1:C:11:MET:HE1	1:C:33:PHE:CZ	2.41	0.55
1:B:11:MET:HE1	1:B:33:PHE:CZ	2.41	0.55
1:B:467:ILE:HG13	1:B:542:MET:CE	2.35	0.55
1:D:27:GLY:HA2	1:F:479:ILE:HD12	1.86	0.55
1:C:269:LEU:O	1:C:296:ARG:NH2	2.39	0.55
1:E:193:ILE:O	1:E:197:VAL:HG12	2.07	0.55
1:B:344:CYS:SG	6:B:1151:HOH:O	2.51	0.55
1:B:471:VAL:HB	1:B:555:LEU:HD11	1.88	0.55
1:E:197:VAL:HG11	1:E:332:VAL:HG11	1.88	0.55
1:D:479:ILE:HD12	1:F:27:GLY:HA2	1.89	0.54
1:A:1:MET:HG2	1:A:174:ASP:HB2	1.87	0.54
1:D:499:ILE:HD12	1:F:521:LYS:HE2	1.89	0.54
1:C:483:GLN:HB3	1:C:488:LEU:HD12	1.90	0.53
1:E:471:VAL:HB	1:E:555:LEU:HD11	1.90	0.53
1:E:246:ASP:HA	1:E:251:MET:HG2	1.88	0.53
1:A:471:VAL:HB	1:A:555:LEU:HD11	1.91	0.53
1:B:92:ALA:HB1	1:B:417:GLN:HG2	1.91	0.52
1:E:381:LYS:NZ	6:E:804:HOH:O	2.42	0.52
1:E:392:THR:HG23	1:E:415:CYS:SG	2.49	0.52
1:D:488:LEU:HD21	1:F:35:SER:HB2	1.91	0.52
1:A:0:GLY:N	6:A:813:HOH:O	2.43	0.52
1:C:392:THR:HG23	1:C:415:CYS:SG	2.50	0.52
1:D:106:ARG:HD3	1:D:165:ASP:OD2	2.09	0.52
1:B:1:MET:HE3	1:B:174:ASP:HB2	1.91	0.51
1:F:92:ALA:HB1	1:F:417:GLN:HG2	1.92	0.51
1:B:251:MET:HE3	1:B:251:MET:C	2.35	0.51
1:D:467:ILE:CG1	1:D:542:MET:HE1	2.40	0.51
5:C:705:UQ0:O1	6:C:803:HOH:O	2.19	0.51
1:A:447:PHE:CG	1:A:476:LEU:HD22	2.46	0.51
1:B:355:ARG:NH2	6:B:803:HOH:O	2.21	0.51
1:C:592:TYR:O	1:C:593:GLU:HB2	2.09	0.50
1:F:465:PRO:HB2	1:F:542:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:PHE:CG	1:B:476:LEU:HD22	2.47	0.50
1:E:237:THR:HG23	1:E:239:MET:H	1.76	0.50
1:D:92:ALA:HB1	1:D:417:GLN:HG2	1.93	0.50
1:F:380:ASN:O	6:F:801:HOH:O	2.19	0.50
1:A:346:LYS:NZ	6:A:815:HOH:O	2.43	0.50
1:B:223:LEU:O	1:B:223:LEU:HG	2.05	0.49
1:E:447:PHE:CG	1:E:476:LEU:HD22	2.48	0.49
1:E:200:LEU:HD12	1:E:273:MET:HE1	1.94	0.49
1:B:251:MET:HE3	1:B:251:MET:O	2.12	0.49
1:B:474:ALA:O	1:B:557:ARG:NH1	2.45	0.49
1:F:524:ARG:HD3	1:F:552:GLU:OE1	2.13	0.49
1:B:198:GLU:OE1	6:B:802:HOH:O	2.20	0.48
1:F:11:MET:HE1	1:F:33:PHE:CZ	2.48	0.48
1:E:533:PRO:O	1:E:537:GLN:HG3	2.13	0.48
1:B:493:GLN:OE1	1:B:557:ARG:NH2	2.47	0.48
1:C:108:ARG:NH2	6:C:812:HOH:O	2.45	0.48
1:E:1:MET:HB3	1:E:174:ASP:HA	1.94	0.48
1:F:16:LYS:NZ	6:F:815:HOH:O	2.47	0.48
1:A:389:TYR:HA	1:A:441:VAL:O	2.15	0.47
1:E:389:TYR:HA	1:E:441:VAL:O	2.15	0.47
1:A:269:LEU:O	1:A:296:ARG:NH2	2.48	0.47
1:B:493:GLN:H	5:B:706:UQ0:CM2	2.27	0.47
1:E:237:THR:CG2	1:E:239:MET:H	2.28	0.47
1:B:385:ARG:HB3	1:B:593:GLU:HB2	1.96	0.47
1:C:17:GLU:OE2	1:C:180:PRO:HB3	2.14	0.47
1:F:593:GLU:HG3	6:F:1063:HOH:O	2.14	0.47
1:A:533:PRO:O	1:A:537:GLN:HG3	2.15	0.46
1:D:87:LEU:HD11	1:D:159:LEU:HD12	1.95	0.46
1:D:447:PHE:CG	1:D:476:LEU:HD22	2.50	0.46
1:D:11:MET:HE1	1:D:33:PHE:CZ	2.49	0.46
1:E:566:GLU:HB2	1:E:569:ASN:HB2	1.98	0.46
1:B:92:ALA:HB1	1:B:417:GLN:CG	2.46	0.46
1:D:92:ALA:HB1	1:D:417:GLN:CG	2.46	0.46
1:E:106:ARG:HD2	1:E:165:ASP:OD2	2.16	0.46
1:E:197:VAL:HG11	1:E:332:VAL:CG1	2.44	0.46
1:B:491:CYS:HA	5:B:706:UQ0:O1	2.16	0.46
1:B:421:LEU:HD11	3:B:702:TPP:C4	2.46	0.46
1:D:465:PRO:HB2	1:D:542:MET:HG3	1.97	0.46
1:D:486:PHE:O	1:D:488:LEU:HD23	2.16	0.46
1:C:488:LEU:HD12	1:C:488:LEU:C	2.41	0.46
1:E:380:ASN:HD21	1:E:405:HIS:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:ASP:OD1	1:E:446:ASP:N	2.49	0.45
1:F:385:ARG:HB2	1:F:593:GLU:HB3	1.99	0.45
1:D:491:CYS:HA	5:D:707:UQO:O2	2.17	0.45
1:E:380:ASN:ND2	6:E:813:HOH:O	2.47	0.45
1:C:27:GLY:HA2	1:E:479:ILE:HD12	1.98	0.45
1:C:103:GLN:HB2	1:C:161:ASP:OD1	2.16	0.45
1:A:546:ARG:HD3	6:A:1134:HOH:O	2.17	0.45
1:C:92:ALA:HB1	1:C:417:GLN:CG	2.47	0.45
1:D:38:ARG:HD3	1:F:488:LEU:HD23	1.99	0.45
1:D:392:THR:HG23	1:D:415:CYS:SG	2.57	0.45
1:B:251:MET:HE2	6:B:863:HOH:O	2.17	0.45
1:F:1:MET:H	1:F:174:ASP:HB2	1.82	0.45
1:F:11:MET:HE1	1:F:33:PHE:CE1	2.52	0.45
1:B:542:MET:HB2	1:B:542:MET:HE3	1.32	0.44
1:C:138:LEU:O	1:C:142:VAL:HG13	2.17	0.44
1:C:112:GLU:HG3	1:E:310:ARG:CZ	2.47	0.44
1:D:38:ARG:HD3	1:F:488:LEU:CD2	2.47	0.44
1:E:237:THR:HG21	2:E:701:FAD:P	2.58	0.44
1:D:0:GLY:N	1:D:176:ASP:OD2	2.47	0.44
1:E:197:VAL:O	1:E:201:ILE:HG23	2.18	0.44
1:B:269:LEU:O	1:B:296:ARG:NH2	2.51	0.44
1:C:521:LYS:HE2	1:E:499:ILE:HD12	2.00	0.44
1:D:223:LEU:O	1:D:223:LEU:HG	2.11	0.44
1:B:473:ASN:O	1:B:557:ARG:HD2	2.18	0.43
1:C:357:ARG:O	1:C:357:ARG:NH1	2.46	0.43
1:B:483:GLN:HB3	1:B:488:LEU:CD1	2.48	0.43
1:C:479:ILE:HD12	1:E:27:GLY:HA2	2.01	0.43
1:F:371:LYS:HD3	1:F:556:GLU:OE2	2.17	0.43
1:C:114:PHE:HE1	2:E:701:FAD:HM83	1.84	0.43
1:E:465:PRO:HB2	1:E:542:MET:CG	2.48	0.43
1:B:524:ARG:NH2	6:B:810:HOH:O	2.39	0.43
1:A:392:THR:HG23	1:A:415:CYS:SG	2.59	0.43
1:C:368:VAL:HG22	1:C:528:PRO:HD3	2.01	0.43
1:F:346:LYS:HG2	6:F:1115:HOH:O	2.19	0.43
1:E:447:PHE:CD2	1:E:476:LEU:HD22	2.54	0.43
1:F:108:ARG:NH1	1:F:108:ARG:HB3	2.34	0.43
1:F:524:ARG:NH2	6:F:821:HOH:O	2.51	0.43
1:C:346:LYS:HE3	1:C:350:ALA:HB2	2.01	0.42
1:D:106:ARG:HD2	1:D:166:VAL:HG23	2.00	0.42
1:C:346:LYS:HA	1:C:346:LYS:HD2	1.63	0.42
1:F:389:TYR:HA	1:F:441:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:THR:HG22	1:D:393:ILE:HG22	2.02	0.42
2:D:701:FAD:HM83	1:F:114:PHE:HE1	1.82	0.42
1:A:392:THR:HG22	1:A:393:ILE:HG22	2.02	0.42
1:E:304:GLU:HG2	1:E:307:GLN:HG2	2.00	0.42
1:A:415:CYS:SG	1:A:420:PRO:HD2	2.59	0.42
1:F:108:ARG:NH2	6:F:823:HOH:O	2.52	0.42
1:C:246:ASP:HA	1:C:251:MET:HG2	2.01	0.42
1:E:199:MET:HE3	1:E:199:MET:HB2	1.84	0.42
1:E:293:THR:HG22	1:E:298:ILE:HD11	2.02	0.42
1:E:345:ARG:HD3	6:E:851:HOH:O	2.18	0.42
1:F:397:GLN:HG3	1:F:398:ILE:N	2.35	0.42
1:A:199:MET:HE1	1:A:316:LEU:HD22	2.02	0.42
1:B:392:THR:HG22	1:B:393:ILE:HG22	2.02	0.42
1:C:112:GLU:HG3	1:E:310:ARG:NH2	2.35	0.42
1:A:365:PHE:HE2	1:A:373:GLN:HG3	1.86	0.41
1:D:389:TYR:HA	1:D:441:VAL:O	2.21	0.41
1:C:447:PHE:CG	1:C:476:LEU:HD22	2.55	0.41
1:A:385:ARG:H	1:A:593:GLU:CG	2.30	0.41
1:E:92:ALA:HB1	1:E:417:GLN:HG2	2.02	0.41
1:C:479:ILE:O	1:C:483:GLN:HG3	2.20	0.41
1:F:106:ARG:HD2	1:F:166:VAL:CG2	2.49	0.41
1:E:338:LYS:HB3	1:E:338:LYS:HE2	1.93	0.41
1:F:92:ALA:HB1	1:F:417:GLN:CG	2.51	0.41
1:A:209:VAL:HA	1:A:235:ILE:O	2.19	0.41
1:D:310:ARG:CZ	1:F:112:GLU:HG3	2.50	0.41
1:B:365:PHE:CD1	1:B:371:LYS:HD2	2.56	0.41
2:D:701:FAD:H9	2:D:701:FAD:H1'1	1.90	0.41
1:E:211:GLY:HA2	1:E:237:THR:HB	2.03	0.41
1:E:392:THR:HG22	1:E:393:ILE:HG22	2.02	0.41
1:C:209:VAL:HA	1:C:235:ILE:O	2.20	0.41
1:D:49:ARG:HD3	1:F:450:GLN:OE1	2.21	0.41
1:F:271:SER:OG	1:F:296:ARG:HD3	2.20	0.41
1:B:389:TYR:HA	1:B:441:VAL:O	2.21	0.40
1:F:223:LEU:O	1:F:223:LEU:HG	2.17	0.40
1:A:106:ARG:HD3	1:A:165:ASP:OD2	2.21	0.40
1:C:92:ALA:HB1	1:C:417:GLN:HG2	2.02	0.40
1:C:446:ASP:HA	1:C:470:LEU:HD11	2.03	0.40
1:D:392:THR:HG21	1:D:420:PRO:O	2.21	0.40
2:F:701:FAD:H9	2:F:701:FAD:H1'1	1.89	0.40
1:D:530:ASP:C	1:D:533:PRO:HD2	2.47	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:OD2	3:B:702:TPP:CM2[8_554]	1.43	0.77
5:A:705:UQ0:CM2	5:B:705:UQ0:CM3[3_555]	1.49	0.71
5:A:706:UQ0:O1	6:A:820:HOH:O[8_554]	2.11	0.09
5:B:706:UQ0:O1	6:B:886:HOH:O[8_554]	2.12	0.08

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%)	583 (98%)	9 (2%)	0	100	100
1	B	592/594 (100%)	581 (98%)	11 (2%)	0	100	100
1	C	591/594 (100%)	583 (99%)	8 (1%)	0	100	100
1	D	592/594 (100%)	582 (98%)	10 (2%)	0	100	100
1	E	591/594 (100%)	580 (98%)	11 (2%)	0	100	100
1	F	592/594 (100%)	584 (99%)	8 (1%)	0	100	100
All	All	3550/3564 (100%)	3493 (98%)	57 (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%)	464 (98%)	11 (2%)	44	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	474/475 (100%)	461 (97%)	13 (3%)	39	41
1	C	475/475 (100%)	456 (96%)	19 (4%)	28	27
1	D	475/475 (100%)	462 (97%)	13 (3%)	39	41
1	E	475/475 (100%)	453 (95%)	22 (5%)	24	22
1	F	475/475 (100%)	462 (97%)	13 (3%)	39	41
All	All	2849/2850 (100%)	2758 (97%)	91 (3%)	34	36

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	113	ASP
1	A	172	GLU
1	A	268	LEU
1	A	297	LYS
1	A	347	GLU
1	A	354	GLN
1	A	406	VAL
1	A	470	LEU
1	A	476	LEU
1	A	505	ASN
1	B	5	ARG
1	B	113	ASP
1	B	124	LYS
1	B	172	GLU
1	B	192	GLN
1	B	223	LEU
1	B	251	MET
1	B	268	LEU
1	B	293	THR
1	B	351	ASP
1	B	354	GLN
1	B	476	LEU
1	B	488	LEU
1	C	1	MET
1	C	108	ARG
1	C	113	ASP
1	C	131	VAL
1	C	142	VAL
1	C	172	GLU

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Mol	Chain	Res	Type
1	C	202	GLN
1	C	223	LEU
1	C	251	MET
1	C	268	LEU
1	C	297	LYS
1	C	346	LYS
1	C	385	ARG
1	C	406	VAL
1	C	475	TYR
1	C	476	LEU
1	C	501	SER
1	C	503	GLU
1	C	593	GLU
1	D	1	MET
1	D	5	ARG
1	D	106	ARG
1	D	113	ASP
1	D	170	GLU
1	D	172	GLU
1	D	223	LEU
1	D	311	VAL
1	D	328	LEU
1	D	385	ARG
1	D	476	LEU
1	D	488	LEU
1	D	569	ASN
1	E	1	MET
1	E	106	ARG
1	E	108	ARG
1	E	113	ASP
1	E	124	LYS
1	E	197	VAL
1	E	199	MET
1	E	234	VAL
1	E	237	THR
1	E	247	ASP
1	E	251	MET
1	E	289	VAL
1	E	299	VAL
1	E	316	LEU
1	E	342	LEU
1	E	406	VAL

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Mol	Chain	Res	Type
1	E	443	ILE
1	E	470	LEU
1	E	476	LEU
1	E	488	LEU
1	E	561	ILE
1	E	585	THR
1	F	3	LYS
1	F	73	LEU
1	F	108	ARG
1	F	109	LEU
1	F	113	ASP
1	F	170	GLU
1	F	172	GLU
1	F	202	GLN
1	F	223	LEU
1	F	257	LEU
1	F	328	LEU
1	F	338	LYS
1	F	397	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	167	GLN
1	A	450	GLN
1	B	167	GLN
1	B	224	GLN
1	B	225	GLN
1	C	167	GLN
1	C	216	ASN
1	C	337	GLN
1	D	110	HIS
1	D	167	GLN
1	D	258	GLN
1	D	337	GLN
1	D	569	ASN
1	E	110	HIS
1	E	167	GLN
1	E	216	ASN
1	F	167	GLN
1	F	202	GLN

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Mol	Chain	Res	Type
1	F	493	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$
5	UQ0	A	705	-	13,13,13	3.58	5 (38%)	16,18,18	1.39	1 (6%)
3	TPP	B	702	4	26,27,27	1.20	4 (15%)	38,40,40	0.93	1 (2%)
2	FAD	E	701	-	58,58,58	0.40	0	85,89,89	0.54	0
5	UQ0	D	707	-	13,13,13	3.58	7 (53%)	16,18,18	1.36	1 (6%)
3	TPP	D	702	4	26,27,27	0.57	0	38,40,40	0.53	0
5	UQ0	C	706	-	13,13,13	3.66	7 (53%)	16,18,18	1.68	1 (6%)
5	UQ0	F	704	-	13,13,13	3.53	7 (53%)	16,18,18	0.92	0
3	TPP	A	702	4	26,27,27	0.43	0	38,40,40	0.50	1 (2%)
5	UQ0	B	705	-	13,13,13	3.42	5 (38%)	16,18,18	1.50	3 (18%)
5	UQ0	A	706	-	13,13,13	3.53	9 (69%)	16,18,18	2.52	2 (12%)
5	UQ0	B	706	-	13,13,13	3.55	8 (61%)	16,18,18	1.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	701	-	58,58,58	0.54	1 (1%)	85,89,89	0.64	3 (3%)
3	TPP	F	702	4	26,27,27	0.80	1 (3%)	38,40,40	0.57	1 (2%)
5	UQ0	D	705	-	13,13,13	3.56	6 (46%)	16,18,18	1.30	1 (6%)
3	TPP	C	702	4	26,27,27	0.46	0	38,40,40	0.44	0
5	UQ0	C	705	-	13,13,13	3.49	9 (69%)	16,18,18	1.12	1 (6%)
2	FAD	D	701	-	58,58,58	0.42	0	85,89,89	0.53	1 (1%)
2	FAD	F	701	-	58,58,58	0.54	1 (1%)	85,89,89	0.54	0
2	FAD	C	701	-	58,58,58	0.41	0	85,89,89	0.61	2 (2%)
5	UQ0	D	706	-	13,13,13	3.62	7 (53%)	16,18,18	1.30	2 (12%)
5	UQ0	E	705	-	13,13,13	3.43	7 (53%)	16,18,18	1.30	2 (12%)
3	TPP	E	702	4	26,27,27	0.73	1 (3%)	38,40,40	0.57	0
5	UQ0	C	704	-	13,13,13	3.51	6 (46%)	16,18,18	1.24	1 (6%)
2	FAD	B	701	-	58,58,58	0.49	1 (1%)	85,89,89	0.61	2 (2%)

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	UQ0	A	705	-	-	0/4/24/24	0/1/1/1
3	TPP	B	702	4	-	2/17/17/17	0/2/2/2
2	FAD	E	701	-	-	9/34/50/50	0/6/6/6
5	UQ0	D	707	-	-	1/4/24/24	0/1/1/1
3	TPP	D	702	4	-	1/17/17/17	0/2/2/2
5	UQ0	C	706	-	-	2/4/24/24	0/1/1/1
5	UQ0	F	704	-	-	0/4/24/24	0/1/1/1
3	TPP	A	702	4	-	1/17/17/17	0/2/2/2
5	UQ0	B	705	-	-	0/4/24/24	0/1/1/1
5	UQ0	A	706	-	-	2/4/24/24	0/1/1/1
5	UQ0	B	706	-	-	1/4/24/24	0/1/1/1
2	FAD	A	701	-	-	8/34/50/50	0/6/6/6
3	TPP	F	702	4	-	1/17/17/17	0/2/2/2
5	UQ0	D	705	-	-	0/4/24/24	0/1/1/1
3	TPP	C	702	4	-	2/17/17/17	0/2/2/2
5	UQ0	C	705	-	-	2/4/24/24	0/1/1/1
2	FAD	D	701	-	-	8/34/50/50	0/6/6/6
2	FAD	F	701	-	-	7/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	701	-	-	7/34/50/50	0/6/6/6
5	UQ0	D	706	-	-	0/4/24/24	0/1/1/1
5	UQ0	E	705	-	-	0/4/24/24	0/1/1/1
3	TPP	E	702	4	-	1/17/17/17	0/2/2/2
5	UQ0	C	704	-	-	0/4/24/24	0/1/1/1
2	FAD	B	701	-	-	5/34/50/50	0/6/6/6

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	705	UQ0	C6-C5	9.52	1.54	1.35
5	F	704	UQ0	C6-C5	9.28	1.53	1.35
5	B	705	UQ0	C6-C5	9.20	1.53	1.35
5	D	707	UQ0	C6-C5	9.04	1.53	1.35
5	C	704	UQ0	C6-C5	9.02	1.53	1.35
5	A	705	UQ0	C6-C5	8.99	1.53	1.35
5	D	706	UQ0	C6-C5	8.90	1.53	1.35
5	C	706	UQ0	C6-C5	8.89	1.53	1.35
5	C	705	UQ0	C6-C5	8.88	1.53	1.35
5	E	705	UQ0	C6-C5	8.86	1.53	1.35
5	B	706	UQ0	C6-C5	8.74	1.52	1.35
5	A	706	UQ0	C6-C5	8.43	1.52	1.35
5	D	706	UQ0	C3-C2	5.34	1.55	1.36
5	C	706	UQ0	C3-C2	5.04	1.54	1.36
5	A	706	UQ0	C5-C4	4.88	1.54	1.47
5	E	705	UQ0	C3-C2	4.83	1.53	1.36
5	C	705	UQ0	C3-C2	4.79	1.53	1.36
5	A	705	UQ0	C3-C2	4.78	1.53	1.36
5	A	706	UQ0	C3-C2	4.77	1.53	1.36
5	B	706	UQ0	C5-C4	4.73	1.54	1.47
5	C	704	UQ0	C3-C2	4.71	1.53	1.36
5	C	706	UQ0	C5-C4	4.68	1.54	1.47
5	D	707	UQ0	C3-C2	4.62	1.53	1.36
5	F	704	UQ0	C3-C2	4.59	1.52	1.36
5	B	706	UQ0	C3-C2	4.51	1.52	1.36
5	D	705	UQ0	C3-C2	4.50	1.52	1.36
5	B	705	UQ0	C5-C4	4.24	1.53	1.47
5	D	707	UQ0	C5-C4	4.22	1.53	1.47
5	A	705	UQ0	C5-C4	4.18	1.53	1.47
5	D	706	UQ0	C5-C4	4.10	1.53	1.47
5	B	705	UQ0	C3-C2	4.08	1.51	1.36
5	C	704	UQ0	C5-C4	3.84	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	705	UQ0	C5-C4	3.78	1.53	1.47
5	C	705	UQ0	C5-C4	3.57	1.52	1.47
5	F	704	UQ0	C5-C4	3.47	1.52	1.47
5	D	705	UQ0	C6-C1	3.45	1.54	1.44
5	F	704	UQ0	C6-C1	3.42	1.54	1.44
5	A	705	UQ0	C2-C1	3.34	1.54	1.46
5	E	705	UQ0	C5-C4	3.30	1.52	1.47
5	A	705	UQ0	C6-C1	3.27	1.53	1.44
5	D	706	UQ0	C2-C1	3.27	1.54	1.46
5	C	706	UQ0	C2-C1	3.24	1.54	1.46
5	C	704	UQ0	C2-C1	3.24	1.54	1.46
5	B	705	UQ0	C6-C1	3.19	1.53	1.44
5	D	707	UQ0	C6-C1	3.18	1.53	1.44
5	C	704	UQ0	C6-C1	3.15	1.53	1.44
5	A	706	UQ0	C6-C1	3.13	1.53	1.44
5	E	705	UQ0	C2-C1	3.11	1.53	1.46
5	C	705	UQ0	C6-C1	3.09	1.53	1.44
5	B	706	UQ0	C6-C1	3.08	1.53	1.44
5	D	707	UQ0	C2-C1	3.08	1.53	1.46
5	C	706	UQ0	C6-C1	3.06	1.53	1.44
2	F	701	FAD	P-O3P	3.02	1.62	1.59
3	B	702	TPP	C5-C4	3.02	1.41	1.35
5	E	705	UQ0	C6-C1	3.01	1.53	1.44
5	D	706	UQ0	C6-C1	3.00	1.53	1.44
5	F	704	UQ0	C2-C1	2.96	1.53	1.46
2	A	701	FAD	P-O2P	-2.91	1.41	1.55
5	C	705	UQ0	C2-C1	2.89	1.53	1.46
5	D	705	UQ0	C2-C1	2.75	1.53	1.46
5	B	706	UQ0	O2-CM2	-2.63	1.39	1.45
5	B	706	UQ0	C2-C1	2.45	1.52	1.46
3	B	702	TPP	C7'-C5'	2.44	1.55	1.51
5	C	706	UQ0	O3-C3	2.38	1.42	1.36
5	D	707	UQ0	O2-CM2	-2.36	1.40	1.45
2	B	701	FAD	P-O2P	-2.31	1.44	1.55
5	A	706	UQ0	C2-C1	2.28	1.52	1.46
5	A	706	UQ0	O1-C1	-2.27	1.18	1.24
5	C	706	UQ0	O2-CM2	-2.23	1.40	1.45
5	E	705	UQ0	O1-C1	-2.22	1.18	1.24
5	F	704	UQ0	O3-CM3	-2.17	1.40	1.45
5	B	705	UQ0	C2-C1	2.15	1.51	1.46
5	F	704	UQ0	O2-CM2	-2.14	1.40	1.45
5	C	705	UQ0	O3-CM3	-2.14	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	702	TPP	PA-O3A	-2.13	1.57	1.59
5	B	706	UQ0	O1-C1	-2.12	1.19	1.24
5	C	705	UQ0	O4-C4	-2.12	1.18	1.23
5	B	706	UQ0	C3-C4	2.11	1.54	1.48
3	B	702	TPP	C2'-N1'	2.10	1.37	1.34
5	E	705	UQ0	O3-CM3	-2.09	1.40	1.45
5	D	705	UQ0	O3-CM3	-2.09	1.40	1.45
5	A	706	UQ0	O2-CM2	-2.08	1.40	1.45
5	D	706	UQ0	O3-CM3	-2.06	1.40	1.45
5	C	705	UQ0	O2-CM2	-2.05	1.40	1.45
5	C	705	UQ0	O1-C1	-2.05	1.19	1.24
5	D	706	UQ0	O3-C3	2.04	1.41	1.36
5	D	707	UQ0	O3-CM3	-2.03	1.40	1.45
3	F	702	TPP	PB-O1B	2.02	1.56	1.50
5	C	704	UQ0	O1-C1	-2.01	1.19	1.24
5	A	706	UQ0	O2-C2	2.01	1.41	1.36
5	A	706	UQ0	C3-C4	2.01	1.54	1.48
3	B	702	TPP	CM2-C2'	2.01	1.55	1.49

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	706	UQ0	CM5-C5-C4	8.95	123.56	117.41
5	B	706	UQ0	CM5-C5-C4	6.17	121.65	117.41
5	C	706	UQ0	CM5-C5-C4	5.74	121.36	117.41
5	D	707	UQ0	CM5-C5-C4	3.91	120.10	117.41
5	D	706	UQ0	CM5-C5-C4	3.56	119.86	117.41
5	A	705	UQ0	CM5-C5-C4	3.36	119.72	117.41
5	E	705	UQ0	C6-C5-C4	3.13	122.18	119.56
5	C	705	UQ0	CM5-C5-C4	2.87	119.39	117.41
5	B	705	UQ0	O1-C1-C2	-2.56	117.74	121.66
3	B	702	TPP	C5'-C7'-N3	2.51	118.38	112.97
5	B	705	UQ0	C6-C5-C4	2.42	121.58	119.56
2	A	701	FAD	O3P-P-O1P	-2.39	103.52	110.70
5	A	706	UQ0	C6-C1-C2	2.37	122.28	115.39
2	A	701	FAD	C4B-O4B-C1B	-2.31	104.36	109.47
2	D	701	FAD	C4B-O4B-C1B	-2.29	104.42	109.47
5	B	705	UQ0	C5-C6-C1	-2.21	118.04	122.65
2	B	701	FAD	O2P-P-O1P	2.11	122.27	112.44
5	D	705	UQ0	C6-C5-C4	2.10	121.32	119.56
5	C	704	UQ0	C6-C5-C4	2.09	121.31	119.56
2	C	701	FAD	O3P-P-O1P	-2.07	104.47	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	TPP	O2A-PA-O1A	2.06	122.05	112.44
5	D	706	UQ0	C6-C5-C4	2.06	121.28	119.56
2	B	701	FAD	C4B-O4B-C1B	-2.05	104.93	109.47
2	C	701	FAD	C4B-O4B-C1B	-2.05	104.94	109.47
5	E	705	UQ0	C5-C6-C1	-2.04	118.40	122.65
3	F	702	TPP	O2B-PB-O3A	2.02	111.40	104.64
2	A	701	FAD	C2B-C1B-N9A	2.01	118.30	113.30

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5B-O5B-PA-O1A
2	D	701	FAD	C5B-O5B-PA-O1A
2	D	701	FAD	C5B-O5B-PA-O3P
2	E	701	FAD	C5'-O5'-P-O1P
2	F	701	FAD	C5B-O5B-PA-O1A
3	C	702	TPP	PA-O3A-PB-O2B
2	D	701	FAD	C2'-C3'-C4'-O4'
2	F	701	FAD	C2'-C3'-C4'-O4'
2	E	701	FAD	O4B-C4B-C5B-O5B
3	A	702	TPP	PA-O3A-PB-O2B
3	B	702	TPP	C5-C6-C7-O7
3	D	702	TPP	C5-C6-C7-O7
2	C	701	FAD	P-O3P-PA-O1A
2	D	701	FAD	P-O3P-PA-O1A
2	E	701	FAD	P-O3P-PA-O1A
2	F	701	FAD	P-O3P-PA-O1A
2	E	701	FAD	C3B-C4B-C5B-O5B
3	B	702	TPP	C6'-C5'-C7'-N3
2	A	701	FAD	C5B-O5B-PA-O1A
2	A	701	FAD	C5B-O5B-PA-O2A
2	A	701	FAD	C5B-O5B-PA-O3P
2	A	701	FAD	C5'-O5'-P-O1P
2	B	701	FAD	C5'-O5'-P-O1P
2	C	701	FAD	C5'-O5'-P-O1P
2	D	701	FAD	C5B-O5B-PA-O2A
2	D	701	FAD	C5'-O5'-P-O1P
2	E	701	FAD	C5B-O5B-PA-O1A
2	E	701	FAD	C5'-O5'-P-O3P
2	F	701	FAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	F	701	FAD	C5B-O5B-PA-O3P
5	C	706	UQ0	C1-C2-O2-CM2
2	C	701	FAD	O4B-C4B-C5B-O5B
2	E	701	FAD	C2B-C1B-N9A-C8A
5	C	706	UQ0	C3-C2-O2-CM2
2	A	701	FAD	C2'-C3'-C4'-O4'
5	A	706	UQ0	C4-C3-O3-CM3
2	A	701	FAD	P-O3P-PA-O1A
2	E	701	FAD	C2'-C3'-C4'-O4'
3	C	702	TPP	C5-C6-C7-O7
3	E	702	TPP	C5-C6-C7-O7
3	F	702	TPP	C5-C6-C7-O7
2	F	701	FAD	C2B-C1B-N9A-C8A
2	A	701	FAD	P-O3P-PA-O2A
2	B	701	FAD	P-O3P-PA-O1A
2	B	701	FAD	P-O3P-PA-O2A
2	C	701	FAD	P-O3P-PA-O2A
2	F	701	FAD	P-O3P-PA-O2A
2	C	701	FAD	C2'-C3'-C4'-O4'
5	C	705	UQ0	C1-C2-O2-CM2
2	A	701	FAD	C2B-C1B-N9A-C8A
2	B	701	FAD	C2B-C1B-N9A-C8A
2	D	701	FAD	C2B-C1B-N9A-C8A
5	A	706	UQ0	C2-C3-O3-CM3
5	D	707	UQ0	C4-C3-O3-CM3
2	C	701	FAD	C2B-C1B-N9A-C8A
2	D	701	FAD	C2'-C3'-C4'-C5'
5	B	706	UQ0	C4-C3-O3-CM3
5	C	705	UQ0	C4-C3-O3-CM3
2	E	701	FAD	P-O3P-PA-O2A

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	UQ0	0	1
3	B	702	TPP	1	1
2	E	701	FAD	3	0
5	D	707	UQ0	1	0
5	B	705	UQ0	0	1
5	A	706	UQ0	1	1
5	B	706	UQ0	2	1

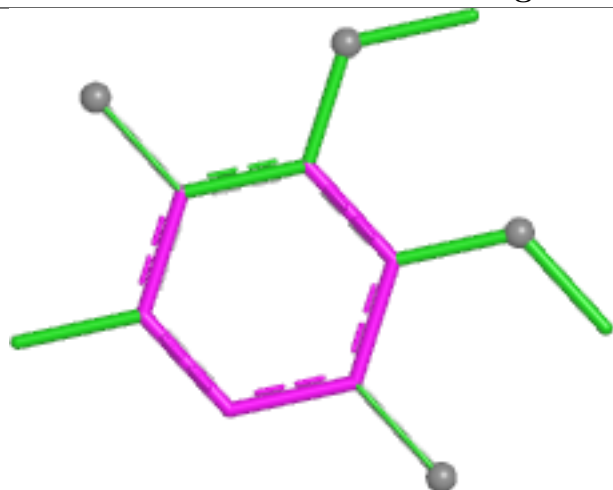
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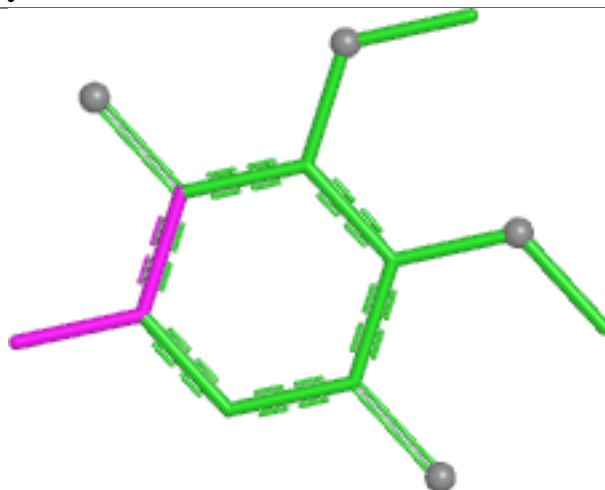
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	705	UQ0	2	0
2	D	701	FAD	2	0
2	F	701	FAD	1	0

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.

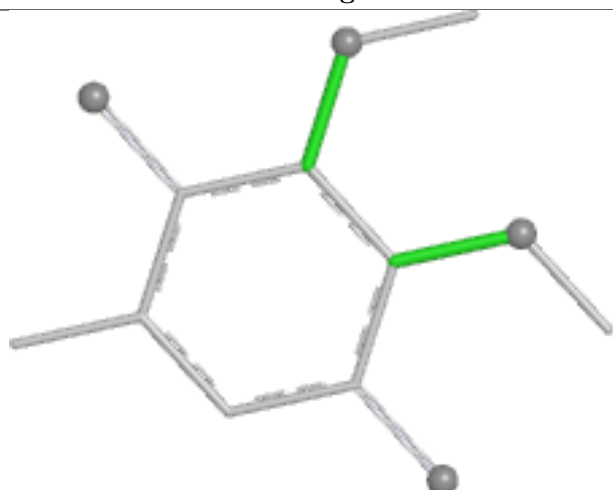
Ligand UQ0 A 705



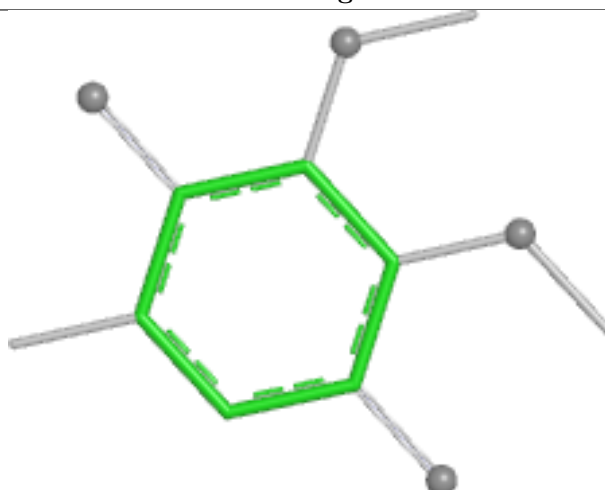
Bond lengths



Bond angles

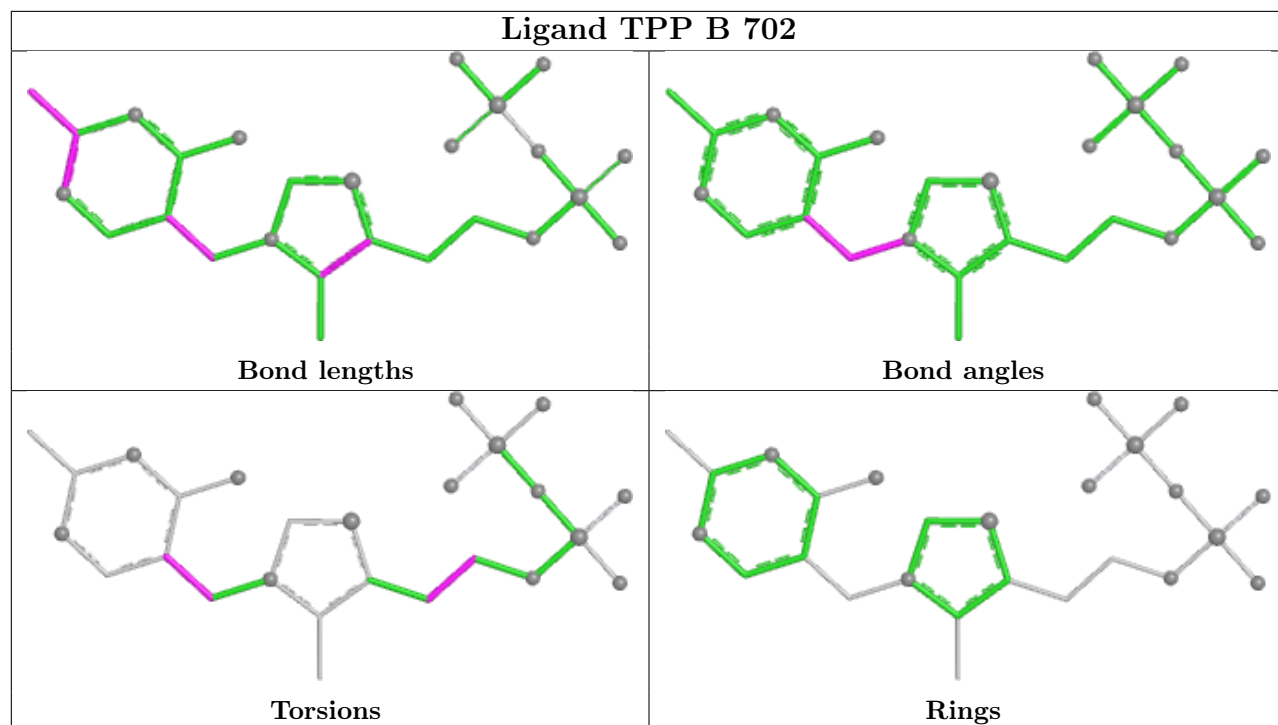


Torsions

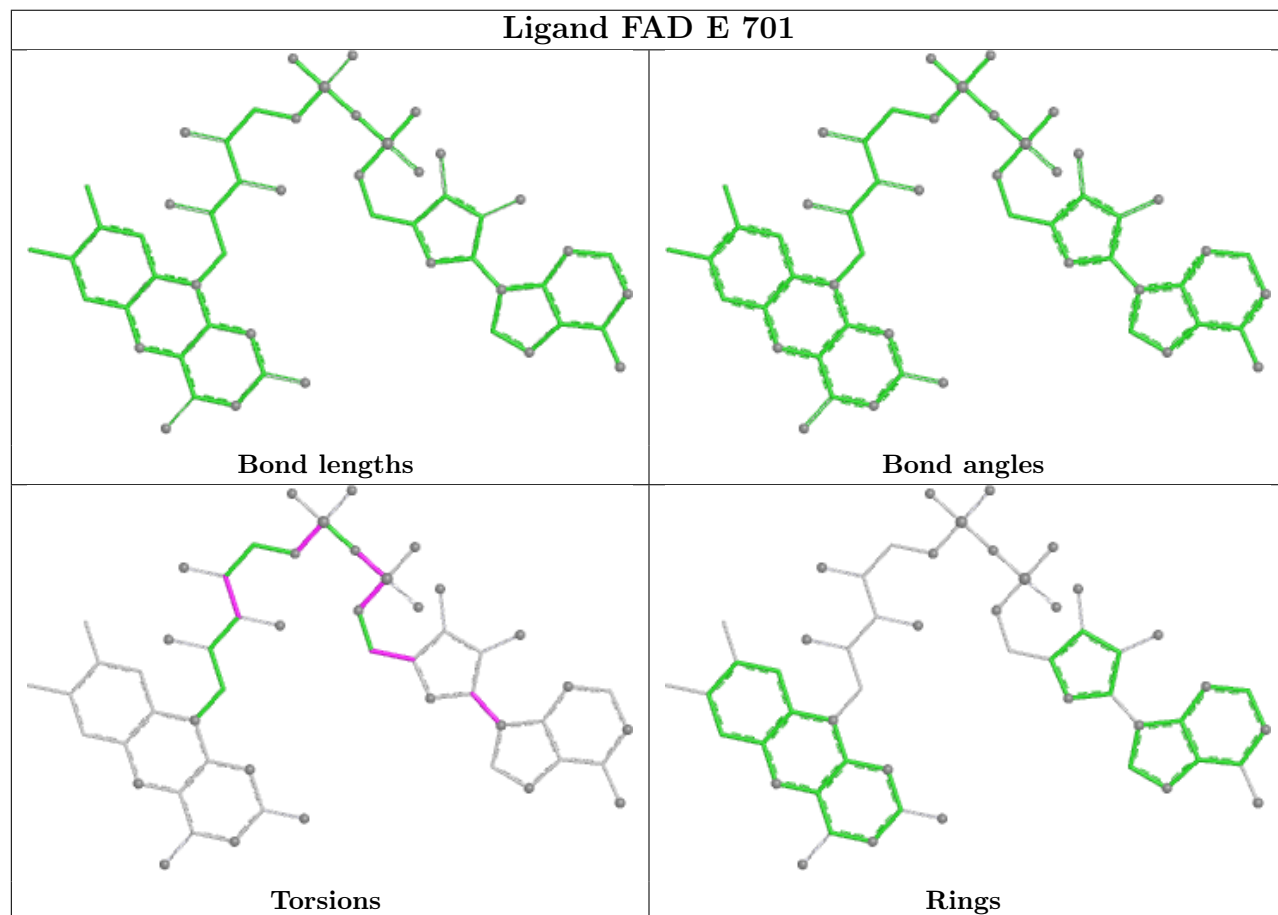


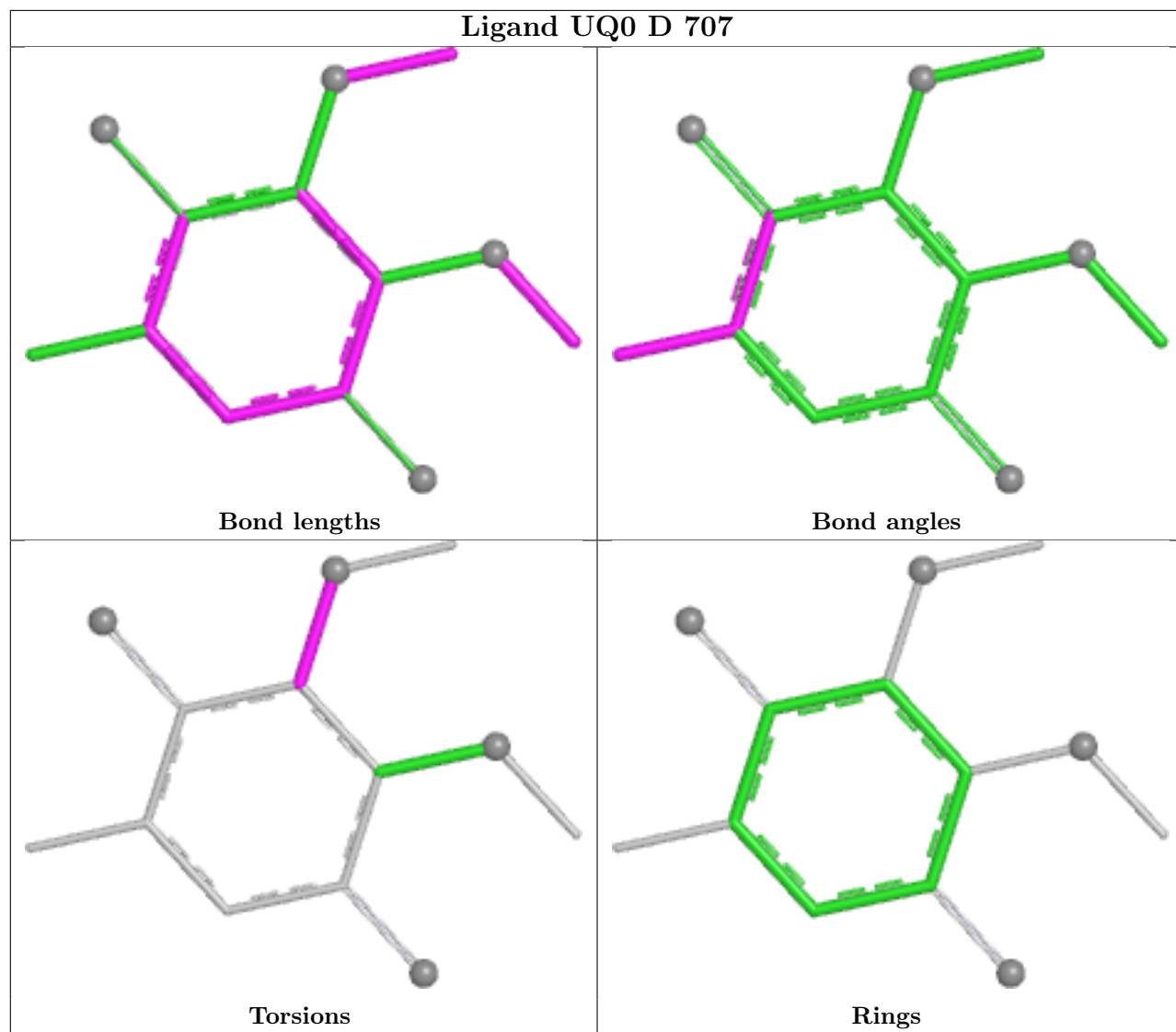
Rings

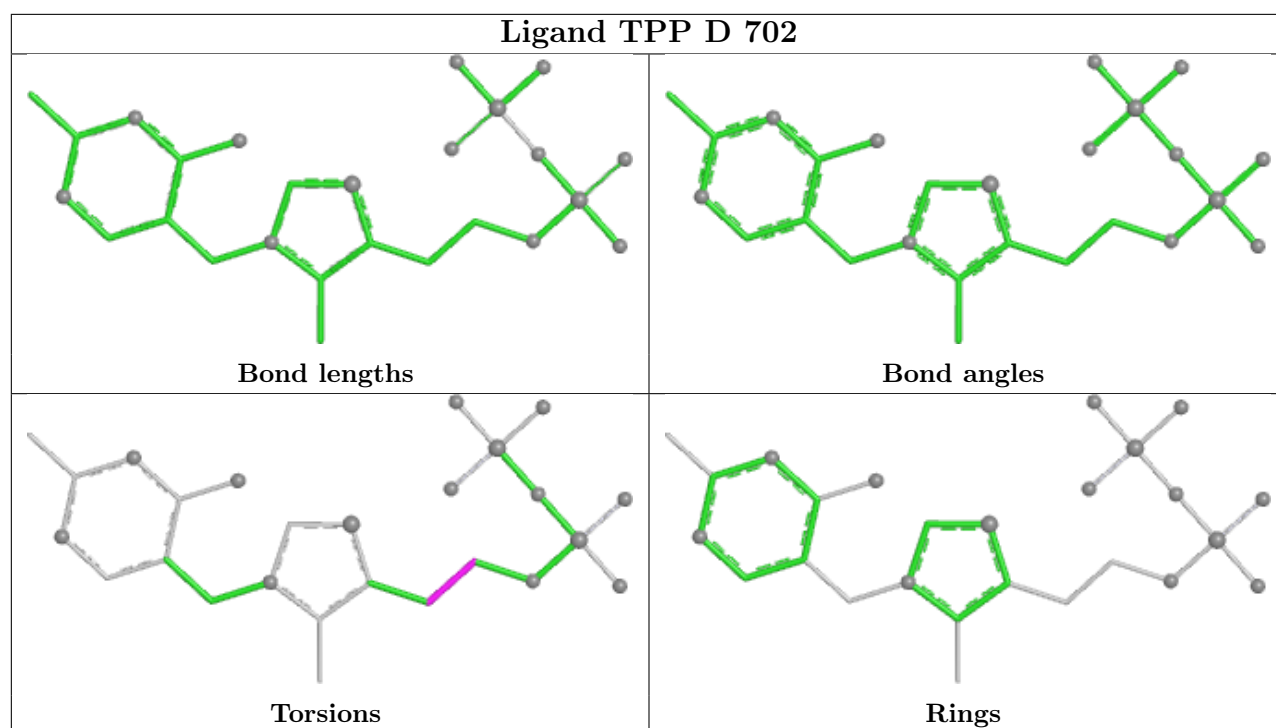
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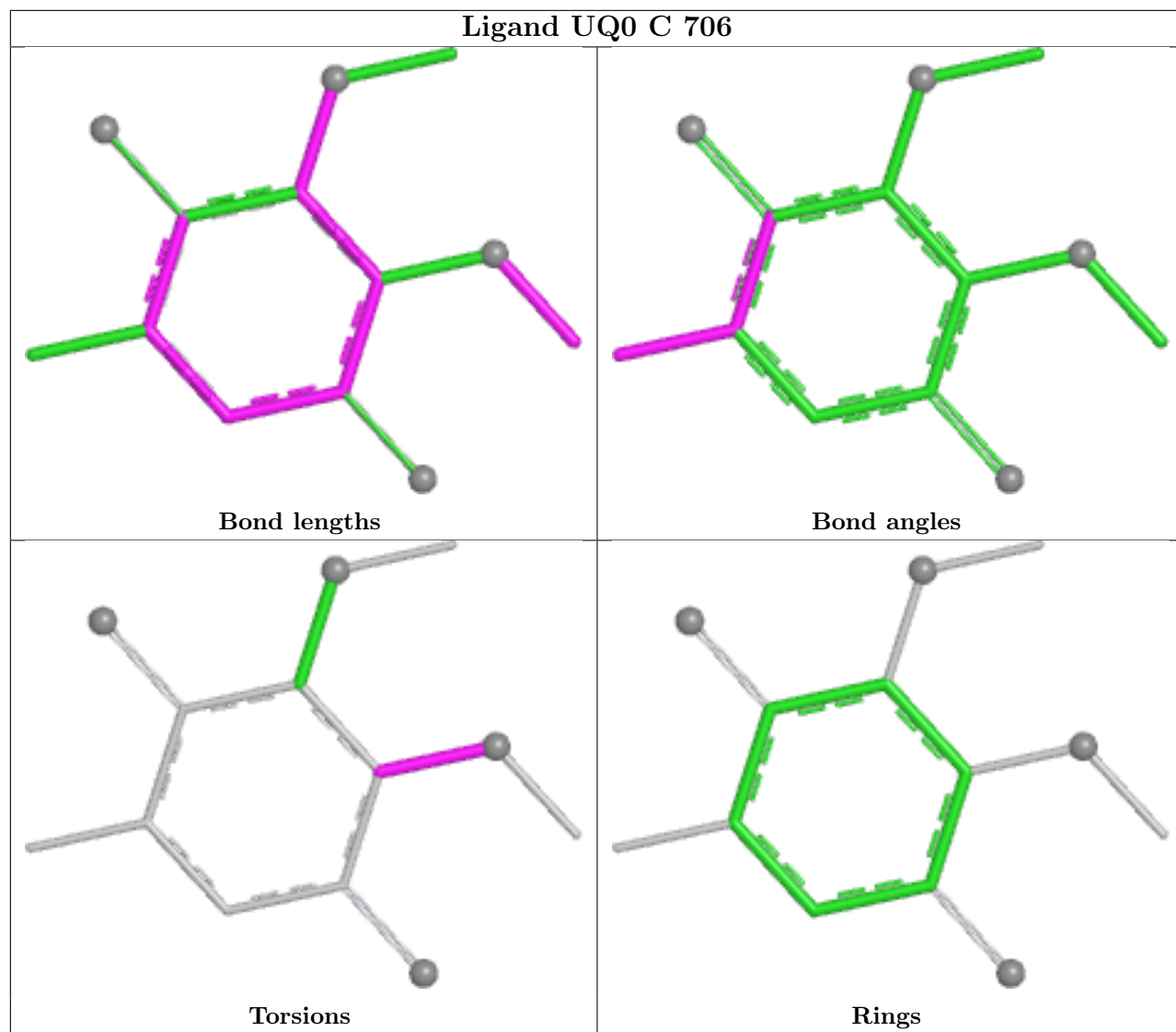
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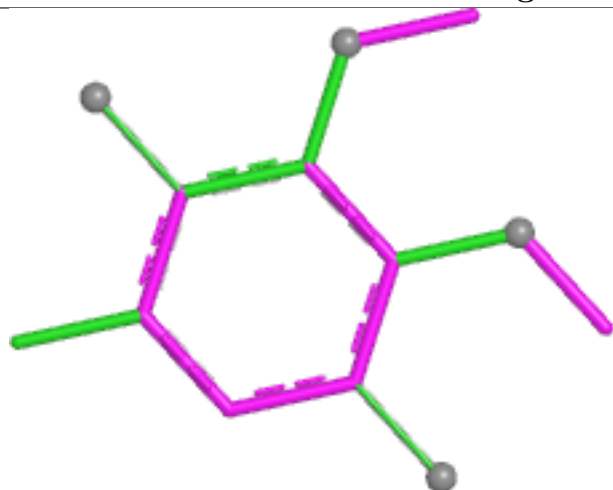




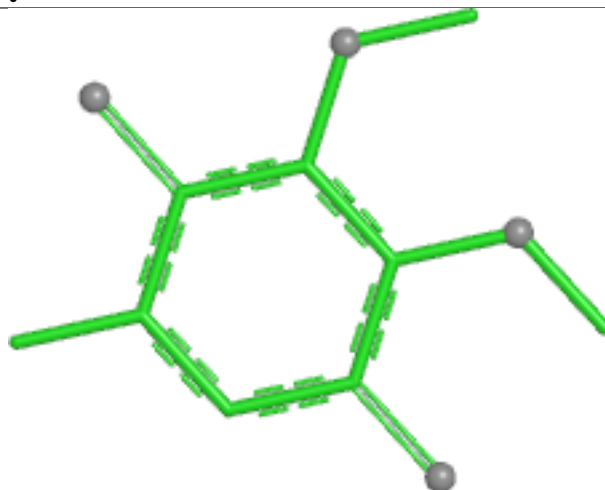
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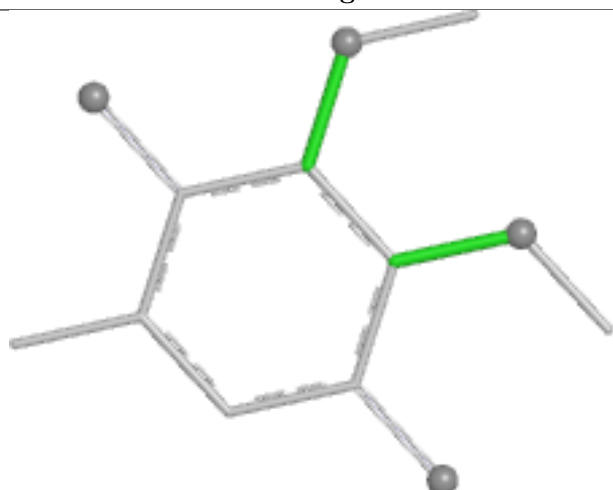
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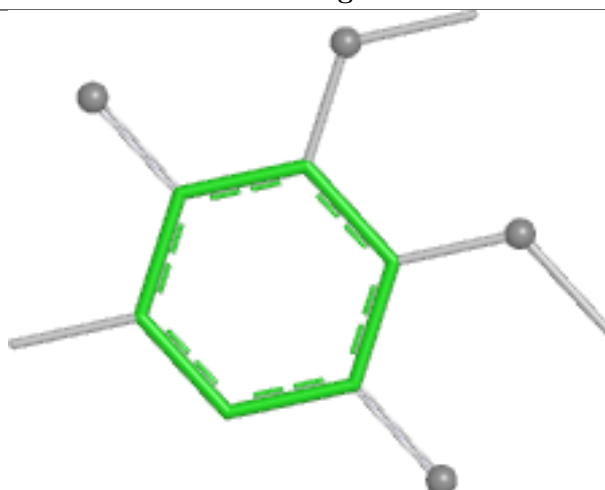
Bond lengths



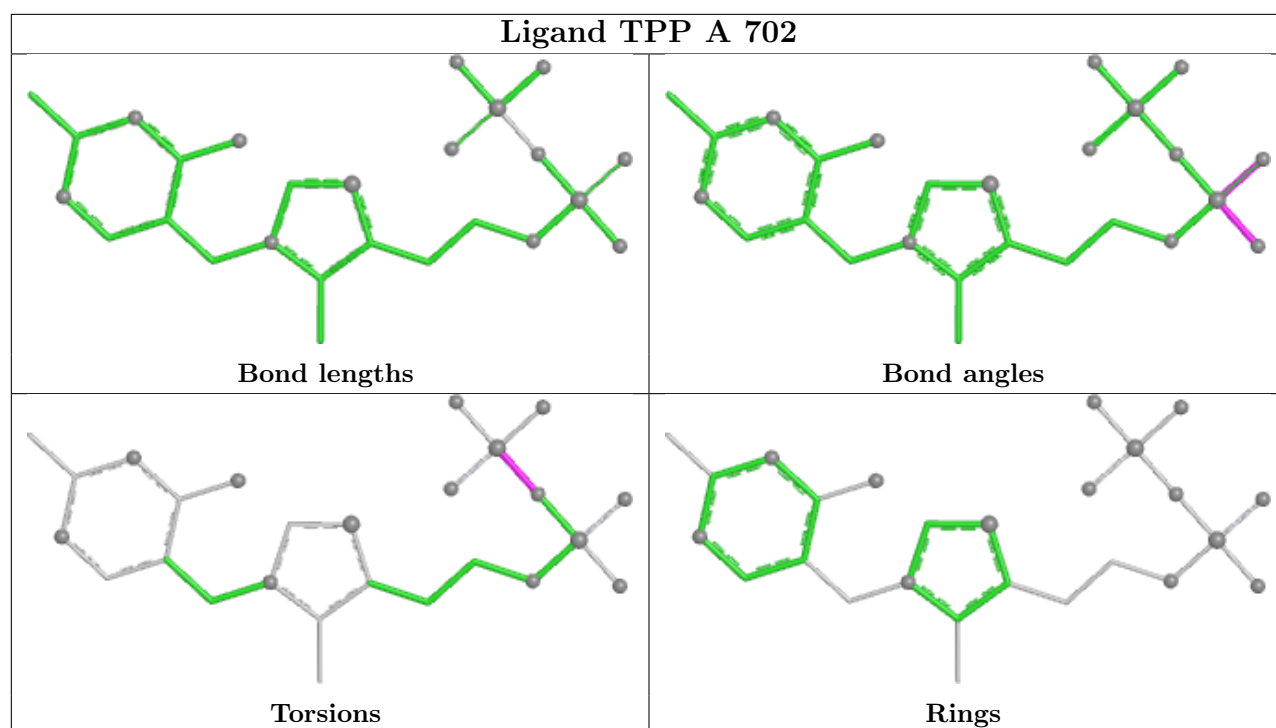
Bond angles



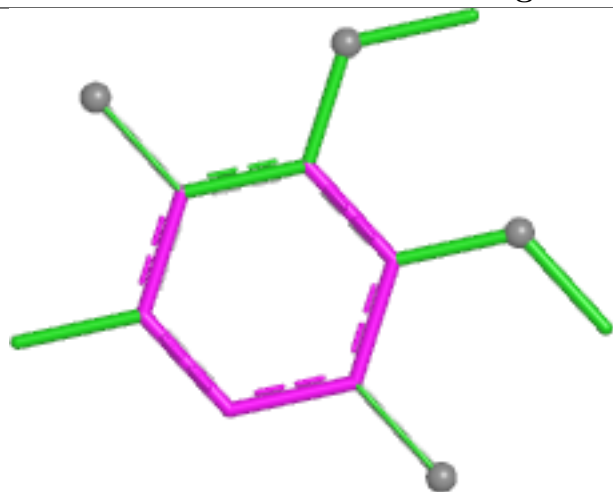
Torsions



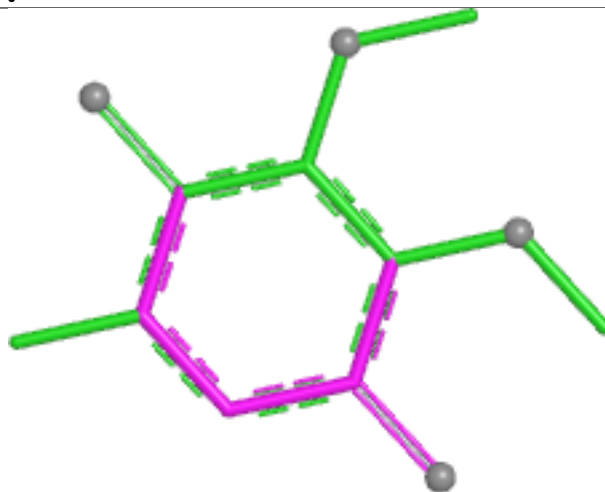
Rings



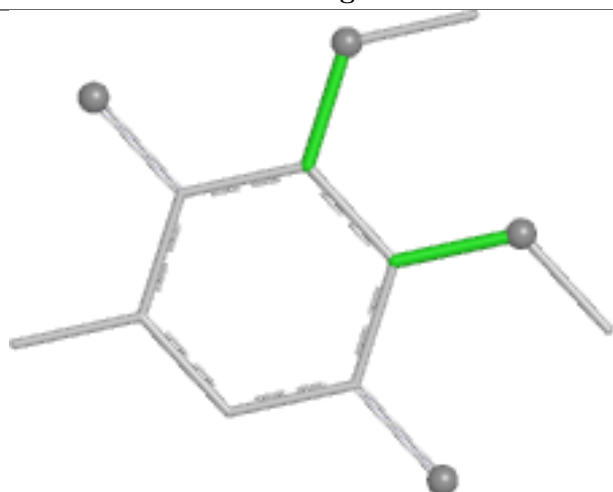
Ligand UQ0 B 705



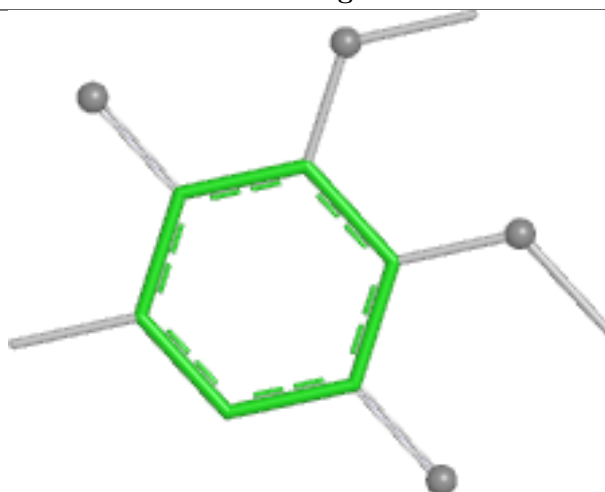
Bond lengths



Bond angles

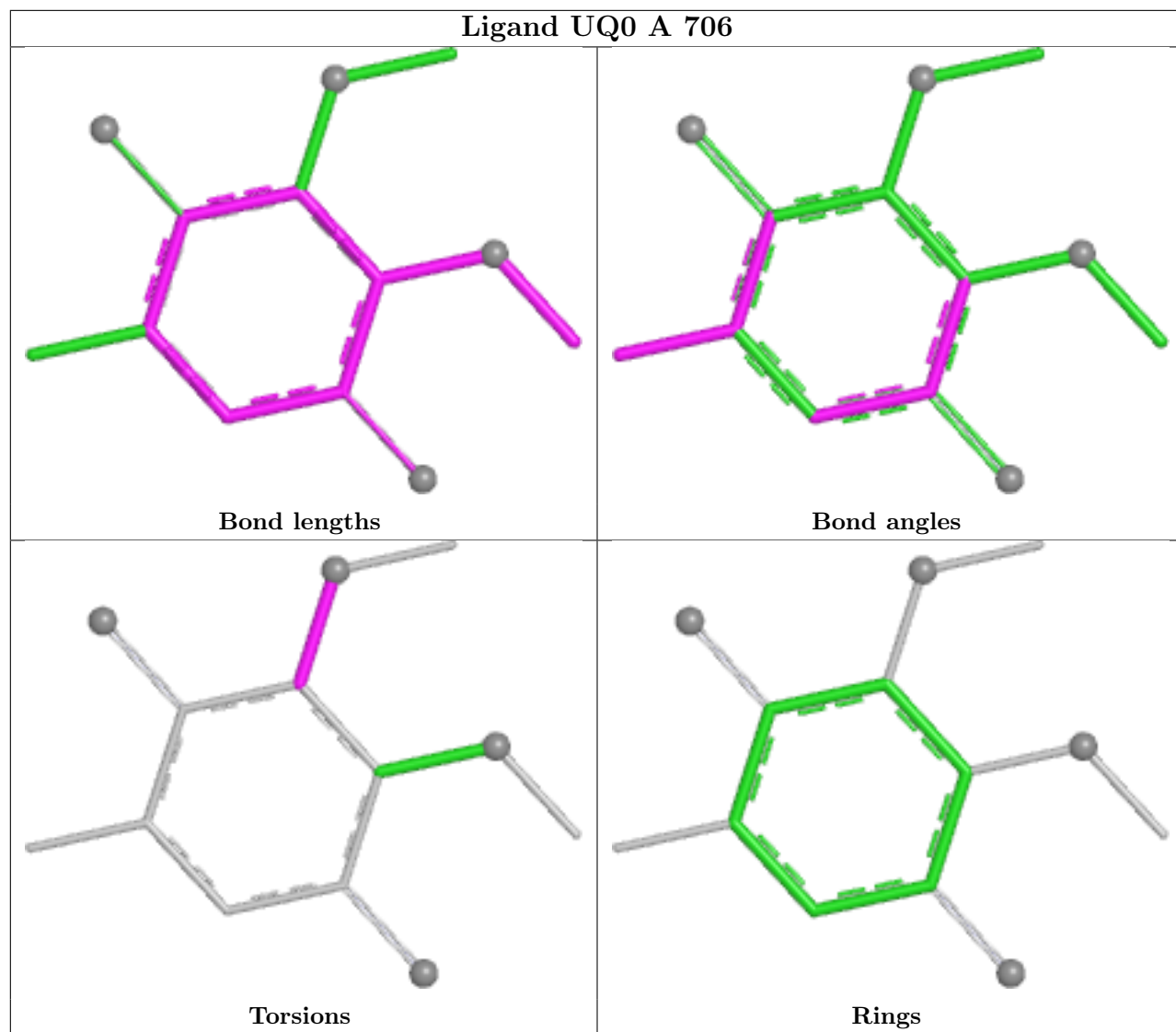


Torsions

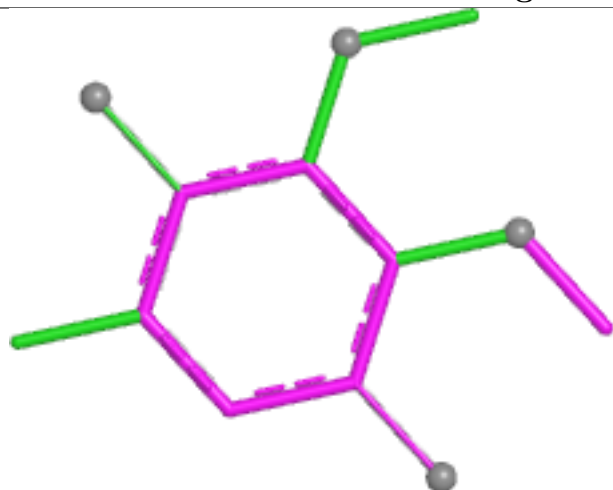


Rings

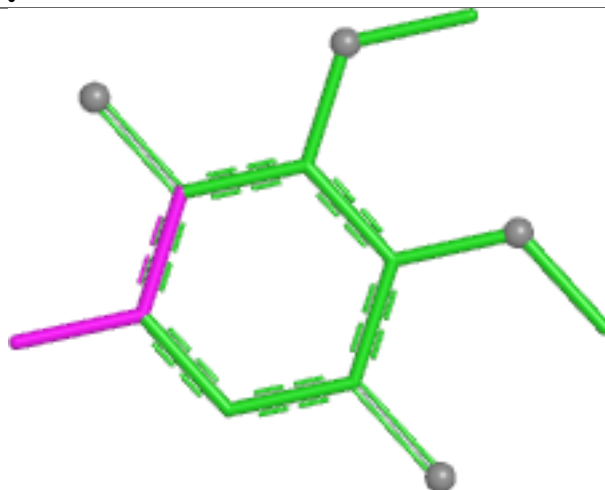
Ligand UQ0 A 706



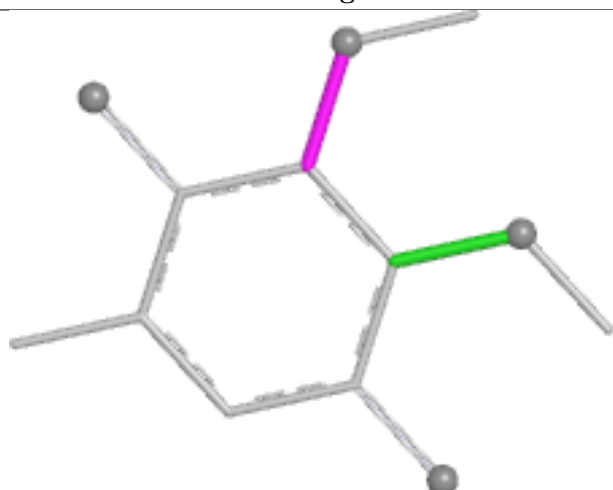
Ligand UQ0 B 706



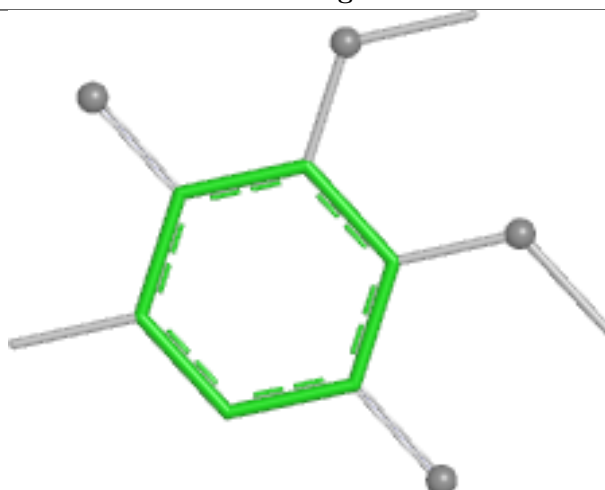
Bond lengths



Bond angles

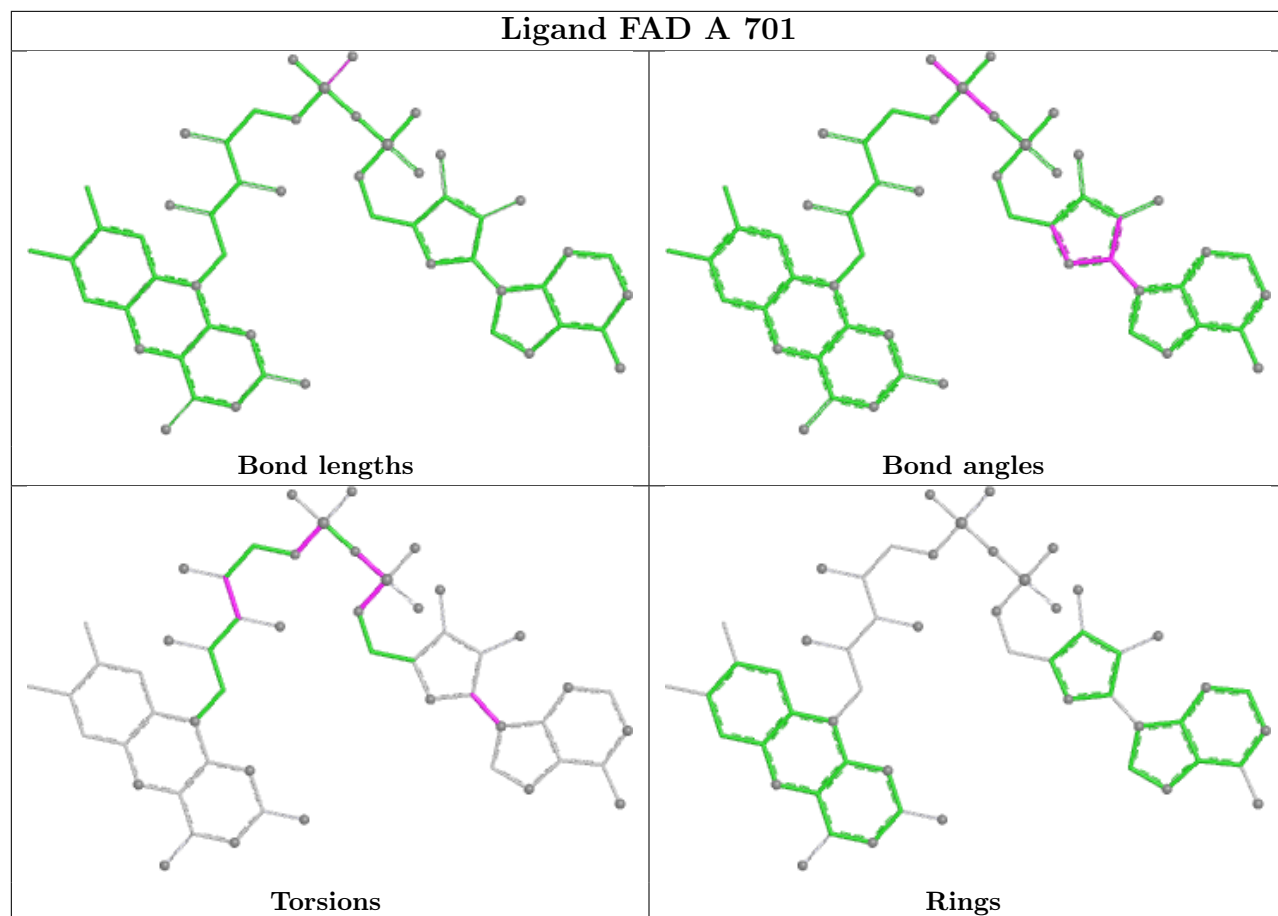


Torsions

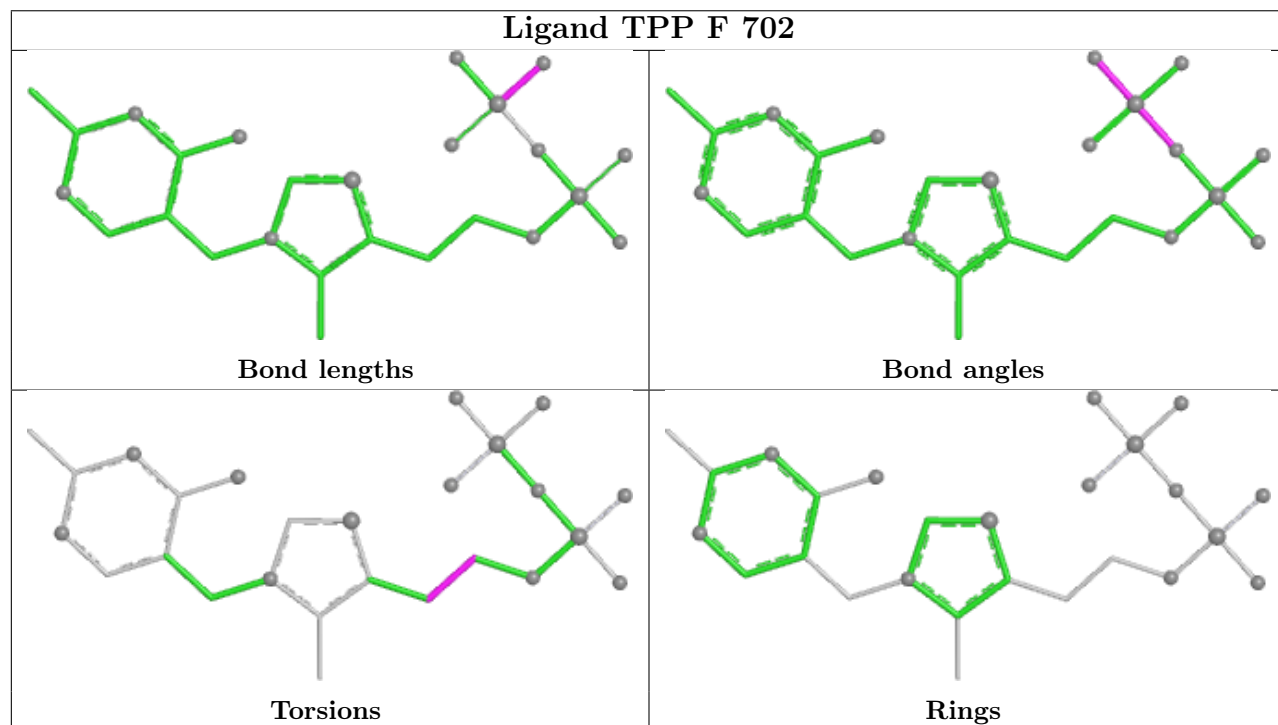


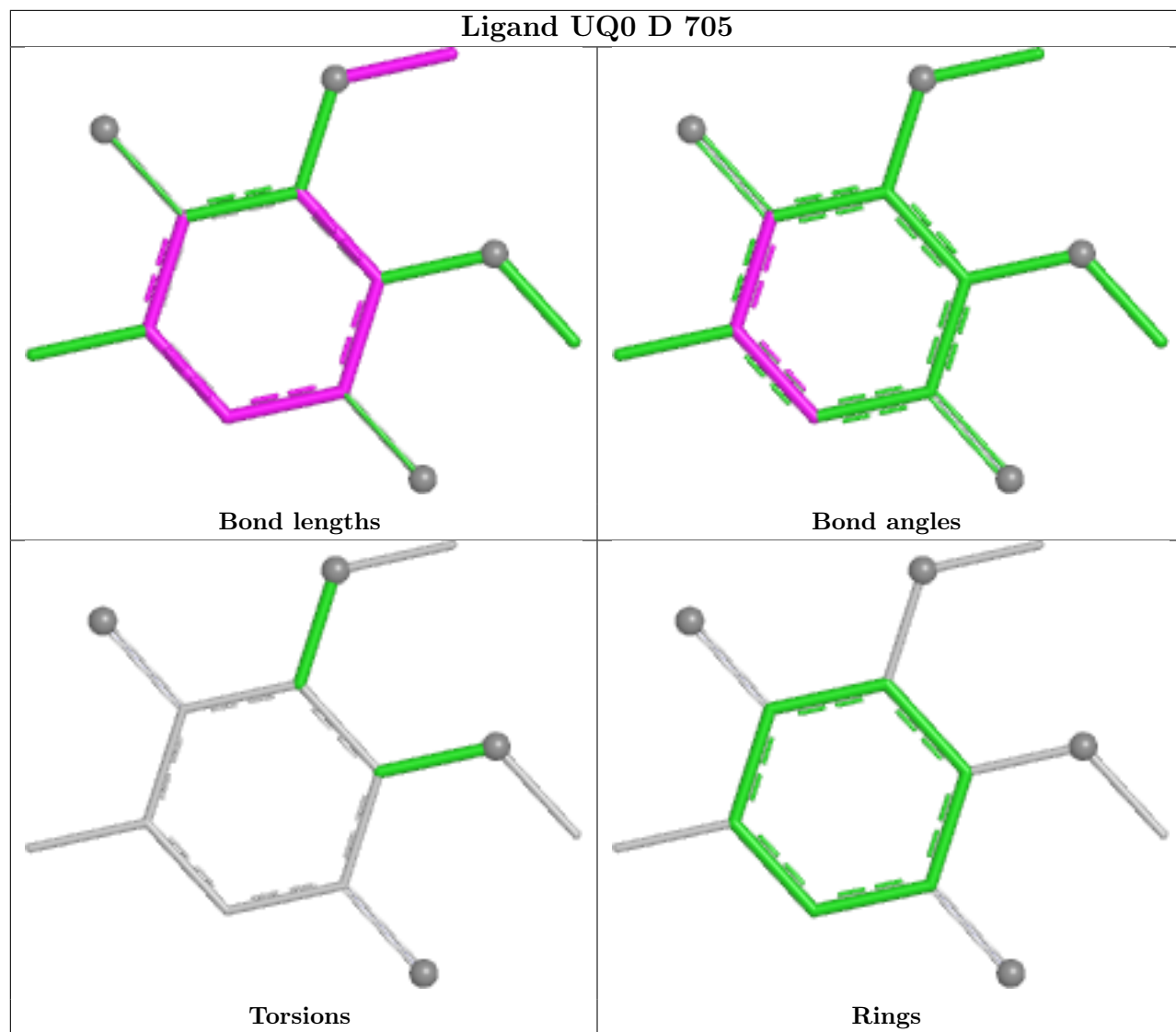
Rings

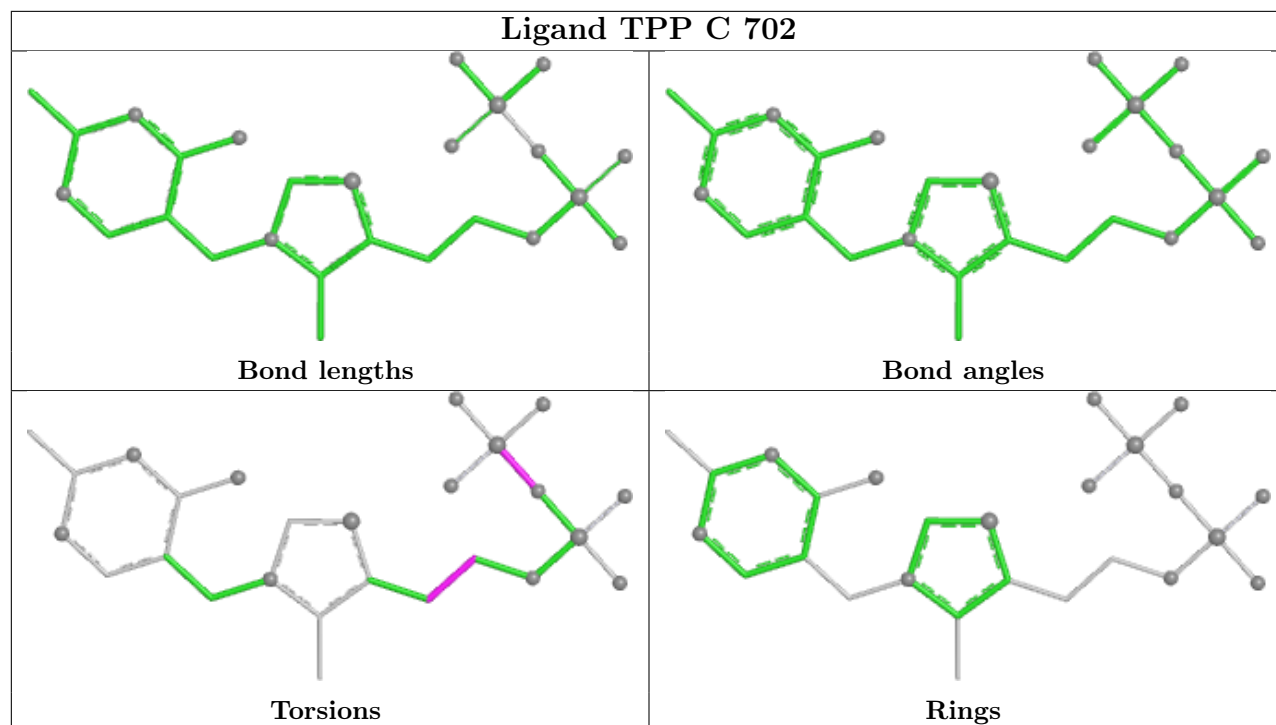
Ligand FAD A 701

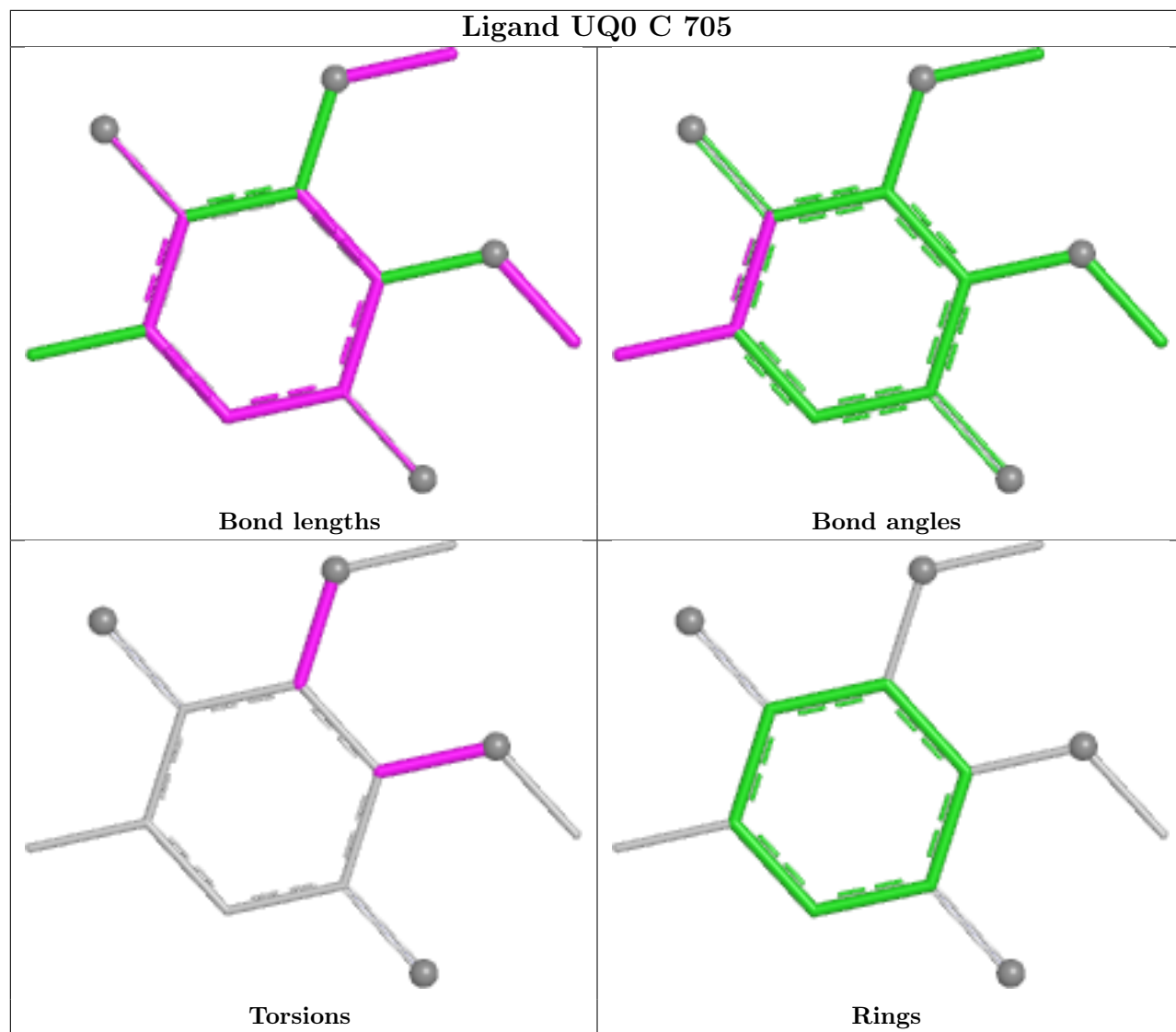


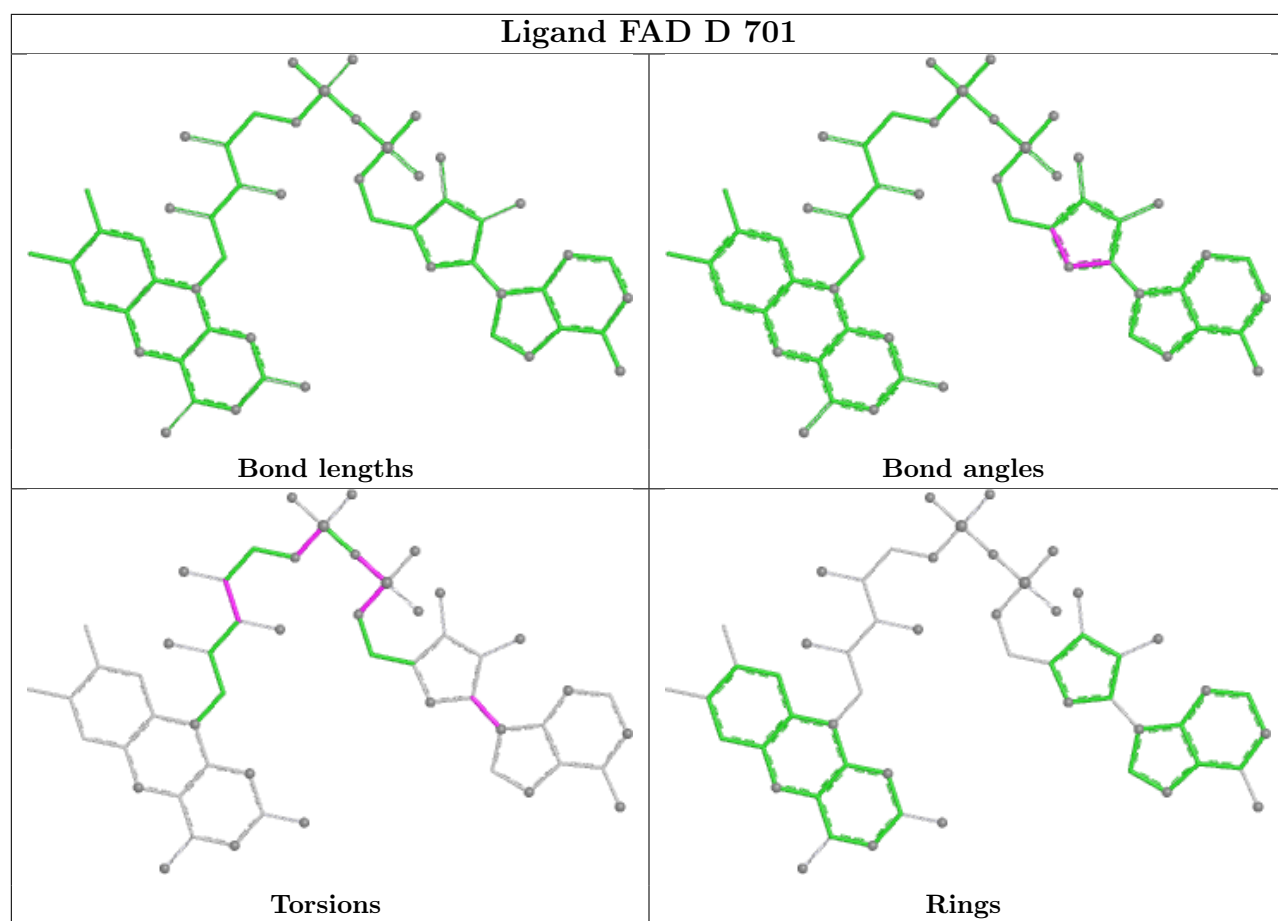
Ligand TPP F 702

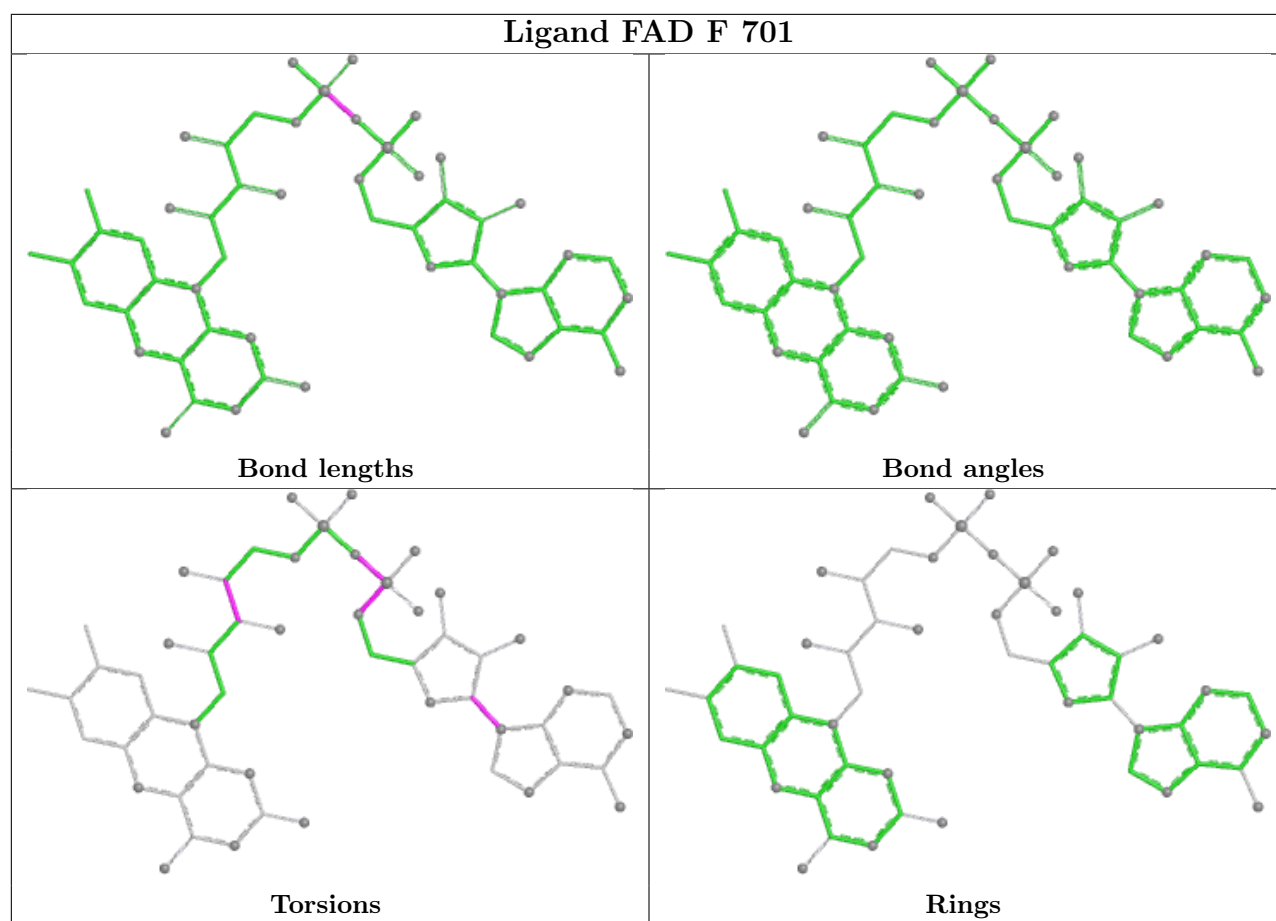


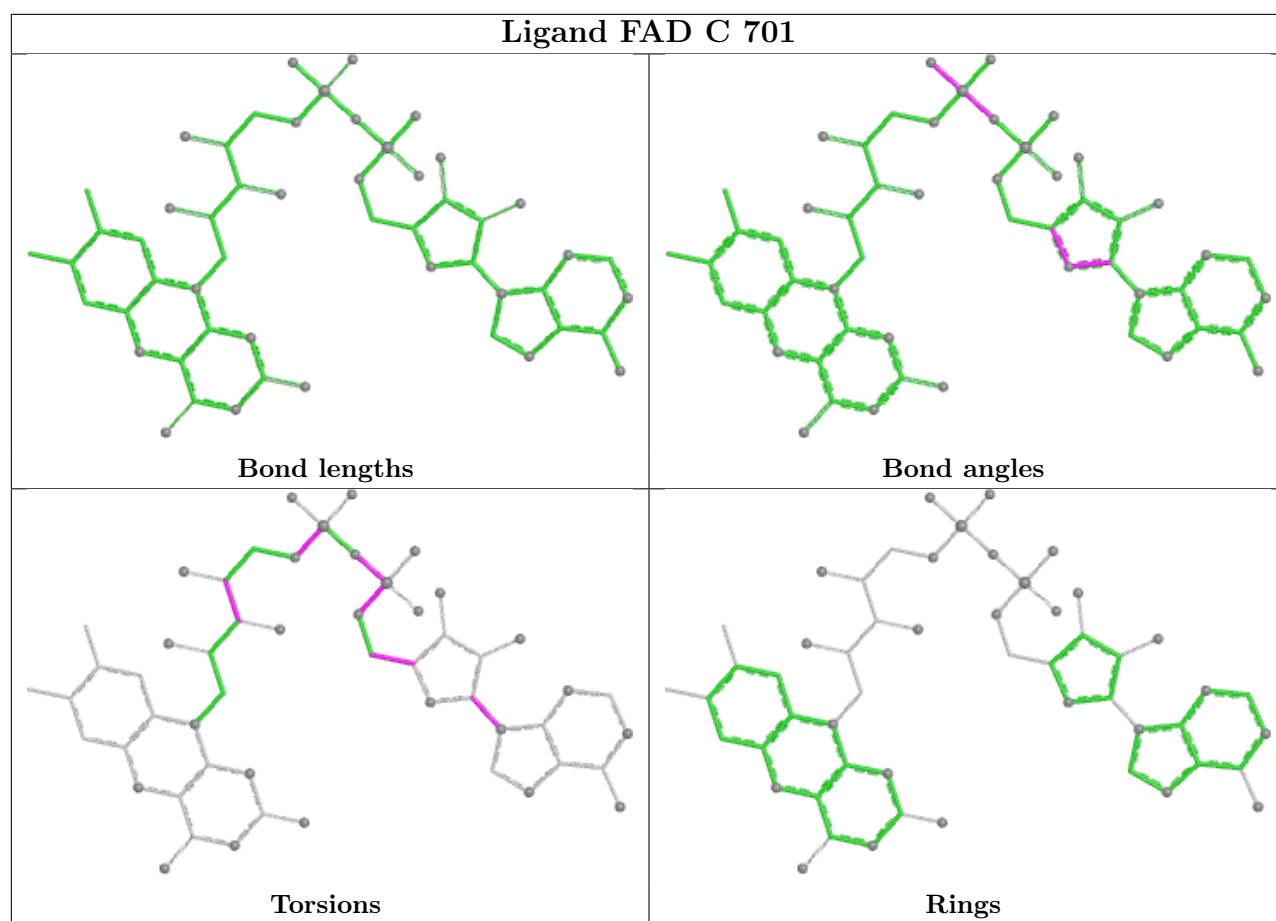


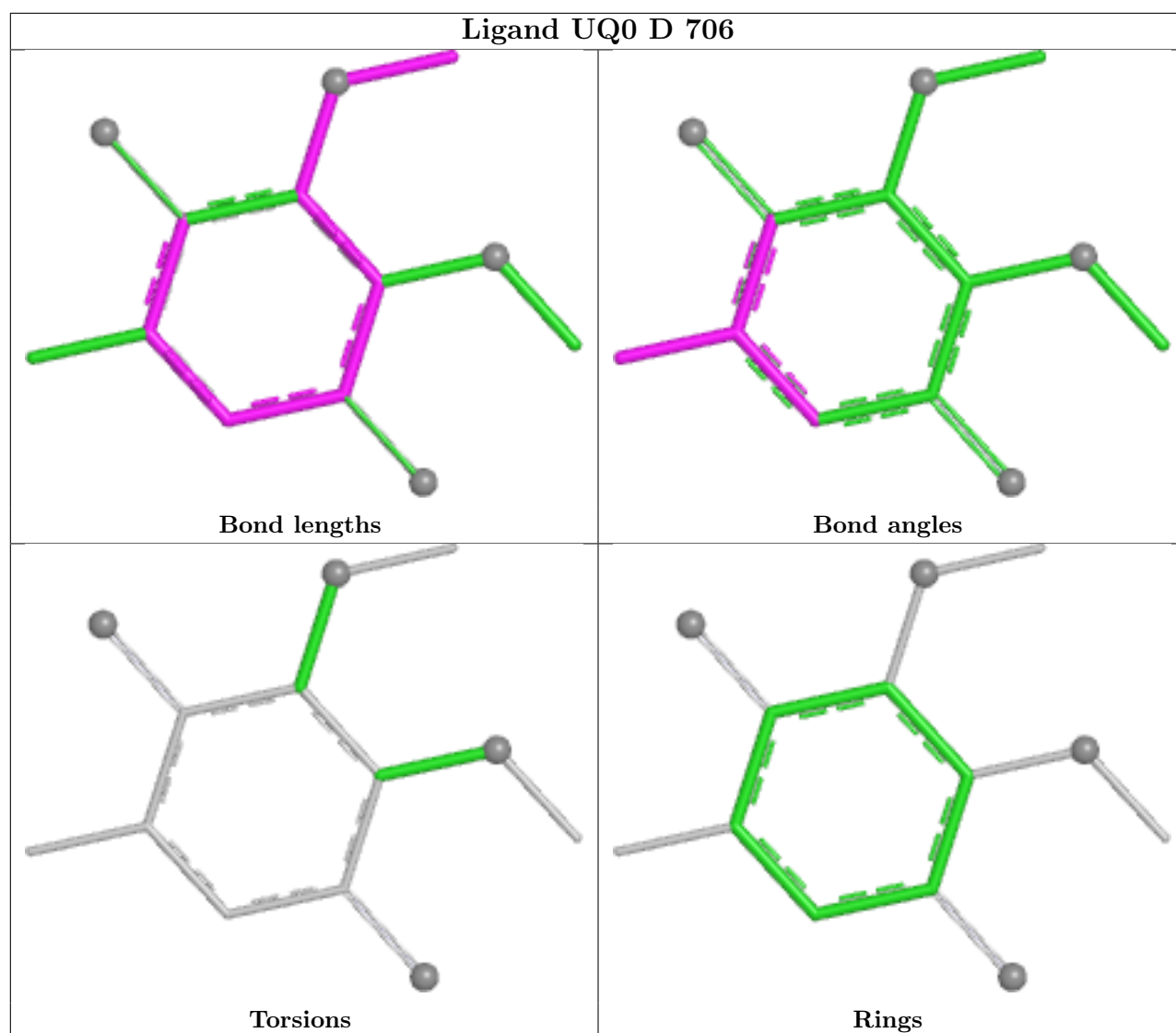




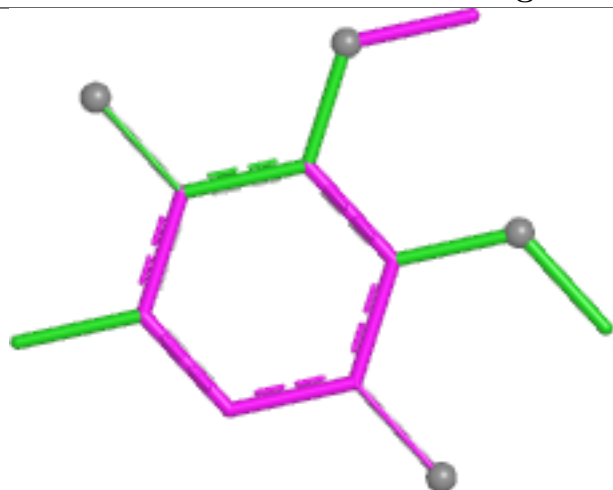




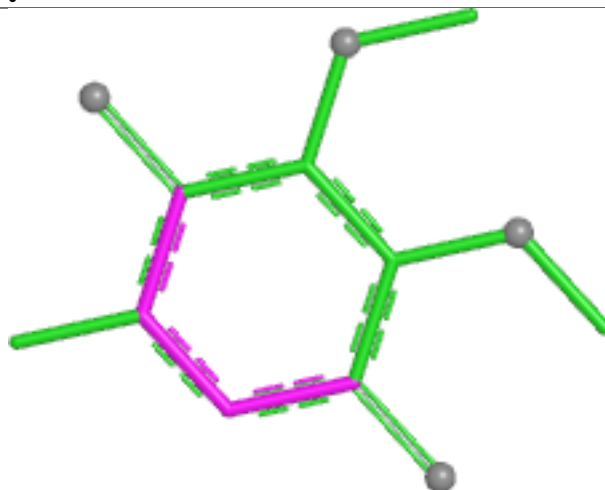




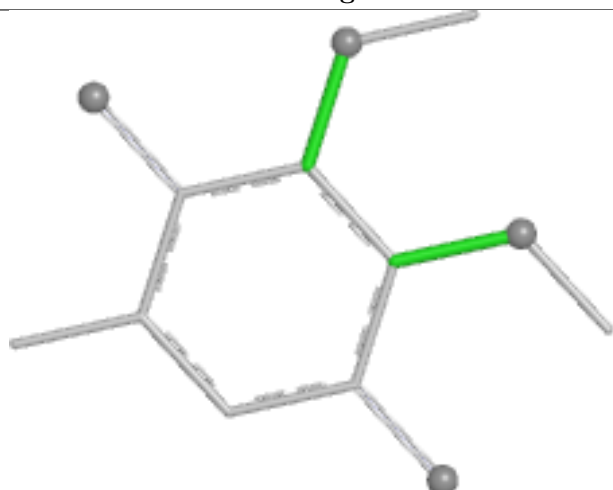
Ligand UQ0 E 705



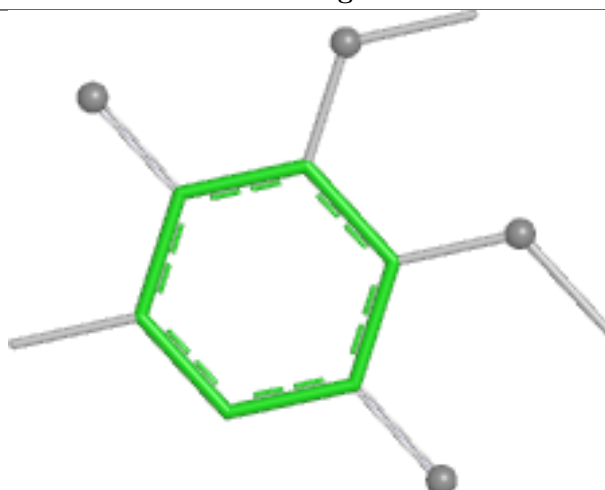
Bond lengths



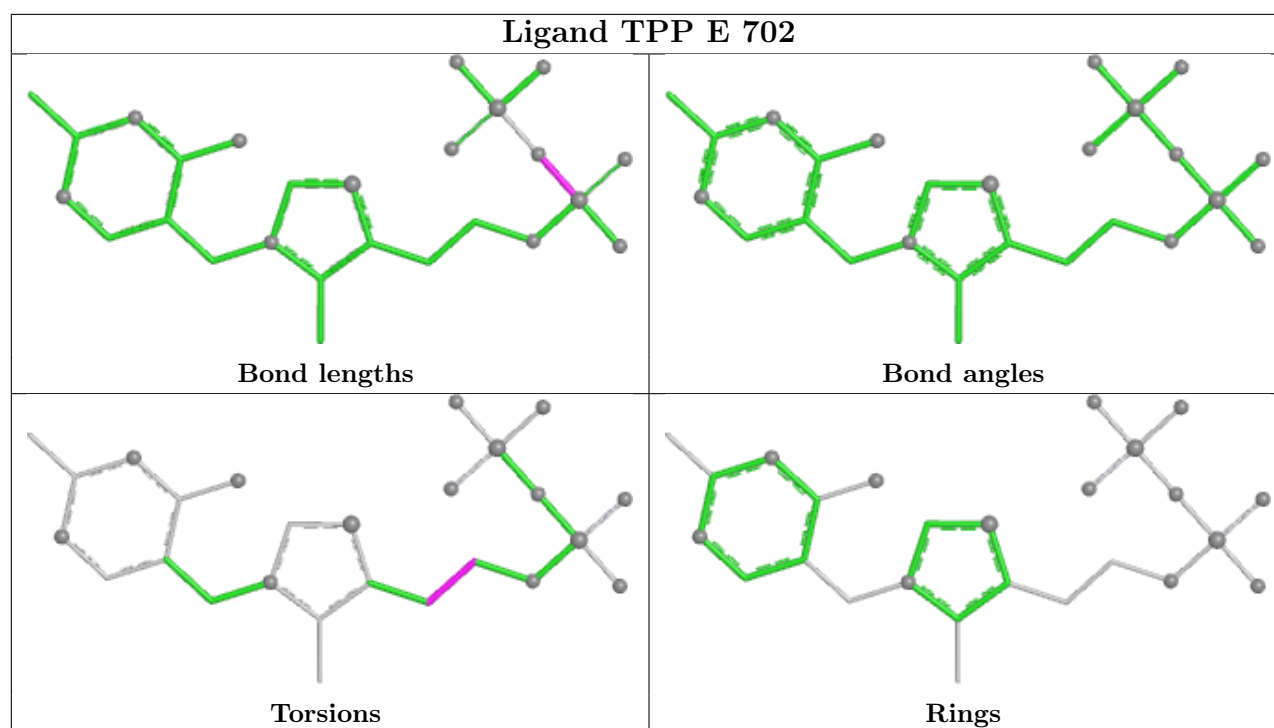
Bond angles

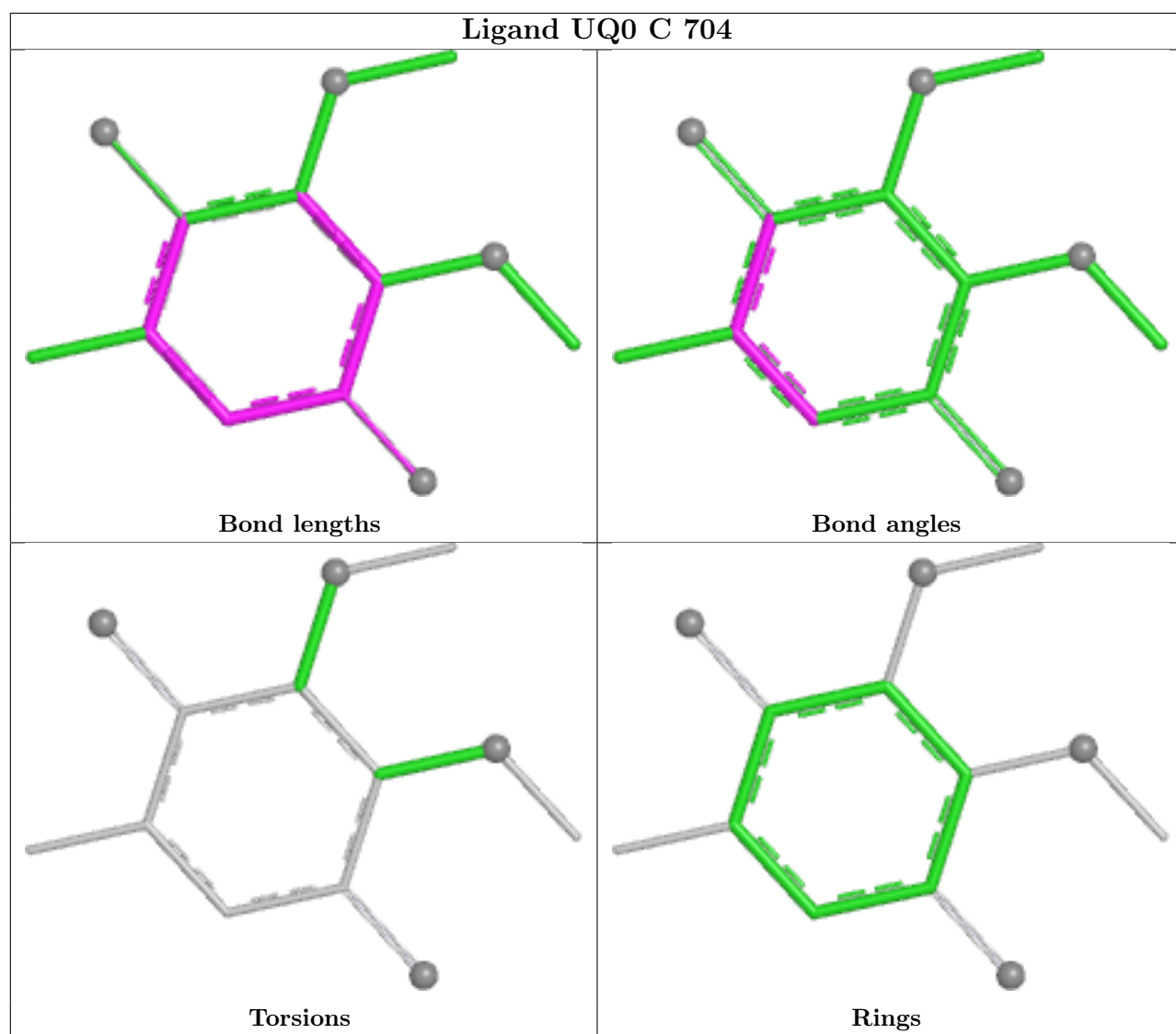


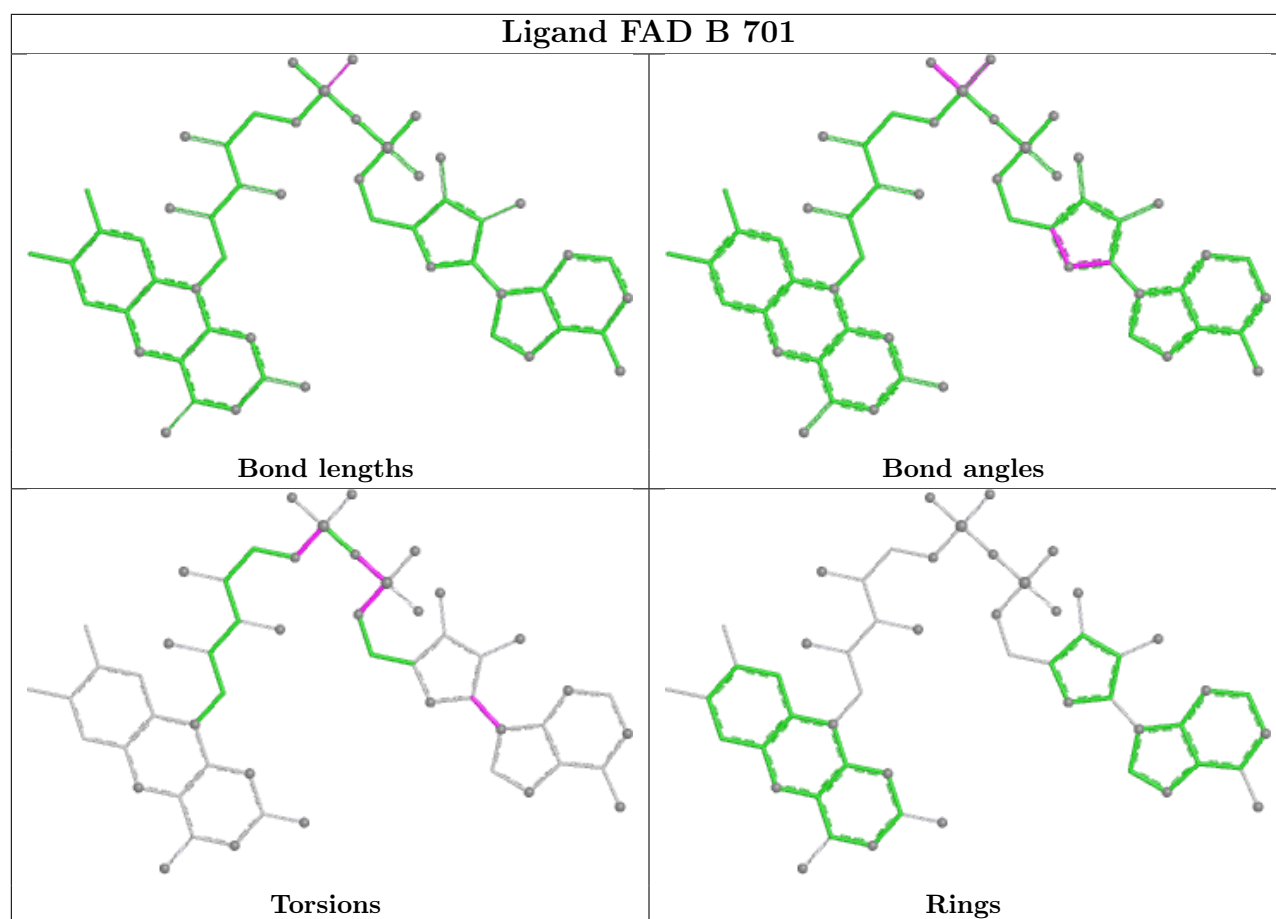
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.52	2 (0%) 90 91	17, 21, 34, 54	0
1	B	594/594 (100%)	-0.37	7 (1%) 76 79	17, 23, 38, 62	0
1	C	593/594 (99%)	-0.32	4 (0%) 84 85	20, 28, 42, 66	0
1	D	594/594 (100%)	-0.29	3 (0%) 87 89	20, 29, 45, 72	0
1	E	593/594 (99%)	-0.21	3 (0%) 87 89	21, 30, 46, 66	0
1	F	594/594 (100%)	-0.09	14 (2%) 59 63	21, 31, 50, 74	0
All	All	3562/3564 (99%)	-0.30	33 (0%) 81 83	17, 27, 44, 74	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	593	GLU	4.1
1	F	504	VAL	3.5
1	F	485	ALA	3.1
1	E	488	LEU	3.1
1	A	593	GLU	3.1
1	E	1	MET	3.1
1	F	593	GLU	3.0
1	B	504	VAL	2.9
1	D	0	GLY	2.8
1	F	474	ALA	2.8
1	F	478	LEU	2.8
1	D	593	GLU	2.7
1	F	1	MET	2.7
1	F	488	LEU	2.6
1	C	111	LYS	2.6
1	C	593	GLU	2.6
1	B	491	CYS	2.5
1	F	491	CYS	2.4
1	F	482	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	0	GLY	2.4
1	B	0	GLY	2.3
1	D	488	LEU	2.3
1	A	488	LEU	2.3
1	C	571	MET	2.3
1	F	475	TYR	2.3
1	B	338	LYS	2.2
1	B	82	ASP	2.2
1	C	110	HIS	2.1
1	B	474	ALA	2.1
1	F	347	GLU	2.1
1	F	337	GLN	2.1
1	E	593	GLU	2.0
1	F	569	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	D	706	13/13	0.42	0.33	78,86,103,106	0
5	UQ0	C	705	13/13	0.46	0.36	93,104,121,123	0
5	UQ0	C	706	13/13	0.51	0.32	73,78,92,94	0
5	UQ0	A	706	13/13	0.56	0.27	64,69,77,84	0
5	UQ0	D	707	13/13	0.58	0.31	91,97,106,112	0
5	UQ0	B	706	13/13	0.64	0.27	77,82,96,97	0
5	UQ0	E	705	13/13	0.78	0.20	72,79,82,84	0
5	UQ0	C	704	13/13	0.80	0.16	58,62,65,65	0
5	UQ0	A	705	13/13	0.80	0.16	46,54,58,60	0

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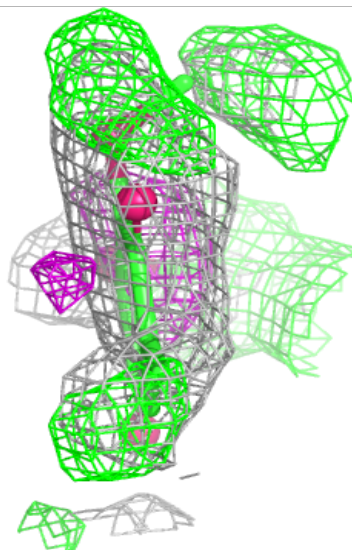
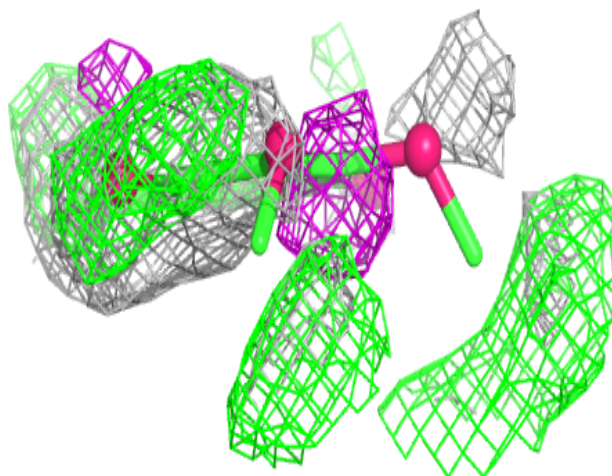
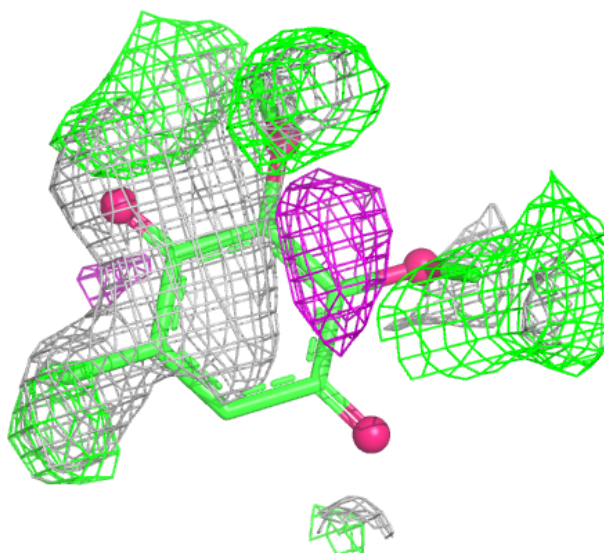
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	UQ0	D	705	13/13	0.87	0.13	43,47,55,57	0
5	UQ0	B	705	13/13	0.90	0.11	36,41,47,51	0
3	TPP	F	702	26/26	0.91	0.10	26,36,41,43	0
5	UQ0	F	704	13/13	0.91	0.14	46,55,65,67	0
3	TPP	B	702	26/26	0.92	0.10	21,26,30,33	0
3	TPP	E	702	26/26	0.95	0.08	27,31,36,38	0
3	TPP	D	702	26/26	0.96	0.08	24,30,33,35	0
2	FAD	C	701	53/53	0.97	0.06	21,24,26,27	0
2	FAD	D	701	53/53	0.97	0.05	22,24,27,28	0
2	FAD	E	701	53/53	0.97	0.06	23,26,31,32	0
2	FAD	F	701	53/53	0.97	0.06	19,25,30,32	0
2	FAD	A	701	53/53	0.97	0.06	19,19,21,24	0
4	MG	D	704	1/1	0.98	0.12	30,30,30,30	0
4	MG	E	704	1/1	0.98	0.11	29,29,29,29	0
3	TPP	A	702	26/26	0.98	0.05	18,20,23,25	0
2	FAD	B	701	53/53	0.98	0.05	16,18,22,23	0
3	TPP	C	702	26/26	0.98	0.05	21,26,29,31	0
4	MG	A	704	1/1	0.98	0.02	17,17,17,17	1
4	MG	D	703	1/1	0.98	0.08	28,28,28,28	0
4	MG	C	703	1/1	0.99	0.04	21,21,21,21	0
4	MG	A	703	1/1	0.99	0.07	19,19,19,19	0
4	MG	B	703	1/1	0.99	0.03	23,23,23,23	0
4	MG	E	703	1/1	0.99	0.02	26,26,26,26	0
4	MG	B	704	1/1	0.99	0.07	18,18,18,18	1
4	MG	F	703	1/1	0.99	0.04	33,33,33,33	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.

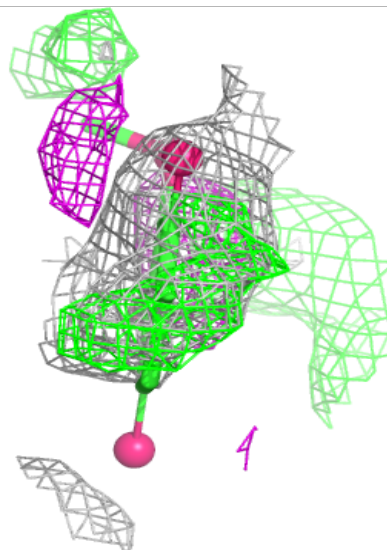
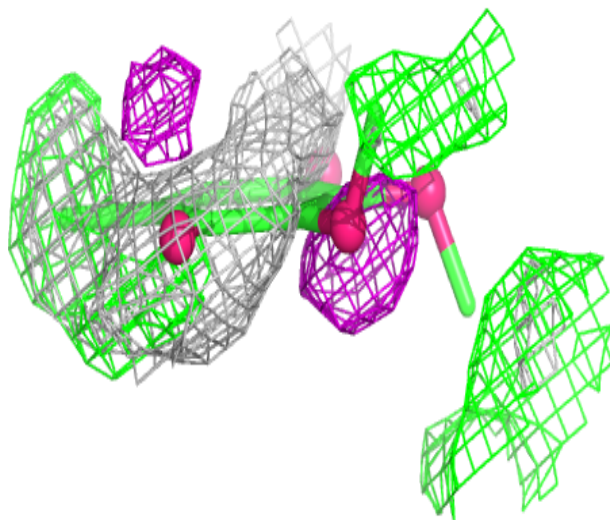
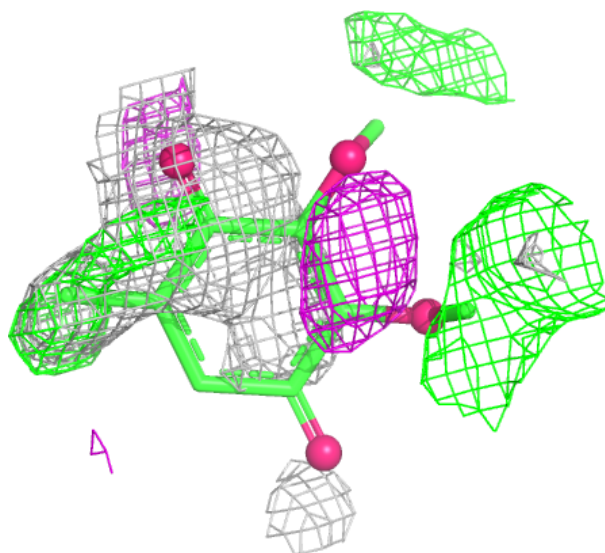
Electron density around UQ0 D 706:

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



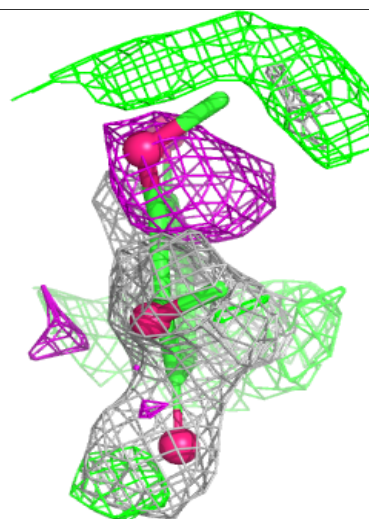
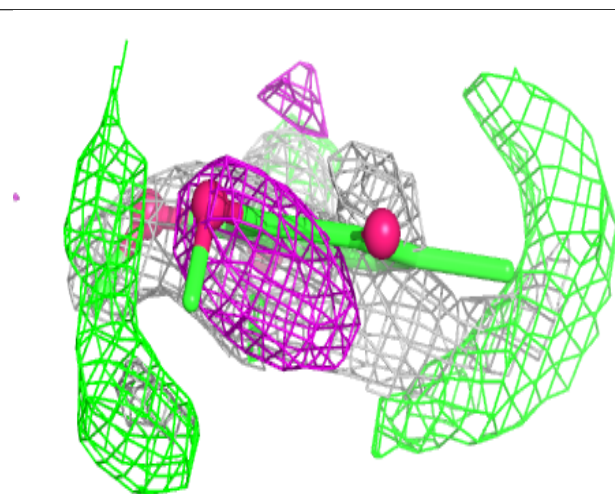
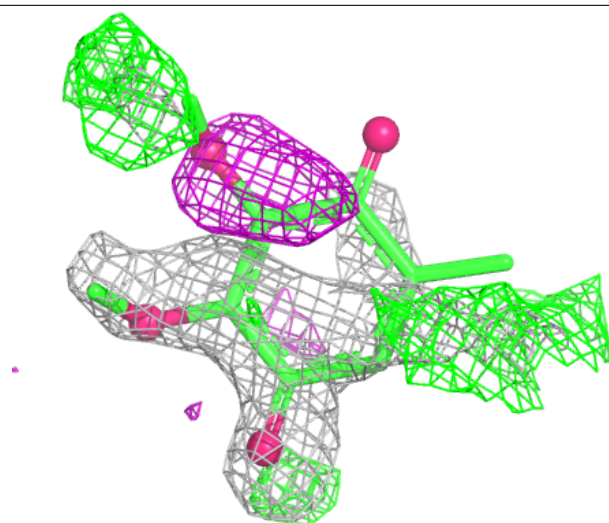
Electron density around UQ0 C 705:

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and green (positive)



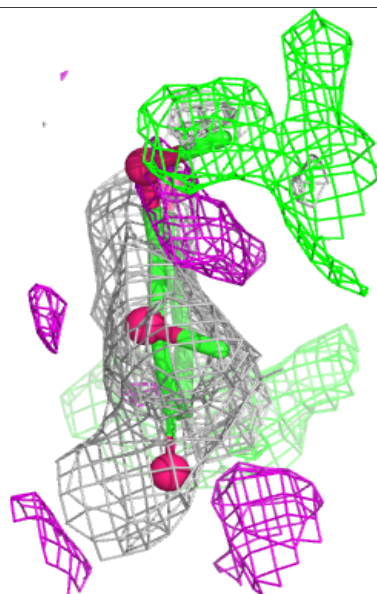
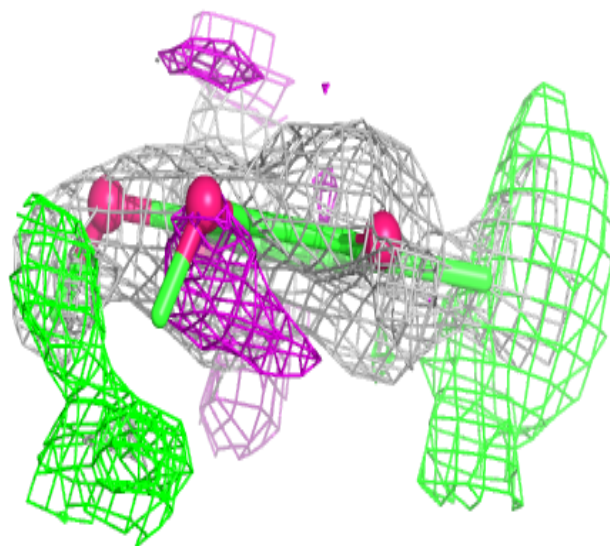
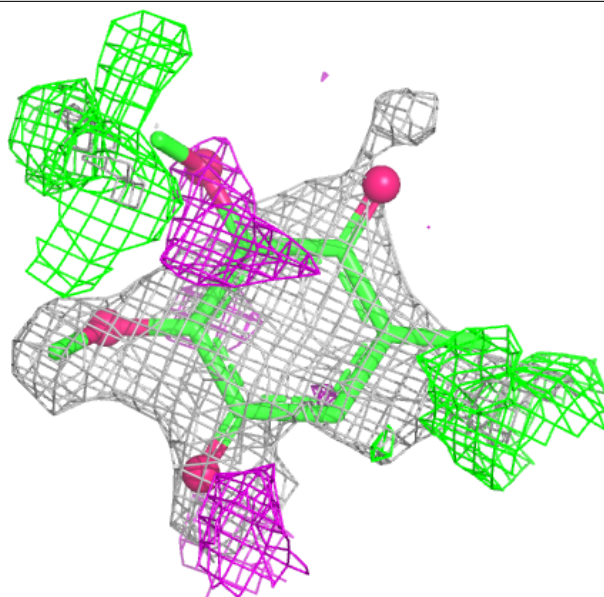
Electron density around UQ0 C 706:

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and green (positive)



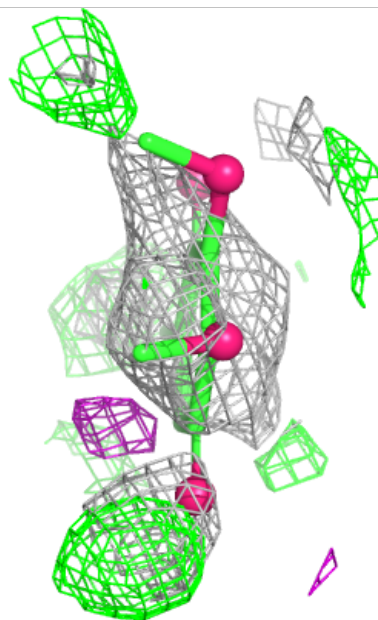
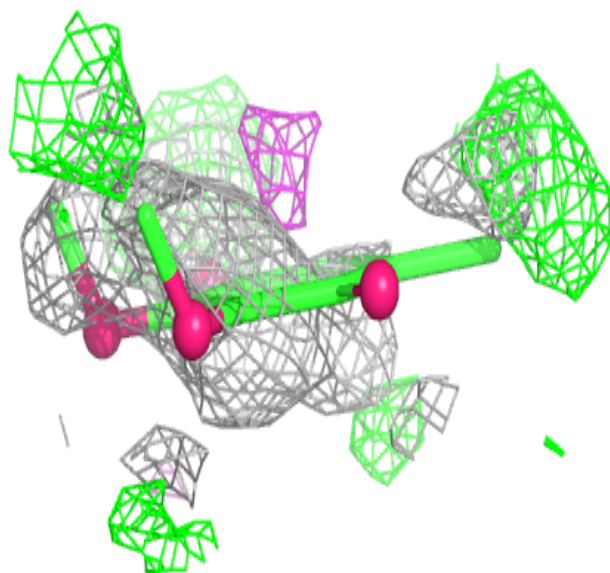
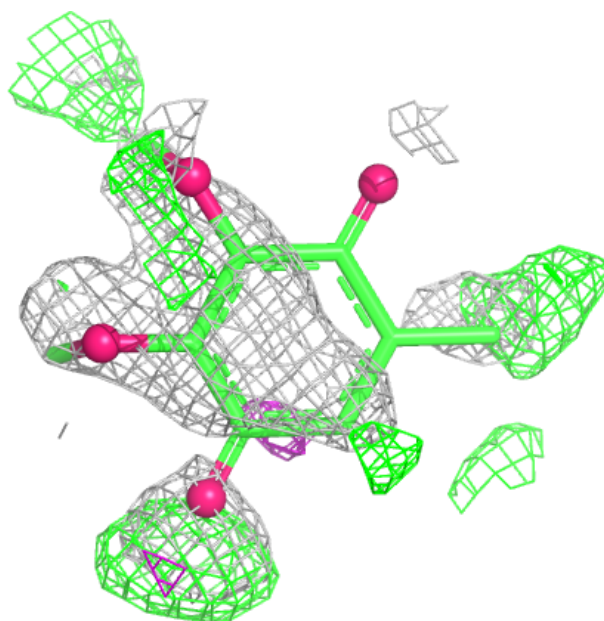
Electron density around UQ0 A 706:

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and green (positive)



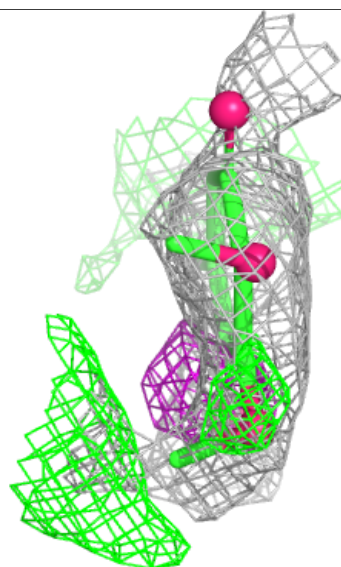
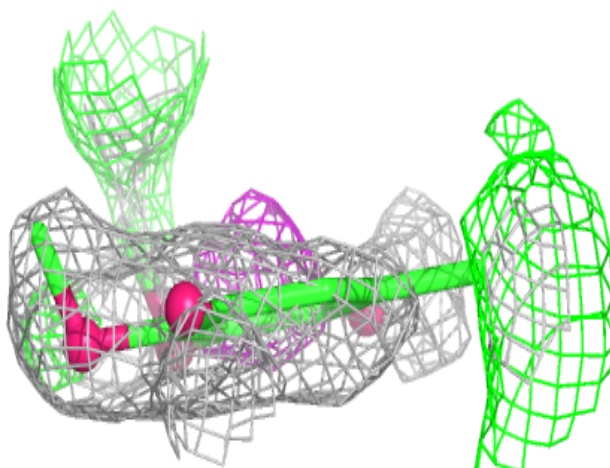
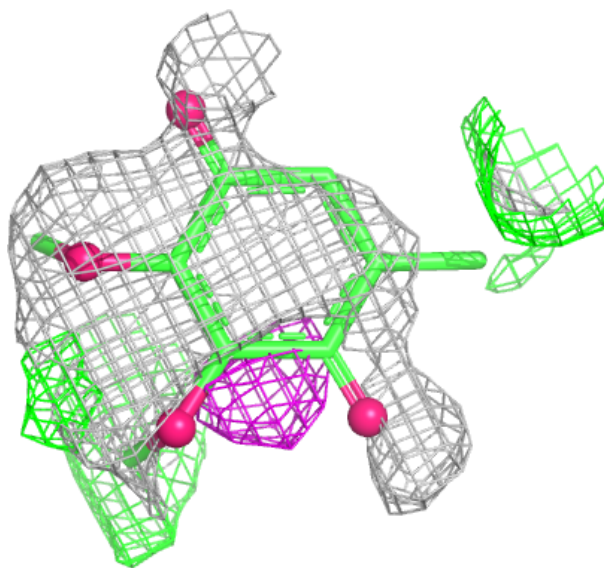
Electron density around UQ0 D 707:

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and green (positive)



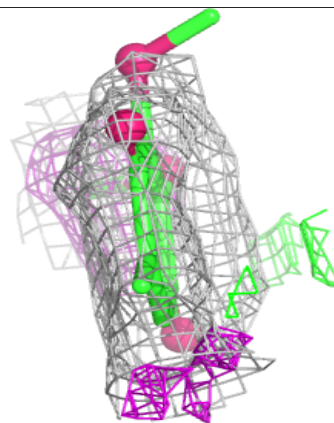
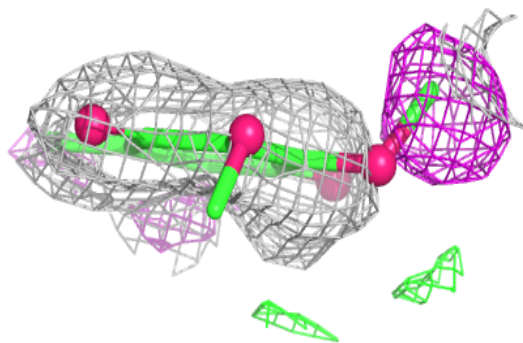
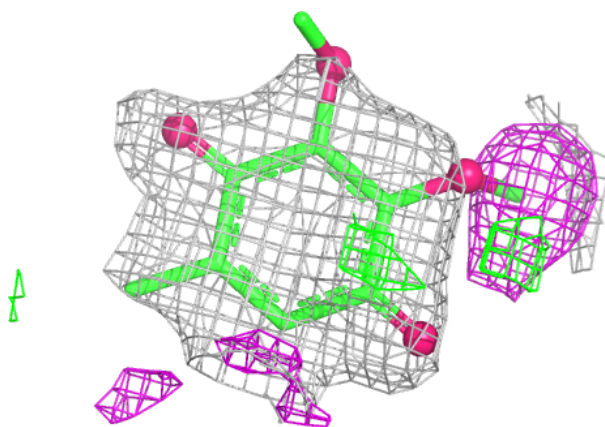
Electron density around UQ0 B 706:

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and green (positive)



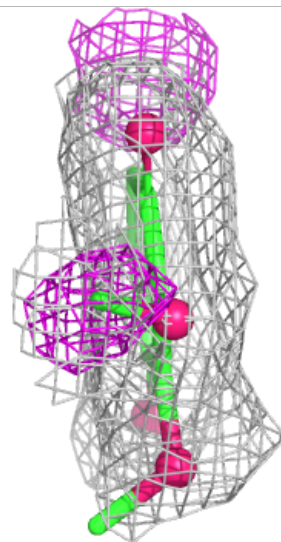
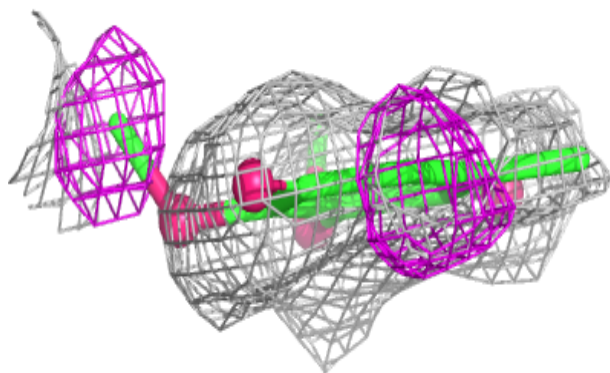
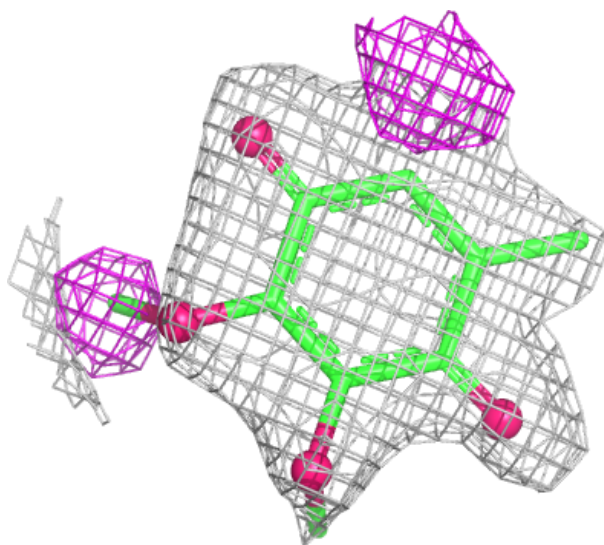
Electron density around UQ0 E 705:

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and green (positive)



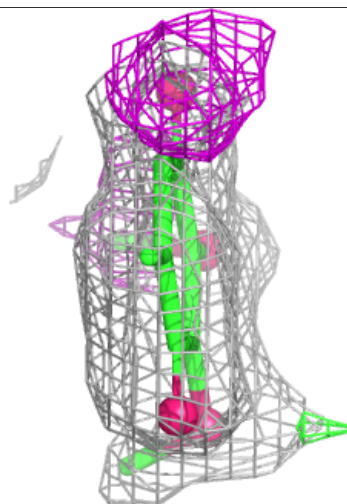
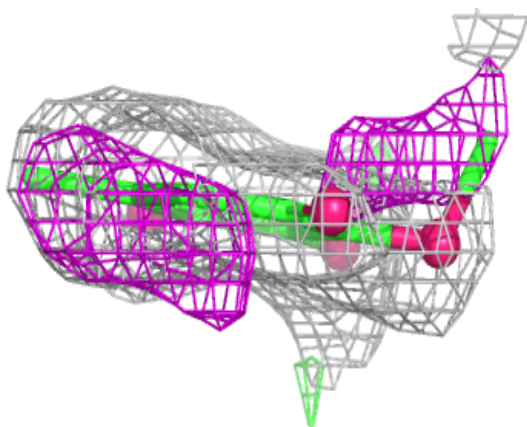
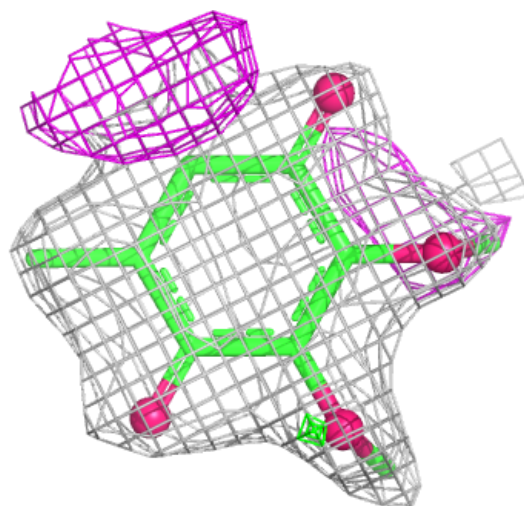
Electron density around UQ0 C 704:

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and green (positive)



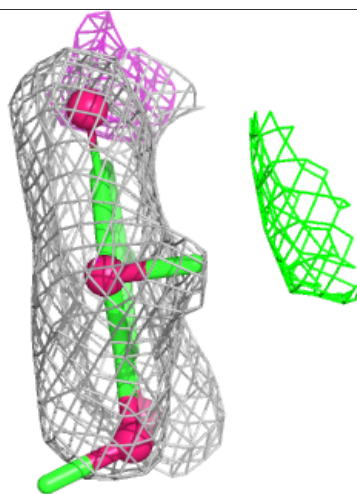
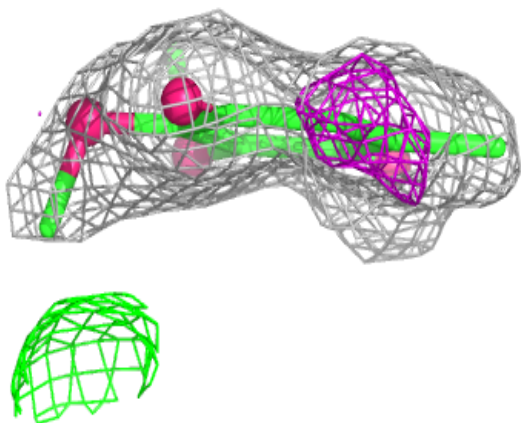
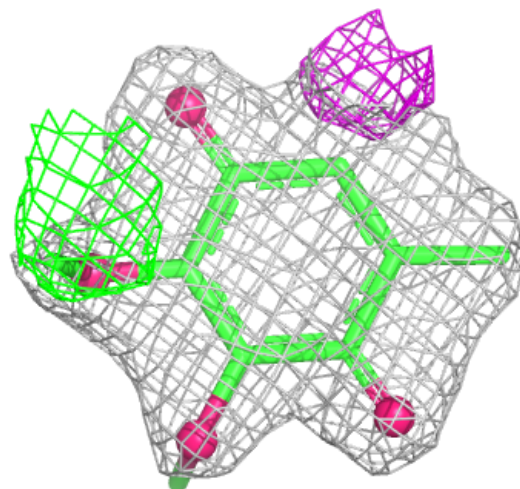
Electron density around UQ0 A 705:

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and green (positive)



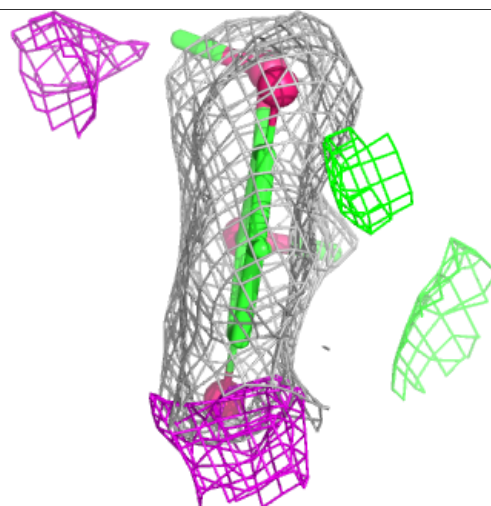
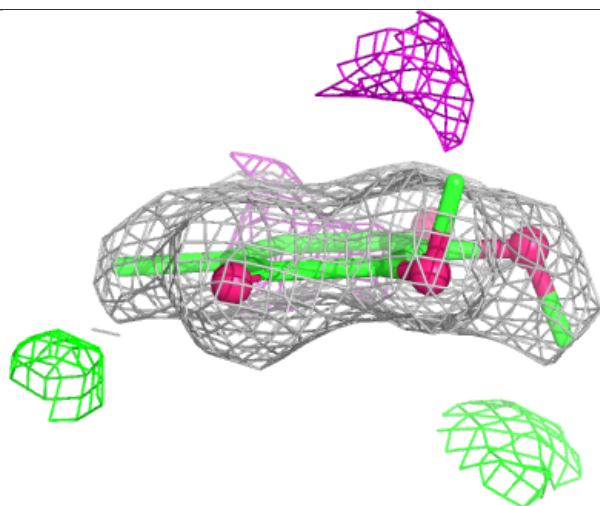
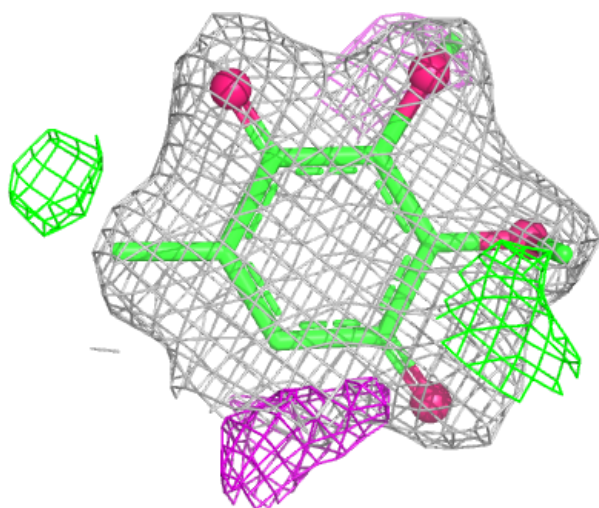
Electron density around UQ0 D 705:

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and green (positive)



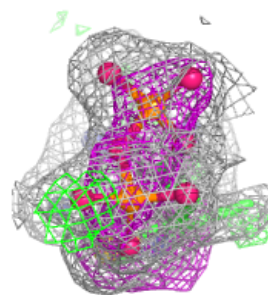
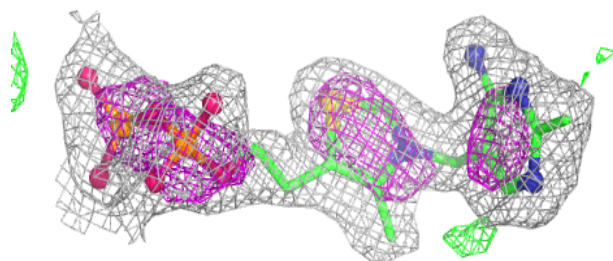
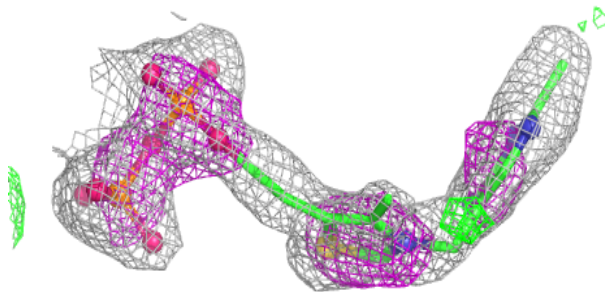
Electron density around UQ0 B 705:

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



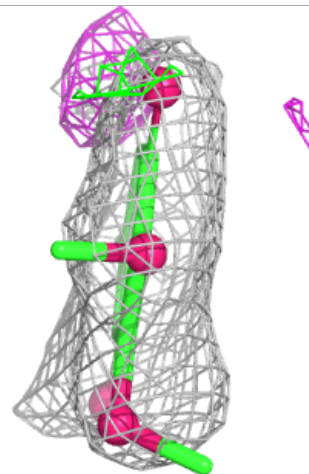
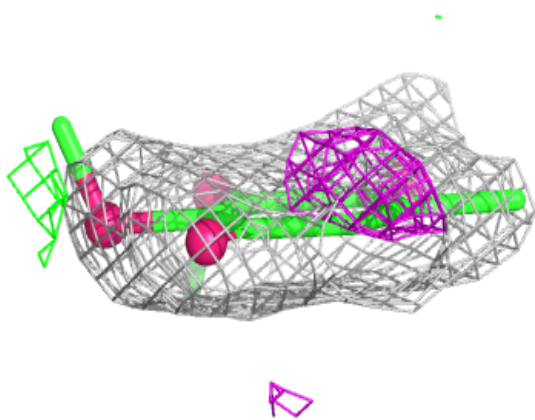
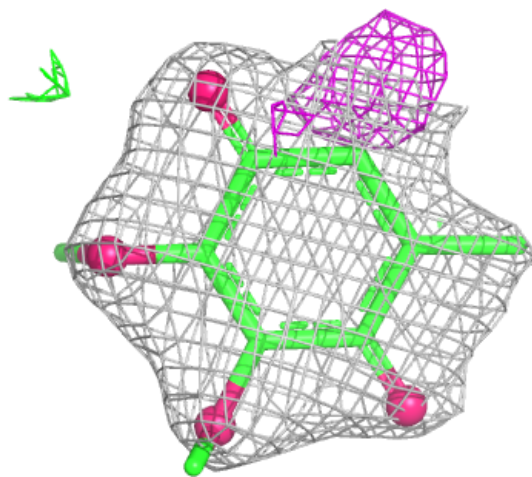
Electron density around TPP F 702:

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



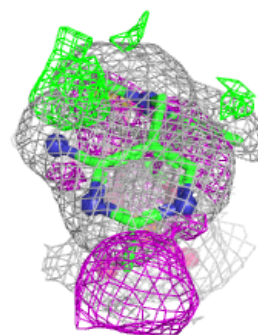
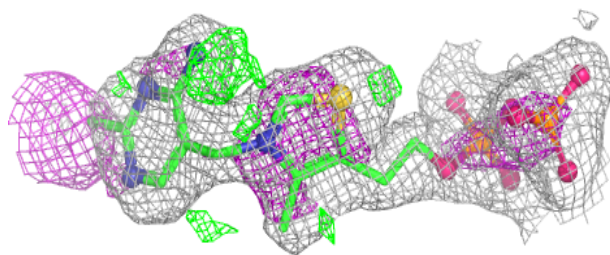
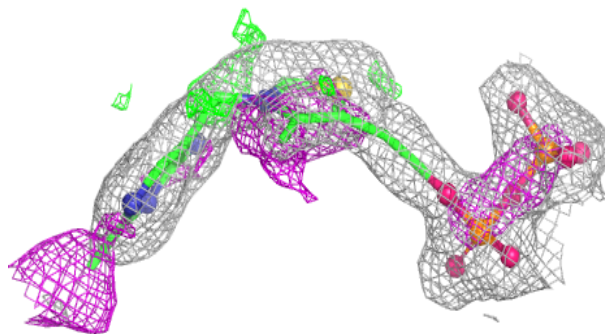
Electron density around UQ0 F 704:

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

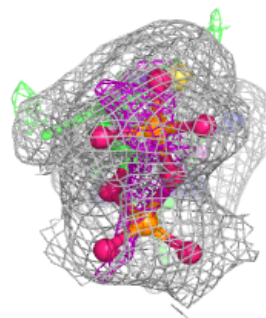
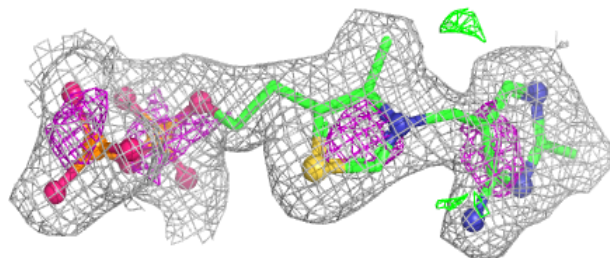
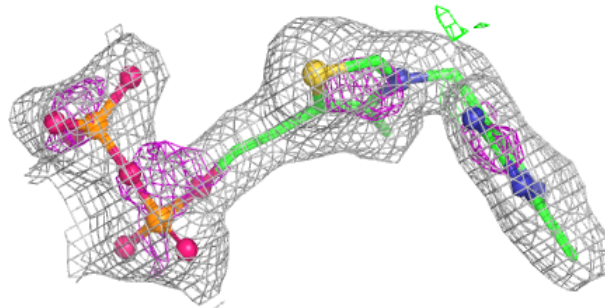


Electron density around TPP B 702:

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

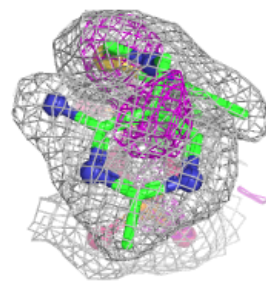
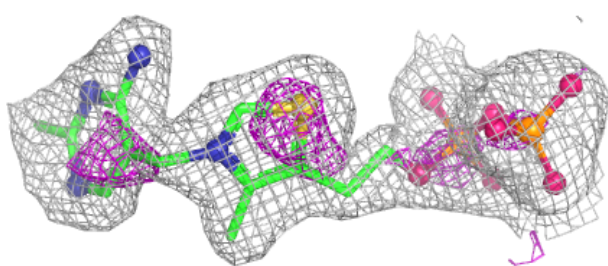
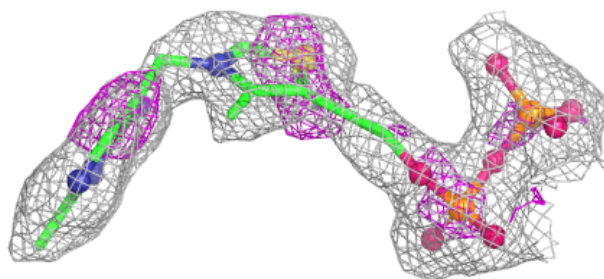
**Electron density around TPP E 702:**

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

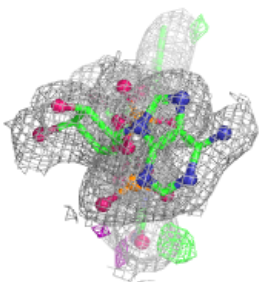
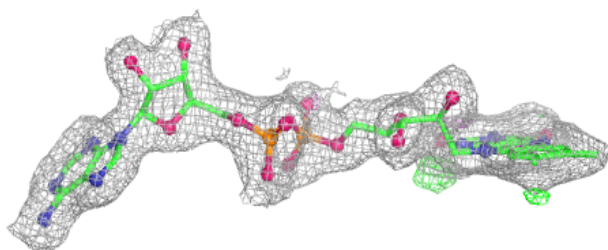
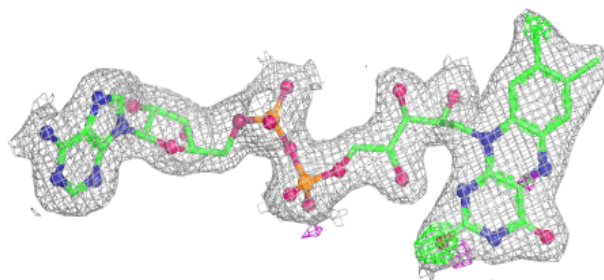


Electron density around TPP D 702:

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

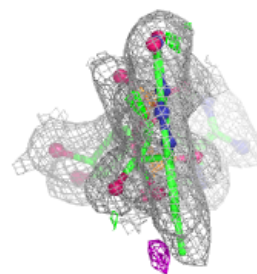
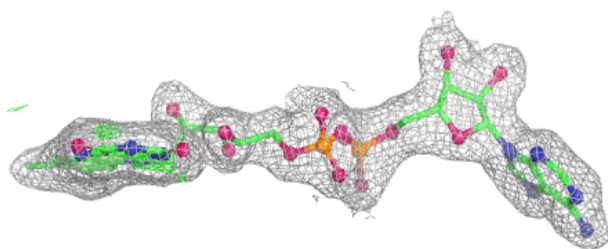
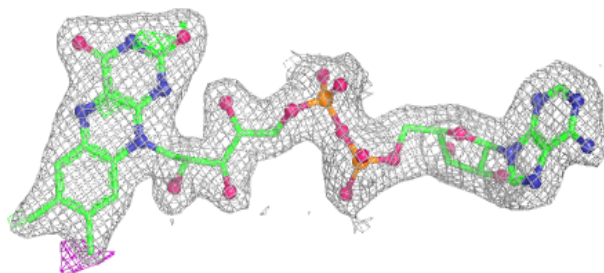
**Electron density around FAD C 701:**

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

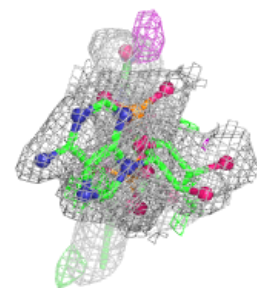
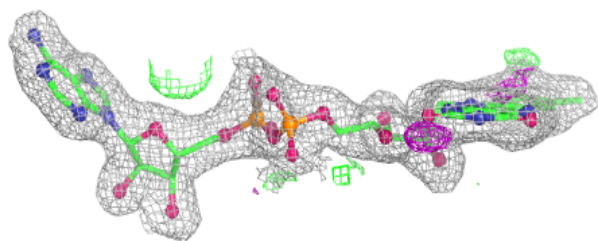
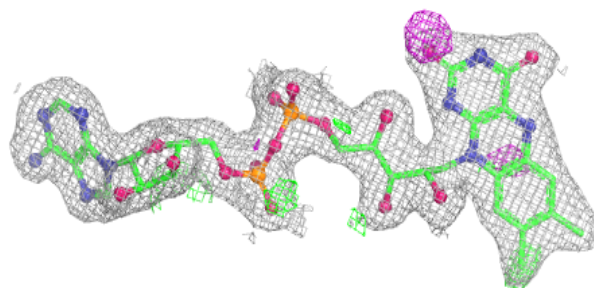


Electron density around FAD D 701:

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

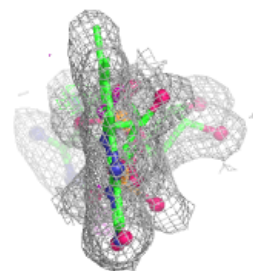
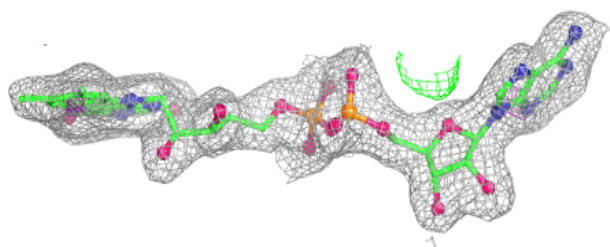
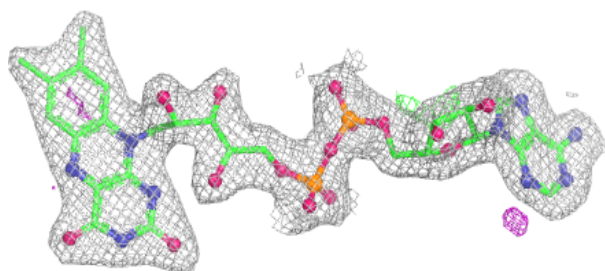
**Electron density around FAD E 701:**

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

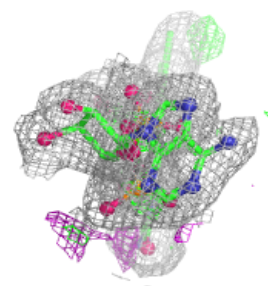
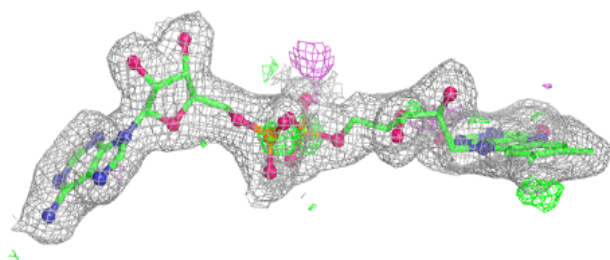
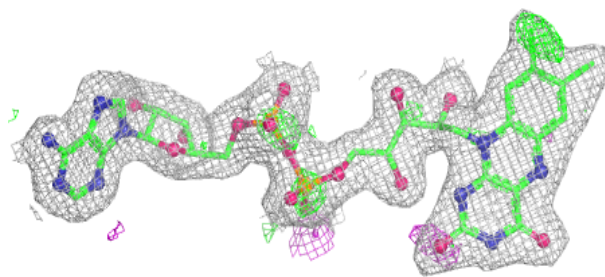


Electron density around FAD F 701:

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

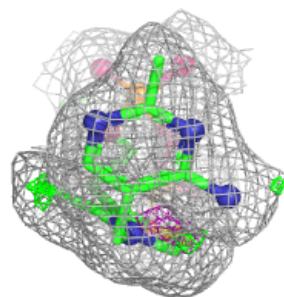
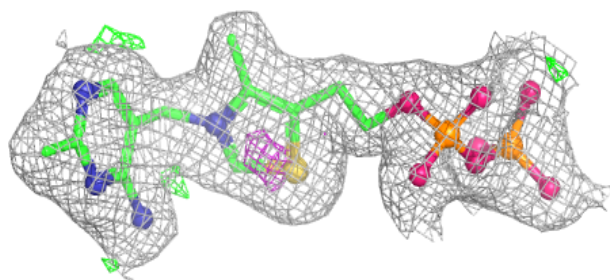
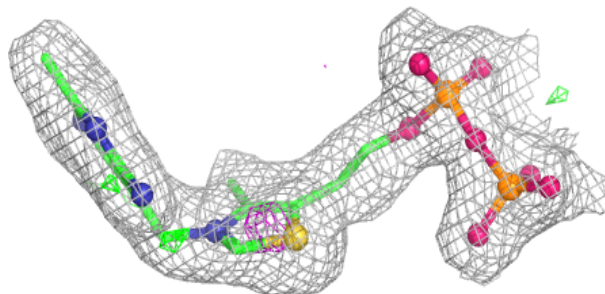
**Electron density around FAD A 701:**

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

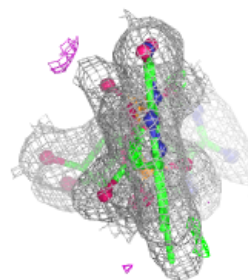
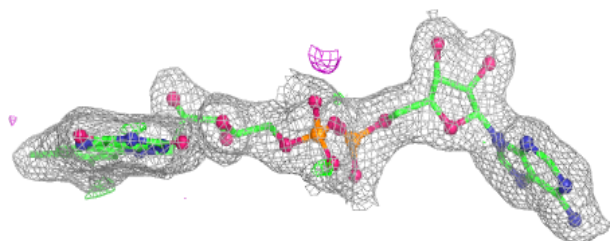
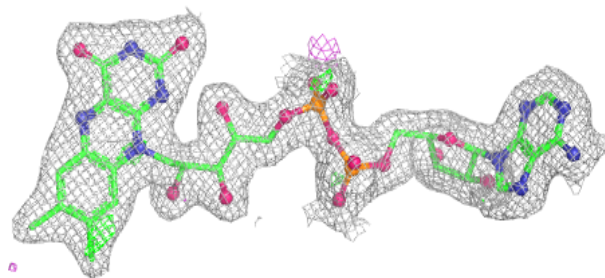


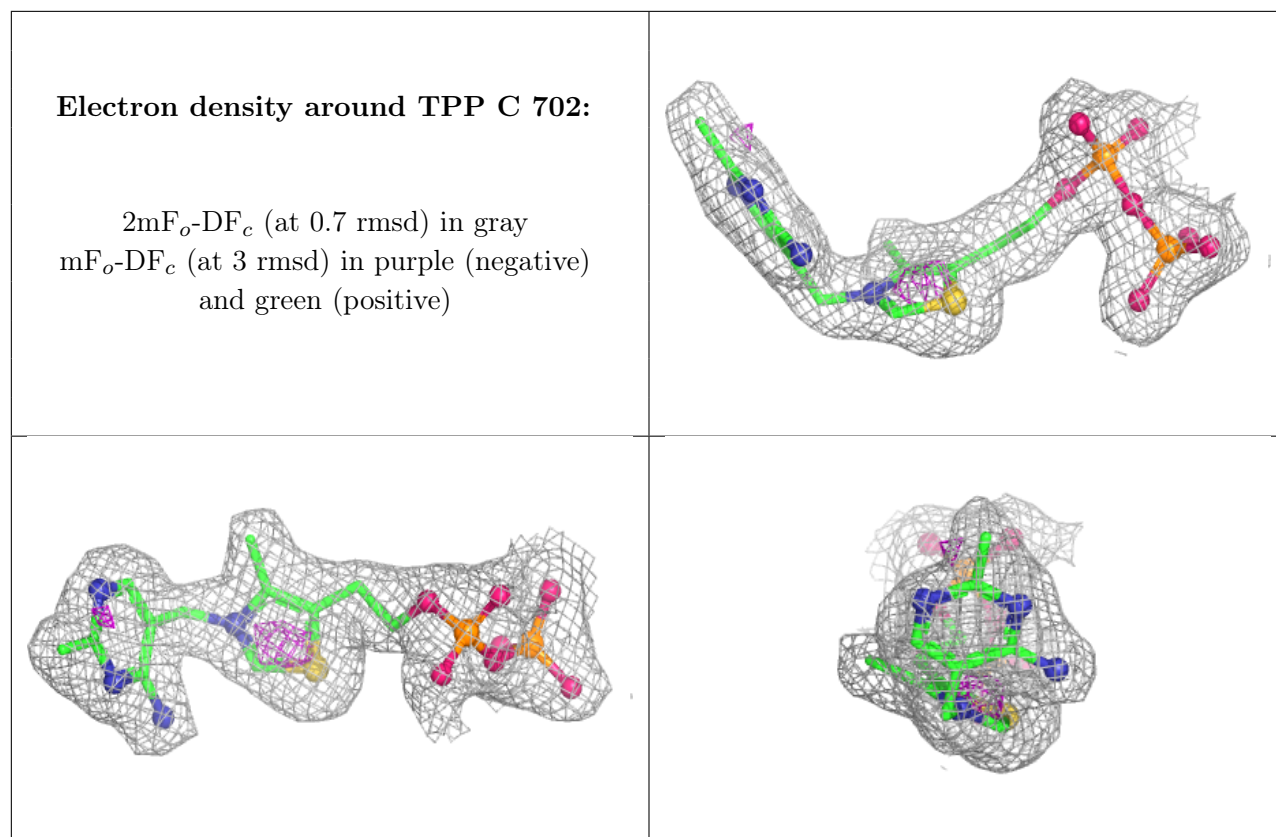
Electron density around TPP A 702:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.