



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:24 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 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:

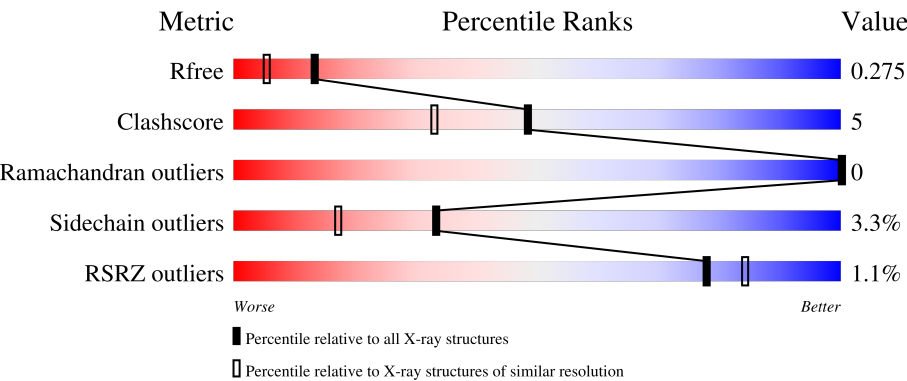
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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%.

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Mol	Chain	Length	Quality of chain
1	F	594	2% 88% 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:

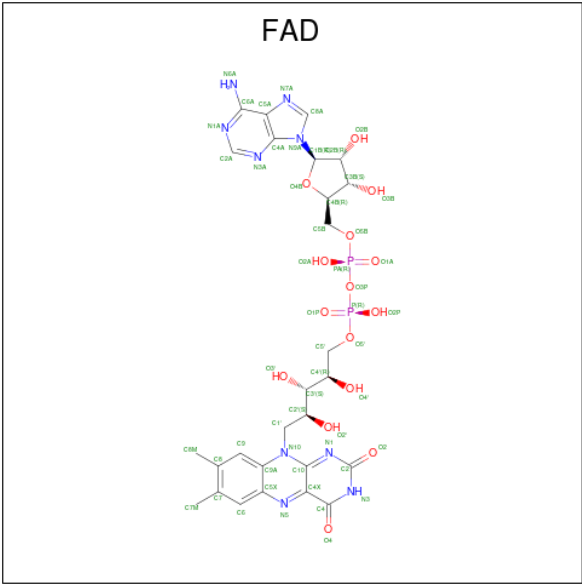
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P0AEP7
A	283	GLN	ASN	engineered mutation	UNP P0AEP7
A	478	MET	LEU	engineered mutation	UNP P0AEP7
A	484	MET	ARG	engineered mutation	UNP P0AEP7
A	488	LEU	MET	engineered mutation	UNP P0AEP7
B	0	GLY	-	expression tag	UNP P0AEP7
B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

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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

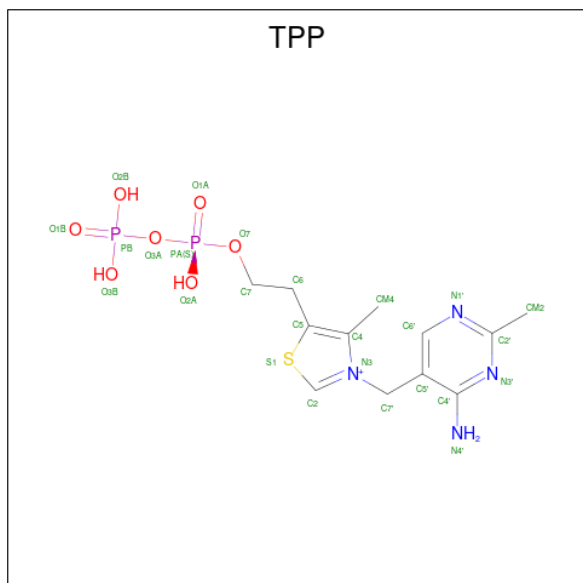
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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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).

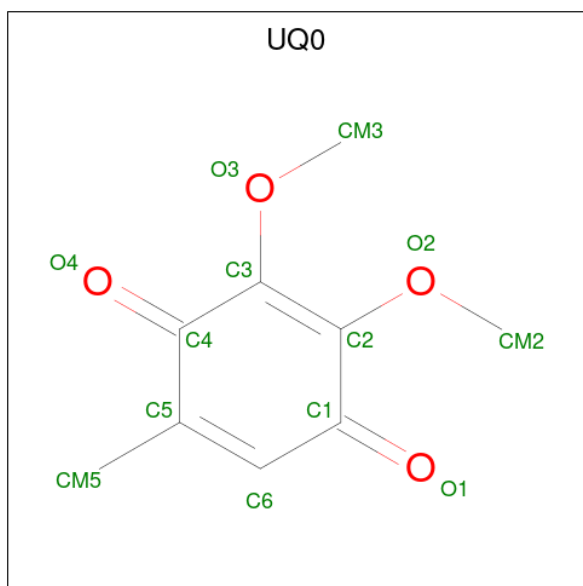


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- 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 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- 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 13 9 4	0	0
5	A	1	Total C O 13 9 4	0	0
5	B	1	Total C O 13 9 4	0	0
5	B	1	Total C O 13 9 4	0	0
5	C	1	Total C O 13 9 4	0	0

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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

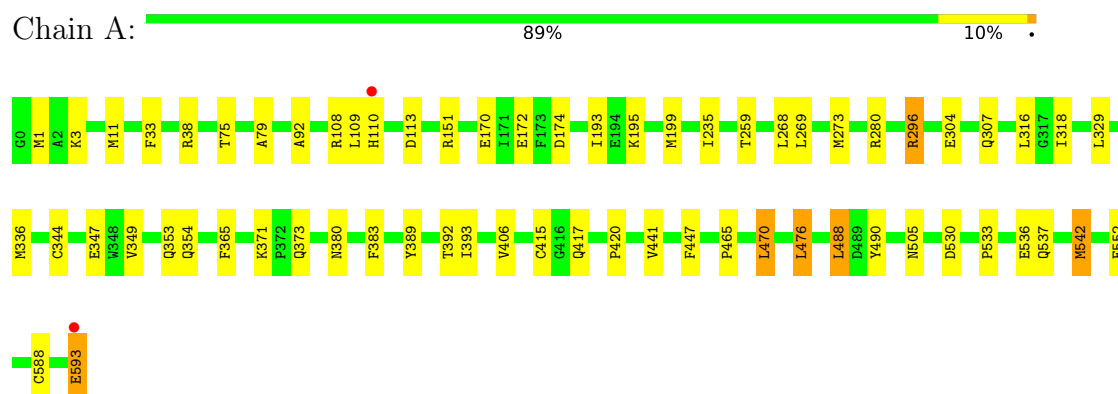
- Molecule 6 is water.

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

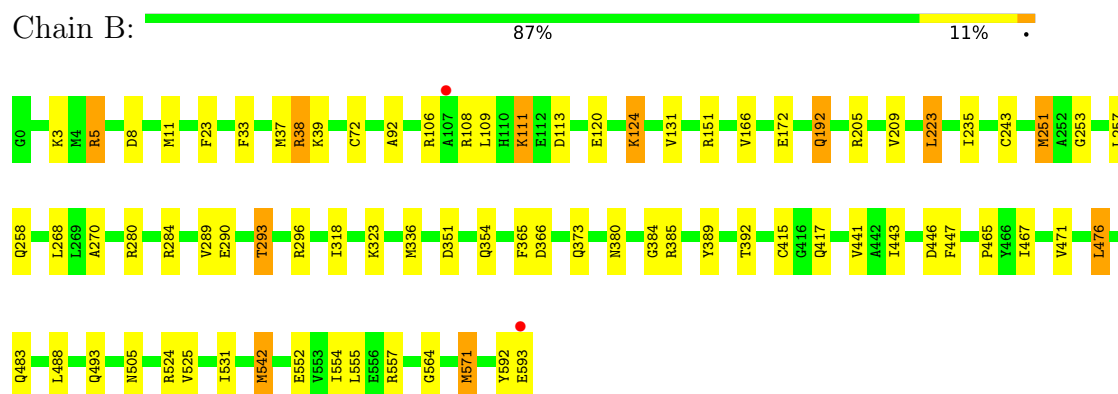
3 Residue-property plots

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.

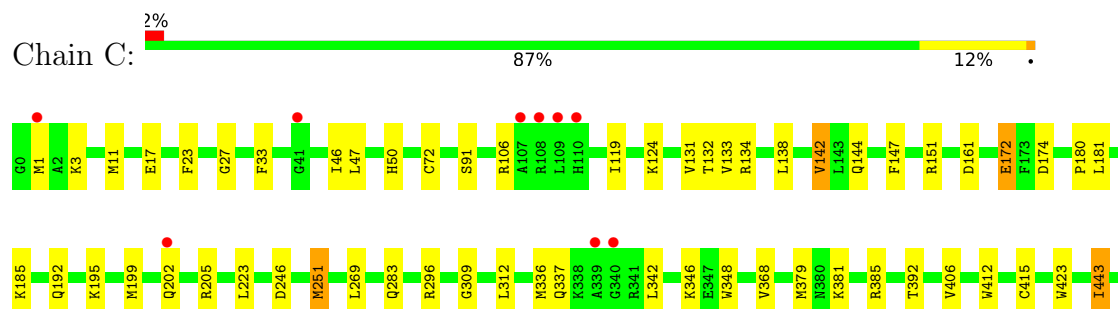
• Molecule 1: Glyoxylate carboligase



• Molecule 1: Glyoxylate carboligase

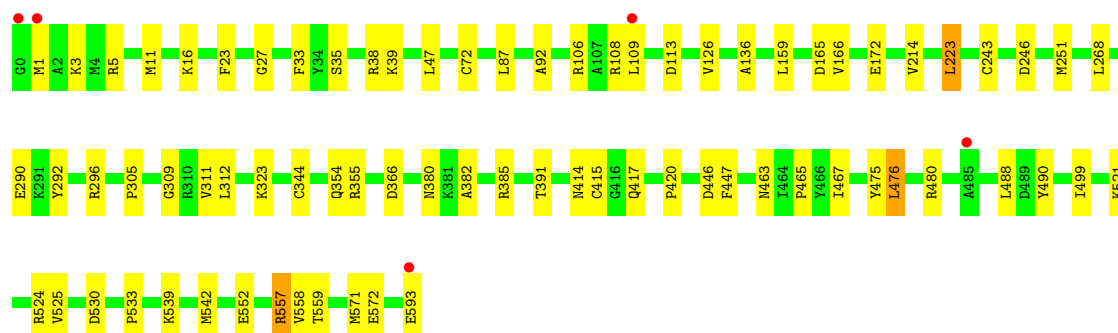
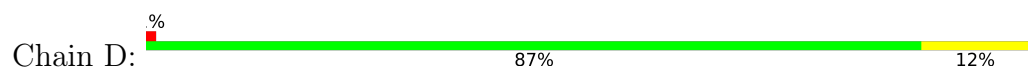


• Molecule 1: Glyoxylate carboligase

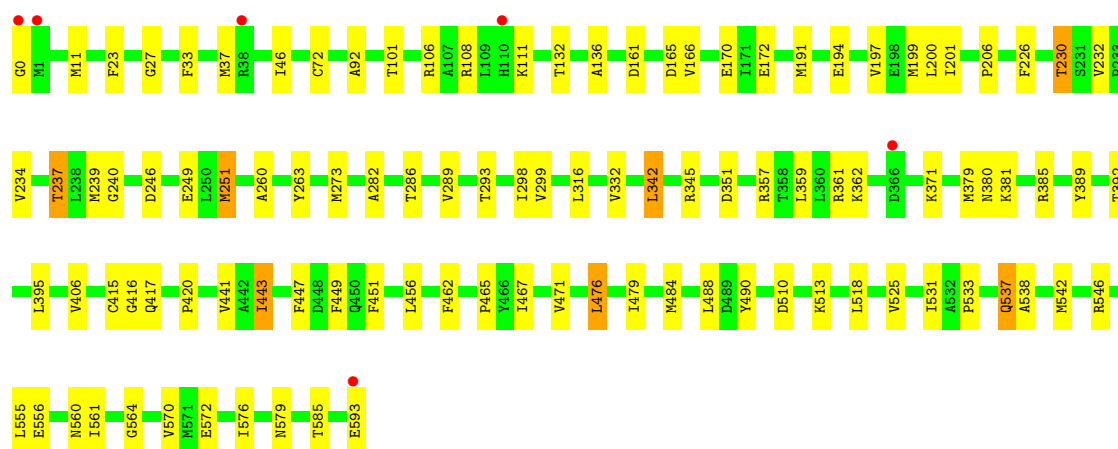
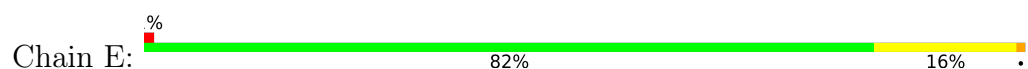




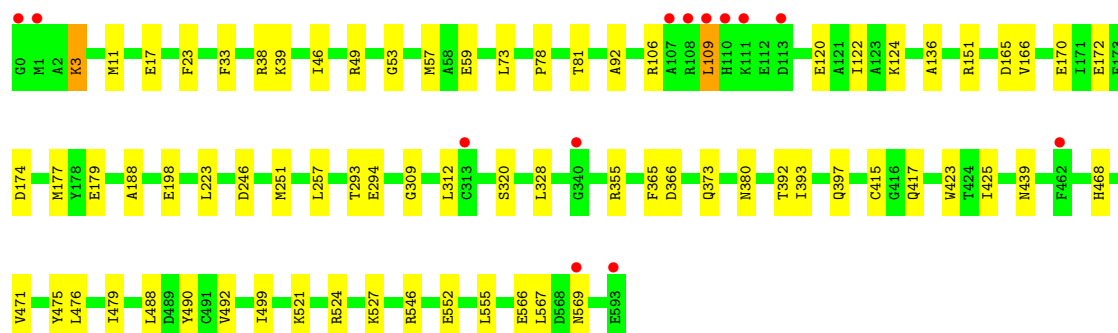
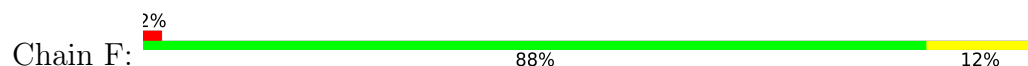
• Molecule 1: Glyoxylate carboligase



• 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)	Xtrriage
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	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.

All (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
1	A	280	ARG	C-N-CA	-6.50	112.72	123.37
1	A	280	ARG	N-CA-C	-5.62	101.08	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	542	MET	CG-SD-CE	-5.14	89.60	100.90

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:D:385:ARG:H	1:D:593:GLU:HG3	1.46	0.81
1:D:292:TYR:O	1:D:296:ARG:NH1	2.14	0.80
1:F:546:ARG:NH2	6:F:702:HOH:O	2.15	0.80
1:E:200:LEU:HA	1:E:273:MET:HE1	1.64	0.77
1:E:361:ARG:HD3	1:E:572:GLU:OE2	1.84	0.76
1:A:380:ASN:O	6:A:802:HOH:O	2.05	0.74
1:E:237:THR:HG21	2:E:602:FAD:O2P	1.88	0.73
1:C:17:GLU:HG2	1:C:147:PHE:CG	2.25	0.72
1:B:557:ARG:NH2	6:B:805:HOH:O	2.24	0.70
1:B:384:GLY:HA2	1:B:593:GLU:HG2	1.74	0.70
1:F:488:LEU:HD22	1:F:490:TYR:HB2	1.73	0.70
1:D:106:ARG:HD3	1:D:165:ASP:OD2	1.92	0.69
1:B:323:LYS:NZ	6:B:808:HOH:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:MET:HE1	1:E:560:ASN:HD21	1.57	0.69
1:D:344:CYS:SG	6:D:1186:HOH:O	2.50	0.69
1:B:505:ASN:ND2	6:B:807:HOH:O	2.26	0.68
1:B:205:ARG:NH1	1:B:270:ALA:O	2.27	0.68
1:F:366:ASP:OD1	6:F:701:HOH:O	2.12	0.68
1:D:344:CYS:SG	6:D:1142:HOH:O	2.50	0.68
1:E:237:THR:HG22	1:E:240:GLY:N	2.07	0.67
1:F:566:GLU:HB2	1:F:569:ASN:HB2	1.77	0.67
1:C:47:LEU:HB2	5:E:601:UQO:CM5	2.24	0.67
1:B:465:PRO:HB2	1:B:542:MET:HG3	1.76	0.67
1:F:521:LYS:NZ	6:F:706:HOH:O	2.27	0.67
1:B:106:ARG:HD2	1:B:166:VAL:HG23	1.76	0.66
1:F:17:GLU:OE1	1:F:151:ARG:NH2	2.28	0.66
1:B:5:ARG:HD3	1:B:8:ASP:OD2	1.95	0.66
1:B:192:GLN:HG2	1:B:318:ILE:HG12	1.77	0.66
1:F:471:VAL:HB	1:F:555:LEU:HD11	1.77	0.65
1:C:592:TYR:O	1:C:593:GLU:HB2	1.97	0.64
1:E:200:LEU:HD11	1:E:232:VAL:HG21	1.79	0.64
1:E:471:VAL:HB	1:E:555:LEU:HD11	1.80	0.64
1:B:524:ARG:HD3	1:B:552:GLU:OE1	1.98	0.64
1:D:27:GLY:HA2	1:F:479:ILE:HD12	1.81	0.63
1:F:380:ASN:O	6:F:704:HOH:O	2.16	0.63
1:A:269:LEU:O	1:A:296:ARG:NH2	2.32	0.63
1:E:246:ASP:HA	1:E:251:MET:HG2	1.80	0.63
1:A:193:ILE:HG23	1:A:329:LEU:HD23	1.80	0.63
1:F:294:GLU:OE1	6:F:703:HOH:O	2.15	0.62
1:A:470:LEU:HD13	1:A:552:GLU:HG3	1.81	0.62
1:A:199:MET:HE1	1:A:316:LEU:HD22	1.82	0.61
1:A:347:GLU:OE1	6:A:804:HOH:O	2.16	0.60
1:B:3:LYS:NZ	6:B:809:HOH:O	2.30	0.60
1:C:17:GLU:OE2	1:C:180:PRO:HB3	2.02	0.60
1:E:206:PRO:HG2	1:E:232:VAL:HG22	1.83	0.60
1:D:465:PRO:HB2	1:D:542:MET:HG3	1.83	0.60
1:A:108:ARG:NH2	6:A:813:HOH:O	2.35	0.59
1:F:198:GLU:OE2	6:F:705:HOH:O	2.17	0.59
1:B:251:MET:HE3	1:B:253:GLY:H	1.68	0.59
1:F:355:ARG:NH2	6:F:713:HOH:O	2.35	0.59
1:E:380:ASN:ND2	6:E:709:HOH:O	2.34	0.59
1:C:479:ILE:HD12	1:E:27:GLY:HA2	1.85	0.58
1:B:11:MET:HE1	1:B:33:PHE:CZ	2.38	0.58
1:B:289:VAL:O	1:B:293:THR:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:ILE:HG13	1:D:542:MET:HE1	1.86	0.57
1:F:136:ALA:HA	1:F:166:VAL:HG13	1.87	0.57
1:E:385:ARG:H	1:E:593:GLU:HB2	1.68	0.57
1:F:151:ARG:HD3	6:F:881:HOH:O	2.04	0.57
1:D:11:MET:HE1	1:D:33:PHE:CZ	2.39	0.57
1:B:471:VAL:HB	1:B:555:LEU:HD11	1.86	0.57
1:E:197:VAL:HG11	1:E:332:VAL:HG11	1.87	0.57
1:E:510:ASP:OD2	1:E:513:LYS:HE3	2.05	0.57
1:A:195:LYS:HE3	1:A:199:MET:HE2	1.87	0.56
1:A:533:PRO:O	1:A:537:GLN:HG3	2.05	0.56
1:F:393:ILE:HA	1:F:397:GLN:HG2	1.86	0.56
1:F:92:ALA:HB1	1:F:417:GLN:HG2	1.85	0.56
1:F:120:GLU:HG2	1:F:124:LYS:HE3	1.88	0.56
1:C:27:GLY:HA2	1:E:479:ILE:HD12	1.88	0.55
1:A:195:LYS:HG3	1:A:199:MET:CE	2.36	0.55
1:F:3:LYS:NZ	6:F:718:HOH:O	2.40	0.55
1:D:16:LYS:NZ	6:D:813:HOH:O	2.38	0.55
1:F:393:ILE:CA	1:F:397:GLN:HG2	2.37	0.55
1:C:471:VAL:HB	1:C:555:LEU:HD11	1.89	0.55
1:A:195:LYS:HG3	1:A:199:MET:HE2	1.88	0.55
1:E:237:THR:HG23	1:E:239:MET:H	1.72	0.55
1:B:467:ILE:CG1	1:B:542:MET:HE1	2.33	0.54
1:D:47:LEU:HB2	5:F:601:UQ0:CM5	2.38	0.54
1:A:488:LEU:HD22	1:A:490:TYR:HB2	1.90	0.54
1:D:415:CYS:SG	1:D:420:PRO:HD2	2.47	0.54
1:E:362:LYS:NZ	6:E:707:HOH:O	2.33	0.53
1:E:379:MET:HE1	1:E:443:ILE:HG12	1.90	0.53
1:B:525:VAL:HG11	1:B:531:ILE:HG12	1.91	0.53
1:A:349:VAL:O	1:A:353:GLN:HG3	2.08	0.53
1:C:246:ASP:HA	1:C:251:MET:HG2	1.91	0.53
1:A:11:MET:HE1	1:A:33:PHE:CZ	2.43	0.53
1:C:579:ASN:ND2	6:C:807:HOH:O	2.40	0.53
1:E:11:MET:HE1	1:E:33:PHE:CZ	2.44	0.53
1:F:524:ARG:HD3	1:F:552:GLU:OE1	2.08	0.53
1:C:11:MET:HE1	1:C:33:PHE:CZ	2.44	0.52
1:D:557:ARG:NH2	6:D:817:HOH:O	2.43	0.52
1:A:383:PHE:O	6:A:802:HOH:O	2.17	0.52
1:D:87:LEU:HD11	1:D:159:LEU:HD12	1.90	0.52
1:A:1:MET:HG2	1:A:174:ASP:HB2	1.91	0.52
1:F:246:ASP:OD1	1:F:251:MET:HE3	2.09	0.52
1:D:447:PHE:CD2	1:D:476:LEU:HD22	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:572:GLU:HG2	1:E:576:ILE:CG2	2.40	0.52
1:A:199:MET:CE	1:A:316:LEU:HD22	2.40	0.52
1:C:23:PHE:O	1:C:72:CYS:HA	2.09	0.52
1:C:385:ARG:HG2	1:C:593:GLU:HG2	1.92	0.52
1:A:3:LYS:HD2	1:A:170:GLU:OE2	2.10	0.51
1:B:251:MET:HE3	1:B:253:GLY:N	2.25	0.51
1:D:3:LYS:HG2	1:D:172:GLU:OE2	2.11	0.51
1:E:136:ALA:HA	1:E:166:VAL:HG13	1.93	0.51
1:B:365:PHE:HE2	1:B:373:GLN:HG3	1.76	0.50
1:E:197:VAL:O	1:E:201:ILE:HG23	2.10	0.50
1:E:572:GLU:OE1	6:E:701:HOH:O	2.19	0.50
1:A:344:CYS:SG	6:A:1408:HOH:O	2.49	0.50
1:C:269:LEU:O	1:C:296:ARG:NH2	2.44	0.50
1:C:412:TRP:O	6:C:802:HOH:O	2.19	0.50
1:E:0:GLY:HA2	1:E:172:GLU:HB3	1.93	0.50
1:A:365:PHE:CE2	1:A:373:GLN:HG3	2.46	0.50
1:B:108:ARG:NH2	6:B:820:HOH:O	2.42	0.50
1:D:380:ASN:O	6:D:802:HOH:O	2.20	0.50
1:E:92:ALA:HB1	1:E:417:GLN:HG2	1.94	0.49
1:D:5:ARG:NH2	1:D:35:SER:OG	2.45	0.49
1:E:226:PHE:O	1:E:230:THR:HB	2.13	0.49
1:A:365:PHE:CD1	1:A:371:LYS:HD2	2.47	0.49
1:B:467:ILE:HG13	1:B:542:MET:CE	2.35	0.49
1:F:38:ARG:NH2	6:F:724:HOH:O	2.46	0.49
1:E:488:LEU:HD22	1:E:490:TYR:HB2	1.95	0.49
1:B:465:PRO:HB2	1:B:542:MET:CG	2.43	0.49
1:C:381:LYS:NZ	6:C:811:HOH:O	2.42	0.49
1:A:113:ASP:OD2	6:A:805:HOH:O	2.17	0.49
1:A:447:PHE:CG	1:A:476:LEU:HD22	2.48	0.48
1:E:237:THR:HG21	2:E:602:FAD:P	2.53	0.48
1:A:316:LEU:HD21	1:A:318:ILE:HD11	1.95	0.48
1:E:371:LYS:HE3	1:E:556:GLU:OE2	2.13	0.48
1:B:39:LYS:NZ	6:B:821:HOH:O	2.43	0.48
1:C:138:LEU:O	1:C:142:VAL:HG12	2.13	0.48
1:C:17:GLU:HG2	1:C:147:PHE:CD1	2.48	0.48
1:D:92:ALA:HB1	1:D:417:GLN:CG	2.44	0.48
1:E:191:MET:HE2	1:F:179:GLU:OE2	2.13	0.48
1:D:92:ALA:HB1	1:D:417:GLN:HG2	1.95	0.47
1:C:512:VAL:O	1:C:516:GLU:HG3	2.14	0.47
1:E:392:THR:HG21	1:E:420:PRO:O	2.14	0.47
1:D:463:ASN:ND2	6:D:810:HOH:O	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:ASP:OD2	1:F:177:MET:HG2	2.15	0.47
1:A:415:CYS:SG	1:A:420:PRO:HD2	2.54	0.47
1:B:365:PHE:CE2	1:B:373:GLN:HG3	2.50	0.47
1:E:447:PHE:CG	1:E:476:LEU:HD22	2.49	0.47
1:F:11:MET:HE1	1:F:33:PHE:CZ	2.50	0.47
1:B:483:GLN:HB3	1:B:488:LEU:HD12	1.97	0.47
1:F:11:MET:HE1	1:F:33:PHE:CE1	2.50	0.46
1:B:447:PHE:CG	1:B:476:LEU:HD22	2.51	0.46
1:D:571:MET:HE3	1:D:572:GLU:H	1.80	0.46
1:F:106:ARG:HD3	1:F:165:ASP:OD2	2.15	0.46
1:D:323:LYS:NZ	6:D:827:HOH:O	2.49	0.46
1:B:23:PHE:O	1:B:72:CYS:HA	2.15	0.46
1:E:546:ARG:NH1	6:E:725:HOH:O	2.48	0.46
1:A:151:ARG:NH1	6:A:801:HOH:O	2.04	0.46
1:A:199:MET:HB3	1:A:273:MET:HE1	1.98	0.46
1:B:120:GLU:HG3	1:B:124:LYS:HZ1	1.80	0.46
1:B:571:MET:HE2	1:B:571:MET:HB2	1.78	0.46
1:B:223:LEU:O	1:B:223:LEU:HG	2.07	0.46
1:C:309:GLY:HA2	1:C:312:LEU:O	2.15	0.46
1:C:337:GLN:HB2	1:C:342:LEU:HD12	1.96	0.46
1:D:290:GLU:CD	1:D:290:GLU:H	2.24	0.45
1:A:151:ARG:NH2	6:A:808:HOH:O	2.41	0.45
1:E:101:THR:HG23	1:E:161:ASP:OD1	2.16	0.45
1:E:230:THR:HG23	1:E:232:VAL:HG23	1.98	0.45
1:A:530:ASP:C	1:A:533:PRO:HD2	2.42	0.45
1:E:260:ALA:O	1:E:361:ARG:NH2	2.48	0.45
1:A:92:ALA:HB1	1:A:417:GLN:CG	2.47	0.45
1:B:336:MET:HE2	1:B:336:MET:HA	1.98	0.45
1:C:17:GLU:HG2	1:C:147:PHE:CD2	2.52	0.45
1:D:251:MET:HE1	6:D:927:HOH:O	2.15	0.45
1:E:197:VAL:HG11	1:E:332:VAL:CG1	2.46	0.45
1:C:3:LYS:HE3	1:C:172:GLU:OE2	2.15	0.45
1:A:365:PHE:HE2	1:A:373:GLN:HG3	1.80	0.45
1:A:536:GLU:HG2	6:A:1046:HOH:O	2.16	0.45
1:F:92:ALA:HB1	1:F:417:GLN:CG	2.47	0.45
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.75	0.45
1:E:282:ALA:O	1:E:286:THR:HG23	2.17	0.45
1:A:304:GLU:HG2	1:A:307:GLN:HG2	1.99	0.45
1:B:151:ARG:NE	6:B:804:HOH:O	2.23	0.45
1:D:465:PRO:CB	1:D:542:MET:HG3	2.46	0.45
1:D:524:ARG:HD3	1:D:552:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:TYR:HA	1:E:441:VAL:O	2.17	0.45
1:D:467:ILE:CG1	1:D:542:MET:HE1	2.47	0.45
1:C:185:LYS:HE2	6:C:1061:HOH:O	2.16	0.44
1:C:336:MET:HE2	1:C:336:MET:HA	1.98	0.44
1:D:309:GLY:HA2	1:D:312:LEU:O	2.17	0.44
1:C:530:ASP:C	1:C:533:PRO:HD2	2.43	0.44
1:D:447:PHE:CG	1:D:476:LEU:HD22	2.53	0.44
1:E:194:GLU:HA	1:E:197:VAL:HG12	2.00	0.44
1:F:59:GLU:CD	1:F:423:TRP:HE1	2.26	0.44
1:F:392:THR:HG23	1:F:415:CYS:SG	2.58	0.44
1:E:23:PHE:O	1:E:72:CYS:HA	2.18	0.44
1:D:447:PHE:HE1	1:F:49:ARG:HA	1.82	0.44
1:E:263:TYR:HA	1:E:359:LEU:HD12	1.99	0.44
1:E:392:THR:HG23	1:E:415:CYS:SG	2.57	0.44
1:F:106:ARG:HA	1:F:109:LEU:HD22	2.00	0.44
1:F:476:LEU:HB2	1:F:492:VAL:HB	1.98	0.44
1:D:366:ASP:HB2	6:D:1242:HOH:O	2.17	0.44
1:A:389:TYR:HA	1:A:441:VAL:O	2.18	0.44
1:B:524:ARG:HD2	1:B:554:ILE:HD11	2.00	0.44
1:D:246:ASP:HA	1:D:251:MET:HG3	2.00	0.44
1:C:133:VAL:HG22	1:C:142:VAL:HG11	2.00	0.43
1:C:368:VAL:HG22	1:C:528:PRO:HD3	2.00	0.43
1:D:223:LEU:HD22	1:D:243:CYS:SG	2.58	0.43
1:B:251:MET:HE3	1:B:251:MET:C	2.43	0.43
1:C:144:GLN:HG2	1:C:181:LEU:HG	2.00	0.43
1:D:525:VAL:HG13	1:D:530:ASP:HB2	2.00	0.43
1:C:106:ARG:HD3	1:C:134:ARG:O	2.18	0.43
1:A:259:THR:OG1	2:A:701:FAD:C4X	2.66	0.43
1:A:465:PRO:HB2	1:A:542:MET:HG2	2.00	0.43
1:B:380:ASN:O	6:B:802:HOH:O	2.21	0.43
1:B:542:MET:HB2	1:B:542:MET:HE3	1.32	0.43
1:D:530:ASP:C	1:D:533:PRO:HD2	2.44	0.43
1:F:365:PHE:CE1	1:F:373:GLN:HG3	2.53	0.43
1:A:336:MET:HE1	6:A:906:HOH:O	2.18	0.43
1:C:392:THR:OG1	1:C:423:TRP:HB3	2.19	0.43
1:D:109:LEU:HD23	1:D:109:LEU:HA	1.83	0.43
1:D:355:ARG:NH2	6:D:808:HOH:O	2.52	0.43
1:F:39:LYS:HB2	6:F:724:HOH:O	2.19	0.43
1:B:493:GLN:OE1	1:B:557:ARG:NH2	2.45	0.42
1:E:200:LEU:O	1:E:345:ARG:NH2	2.53	0.42
1:E:467:ILE:HD12	1:E:538:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:PHE:CG	1:C:476:LEU:HD22	2.54	0.42
1:C:379:MET:HE1	1:C:443:ILE:HG12	2.00	0.42
1:D:382:ALA:O	1:D:539:LYS:NZ	2.52	0.42
1:E:564:GLY:HA3	1:E:570:VAL:HA	2.01	0.42
1:B:392:THR:HG23	1:B:415:CYS:SG	2.60	0.42
1:D:136:ALA:HA	1:D:166:VAL:HG13	2.02	0.42
1:E:449:PHE:CZ	1:E:456:LEU:HD11	2.55	0.42
1:B:258:GLN:OE1	1:B:284:ARG:NH1	2.53	0.42
1:B:446:ASP:OD1	1:B:446:ASP:N	2.50	0.42
1:E:165:ASP:OD1	1:E:165:ASP:N	2.49	0.42
1:E:395:LEU:HD13	1:E:561:ILE:HD13	2.02	0.42
1:F:53:GLY:O	1:F:57:MET:HG3	2.19	0.42
1:F:78:PRO:HA	1:F:81:THR:OG1	2.20	0.42
1:A:109:LEU:HD23	1:A:109:LEU:HA	1.79	0.42
1:C:132:THR:HA	1:C:161:ASP:HB3	2.01	0.42
1:D:39:LYS:NZ	6:D:842:HOH:O	2.53	0.42
1:D:214:VAL:HG21	1:D:223:LEU:HD13	2.00	0.42
1:F:439:ASN:HB2	6:F:1008:HOH:O	2.20	0.42
1:D:38:ARG:HD3	1:F:488:LEU:CD2	2.48	0.42
1:B:389:TYR:HA	1:B:441:VAL:O	2.20	0.41
1:C:192:GLN:HG3	6:C:856:HOH:O	2.20	0.41
1:D:499:ILE:HD12	1:F:521:LYS:HE2	2.02	0.41
1:B:38:ARG:NH1	6:B:843:HOH:O	2.53	0.41
1:D:521:LYS:NZ	6:D:844:HOH:O	2.53	0.41
1:E:92:ALA:HB1	1:E:417:GLN:CG	2.49	0.41
1:F:392:THR:OG1	1:F:423:TRP:HB3	2.19	0.41
1:B:111:LYS:HZ3	1:B:111:LYS:HG2	1.73	0.41
1:B:290:GLU:H	1:B:290:GLU:CD	2.29	0.41
1:C:1:MET:HE2	1:C:174:ASP:HB2	2.02	0.41
1:C:119:ILE:HD12	1:C:119:ILE:HA	1.89	0.41
1:C:151:ARG:NE	6:C:801:HOH:O	2.18	0.41
1:D:106:ARG:NH1	6:D:838:HOH:O	2.52	0.41
1:F:109:LEU:HD12	1:F:109:LEU:HA	1.85	0.41
1:A:593:GLU:HB2	6:A:1154:HOH:O	2.19	0.41
1:E:416:GLY:O	2:E:602:FAD:H9	2.20	0.41
1:E:518:LEU:HD23	1:E:518:LEU:HA	1.93	0.41
1:A:392:THR:HG22	1:A:393:ILE:HG22	2.03	0.41
1:D:463:ASN:ND2	6:D:805:HOH:O	2.30	0.41
1:E:132:THR:HA	1:E:161:ASP:HB3	2.02	0.41
1:E:293:THR:HB	1:E:298:ILE:HD11	2.03	0.41
1:B:106:ARG:HA	1:B:109:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ARG:NE	1:B:113:ASP:OD2	2.53	0.41
1:C:50:HIS:HA	1:E:451:PHE:CZ	2.56	0.41
1:E:465:PRO:HB2	1:E:542:MET:HG3	2.02	0.41
1:E:525:VAL:HG11	1:E:531:ILE:HG12	2.02	0.41
1:B:209:VAL:HA	1:B:235:ILE:O	2.20	0.41
1:B:366:ASP:OD1	6:B:803:HOH:O	2.22	0.41
1:C:11:MET:HE1	1:C:33:PHE:CE1	2.56	0.41
1:C:195:LYS:O	1:C:199:MET:HG3	2.21	0.41
1:D:126:VAL:HG13	1:F:122:ILE:HD11	2.02	0.41
1:D:385:ARG:HB3	1:D:593:GLU:HB2	2.03	0.41
1:D:521:LYS:HE2	1:F:499:ILE:HD12	2.02	0.41
1:E:533:PRO:O	1:E:537:GLN:HG3	2.21	0.41
1:E:579:ASN:ND2	6:E:739:HOH:O	2.54	0.41
1:F:188:ALA:HB2	1:F:320:SER:HB2	2.03	0.41
1:F:309:GLY:HA2	1:F:312:LEU:O	2.20	0.41
1:F:425:ILE:HG12	1:F:468:HIS:CE1	2.56	0.41
1:F:521:LYS:NZ	6:F:728:HOH:O	2.49	0.41
1:C:1:MET:H	1:C:174:ASP:HA	1.86	0.41
1:C:181:LEU:HD11	1:D:305:PRO:HG2	2.03	0.41
1:C:205:ARG:HB3	1:C:348:TRP:CD2	2.55	0.41
1:C:541:LEU:HD23	1:C:541:LEU:HA	1.93	0.41
1:E:357:ARG:HG2	6:E:1104:HOH:O	2.21	0.41
1:F:23:PHE:CE2	1:F:46:ILE:HD12	2.56	0.41
1:B:223:LEU:HD22	1:B:243:CYS:SG	2.61	0.40
1:D:391:THR:O	1:D:414:ASN:ND2	2.54	0.40
1:D:480:ARG:CZ	1:D:558:VAL:HG13	2.52	0.40
1:E:488:LEU:HD22	1:E:490:TYR:CB	2.50	0.40
1:B:385:ARG:H	1:B:593:GLU:HB2	1.85	0.40
1:C:488:LEU:HD13	1:C:490:TYR:HB3	2.02	0.40
1:D:465:PRO:HB2	1:D:542:MET:CG	2.50	0.40
1:A:75:THR:O	1:A:79:ALA:HB3	2.21	0.40
1:E:342:LEU:HA	1:E:342:LEU:HD12	1.82	0.40
1:E:447:PHE:CD2	1:E:476:LEU:HD22	2.57	0.40
1:E:465:PRO:HB2	1:E:542:MET:CG	2.51	0.40
1:B:92:ALA:HB1	1:B:417:GLN:HG2	2.03	0.40
1:D:23:PHE:O	1:D:72:CYS:HA	2.21	0.40
1:D:490:TYR:CD1	1:F:38:ARG:HG3	2.57	0.40
1:B:257:LEU:HB3	1:B:564:GLY:O	2.22	0.40
1:C:392:THR:HG23	1:C:415:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
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

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

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	172	GLU
1	A	235	ILE
1	A	268	LEU
1	A	354	GLN
1	A	406	VAL
1	A	470	LEU
1	A	476	LEU
1	A	488	LEU
1	A	505	ASN
1	A	542	MET
1	A	593	GLU
1	B	5	ARG
1	B	37	MET
1	B	38	ARG
1	B	111	LYS
1	B	124	LYS
1	B	131	VAL
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	443	ILE
1	B	476	LEU
1	B	571	MET
1	C	46	ILE
1	C	91	SER
1	C	124	LYS
1	C	131	VAL
1	C	142	VAL
1	C	172	GLU
1	C	202	GLN
1	C	223	LEU
1	C	251	MET
1	C	283	GLN
1	C	346	LYS
1	C	406	VAL
1	C	443	ILE

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Mol	Chain	Res	Type
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	108	ARG
1	D	113	ASP
1	D	223	LEU
1	D	268	LEU
1	D	311	VAL
1	D	354	GLN
1	D	446	ASP
1	D	475	TYR
1	D	476	LEU
1	D	488	LEU
1	D	559	THR
1	E	37	MET
1	E	46	ILE
1	E	106	ARG
1	E	108	ARG
1	E	111	LYS
1	E	170	GLU
1	E	199	MET
1	E	230	THR
1	E	234	VAL
1	E	237	THR
1	E	249	GLU
1	E	251	MET
1	E	289	VAL
1	E	299	VAL
1	E	316	LEU
1	E	342	LEU
1	E	351	ASP
1	E	381	LYS
1	E	406	VAL
1	E	443	ILE
1	E	476	LEU
1	E	537	GLN
1	E	585	THR
1	F	3	LYS
1	F	73	LEU

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Mol	Chain	Res	Type
1	F	109	LEU
1	F	170	GLU
1	F	172	GLU
1	F	223	LEU
1	F	257	LEU
1	F	293	THR
1	F	328	LEU
1	F	475	TYR
1	F	527	LYS
1	F	567	LEU

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	167	GLN
1	A	450	GLN
1	A	500	ASN
1	A	591	HIS
1	B	167	GLN
1	B	225	GLN
1	C	115	GLN
1	C	167	GLN
1	C	216	ASN
1	D	167	GLN
1	D	337	GLN
1	D	544	GLN
1	E	167	GLN
1	E	202	GLN
1	E	354	GLN
1	E	505	ASN
1	F	167	GLN
1	F	202	GLN
1	F	411	HIS
1	F	544	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 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
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

All (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
5	B	706	UQ0	C6-C5	8.84	1.53	1.35
5	E	605	UQ0	C6-C5	8.73	1.52	1.35
5	C	704	UQ0	C6-C5	8.72	1.52	1.35
5	B	705	UQ0	C6-C5	8.70	1.52	1.35
5	E	601	UQ0	C6-C5	8.68	1.52	1.35
5	F	601	UQ0	C6-C5	8.48	1.52	1.35
5	A	705	UQ0	C6-C5	7.29	1.50	1.35
5	A	705	UQ0	C3-C2	4.96	1.54	1.36
5	F	601	UQ0	C3-C2	4.96	1.54	1.36
5	E	605	UQ0	C3-C2	4.91	1.54	1.36
5	F	605	UQ0	C3-C2	4.73	1.53	1.36
5	C	704	UQ0	C3-C2	4.71	1.53	1.36
5	C	706	UQ0	C3-C2	4.63	1.53	1.36
5	E	601	UQ0	C3-C2	4.59	1.52	1.36
5	A	706	UQ0	C5-C4	4.58	1.54	1.47
3	B	702	TPP	PA-O3A	-4.52	1.54	1.59
5	D	706	UQ0	C3-C2	4.51	1.52	1.36
5	A	706	UQ0	C3-C2	4.50	1.52	1.36
5	D	704	UQ0	C3-C2	4.50	1.52	1.36
5	D	706	UQ0	C5-C4	4.39	1.54	1.47
5	C	706	UQ0	C5-C4	4.33	1.53	1.47
5	B	706	UQ0	C3-C2	4.28	1.51	1.36
5	B	706	UQ0	C5-C4	4.19	1.53	1.47
5	B	705	UQ0	C3-C2	4.00	1.50	1.36
5	C	704	UQ0	C5-C4	3.76	1.53	1.47
5	D	704	UQ0	C5-C4	3.52	1.52	1.47
2	C	701	FAD	P-O3P	3.45	1.63	1.59
3	A	702	TPP	PA-O3A	-3.45	1.55	1.59
5	E	601	UQ0	C6-C1	3.42	1.54	1.44
5	F	605	UQ0	C5-C4	3.41	1.52	1.47
5	D	704	UQ0	C6-C1	3.38	1.54	1.44
5	C	706	UQ0	C6-C1	3.38	1.54	1.44
5	B	705	UQ0	C5-C4	3.38	1.52	1.47
5	A	706	UQ0	C6-C1	3.36	1.54	1.44
5	F	605	UQ0	C6-C1	3.29	1.53	1.44
5	E	601	UQ0	C5-C4	3.24	1.52	1.47
5	D	706	UQ0	C6-C1	3.24	1.53	1.44
5	E	605	UQ0	C5-C4	3.18	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	705	UQ0	C6-C1	3.17	1.53	1.44
5	F	601	UQ0	C5-C4	3.14	1.52	1.47
5	B	706	UQ0	C6-C1	3.07	1.53	1.44
5	E	601	UQ0	C2-C1	3.07	1.53	1.46
5	F	601	UQ0	C2-C1	3.03	1.53	1.46
5	D	706	UQ0	C2-C1	2.98	1.53	1.46
5	F	601	UQ0	C6-C1	2.88	1.52	1.44
5	C	706	UQ0	C2-C1	2.86	1.53	1.46
5	E	605	UQ0	C6-C1	2.85	1.52	1.44
5	C	704	UQ0	C6-C1	2.81	1.52	1.44
5	C	704	UQ0	C2-C1	2.81	1.53	1.46
3	D	702	TPP	PA-O3A	-2.79	1.56	1.59
5	B	706	UQ0	C2-C1	2.76	1.53	1.46
5	A	705	UQ0	C2-C1	2.75	1.53	1.46
5	E	605	UQ0	C2-C1	2.75	1.53	1.46
5	D	704	UQ0	C2-C1	2.70	1.52	1.46
5	F	605	UQ0	C2-C1	2.65	1.52	1.46
2	A	701	FAD	P-O3P	2.59	1.62	1.59
3	E	603	TPP	PA-O3A	-2.57	1.56	1.59
2	E	602	FAD	PA-O5B	-2.56	1.49	1.59
5	A	706	UQ0	C2-C1	2.50	1.52	1.46
5	B	706	UQ0	O1-C1	-2.37	1.18	1.24
5	F	605	UQ0	O3-CM3	-2.29	1.40	1.45
5	A	705	UQ0	O4-C4	-2.26	1.18	1.23
5	E	605	UQ0	O3-CM3	-2.24	1.40	1.45
5	D	706	UQ0	O1-C1	-2.23	1.18	1.24
5	A	705	UQ0	O2-CM2	-2.21	1.40	1.45
2	B	701	FAD	P-O2P	-2.20	1.45	1.55
5	F	601	UQ0	O2-CM2	-2.17	1.40	1.45
5	B	705	UQ0	C2-C1	2.16	1.51	1.46
5	A	705	UQ0	C5-C4	2.14	1.50	1.47
5	E	601	UQ0	O1-C1	-2.10	1.19	1.24
5	E	605	UQ0	O1-C1	-2.09	1.19	1.24
2	A	701	FAD	P-O2P	-2.08	1.45	1.55
2	E	602	FAD	P-O2P	-2.05	1.45	1.55
5	F	601	UQ0	O1-C1	-2.04	1.19	1.24
5	E	601	UQ0	O2-CM2	-2.03	1.40	1.45
5	F	605	UQ0	O2-CM2	-2.03	1.40	1.45
5	E	601	UQ0	O3-CM3	-2.03	1.40	1.45
5	D	704	UQ0	O3-CM3	-2.02	1.40	1.45

All (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
5	E	601	UQ0	C6-C5-C4	3.63	122.60	119.56
5	C	704	UQ0	CM5-C5-C4	3.29	119.67	117.41
5	B	705	UQ0	O4-C4-C5	-3.20	117.62	120.91
5	B	706	UQ0	C5-C6-C1	-3.10	116.19	122.65
5	A	706	UQ0	C5-C6-C1	-3.04	116.31	122.65
5	B	705	UQ0	C6-C5-C4	3.02	122.09	119.56
5	B	705	UQ0	O3-C3-C4	3.01	126.78	116.64
5	A	705	UQ0	O4-C4-C5	-2.97	117.86	120.91
5	A	705	UQ0	O1-C1-C2	2.93	126.13	121.66
5	C	706	UQ0	C6-C5-C4	2.93	122.01	119.56
5	E	601	UQ0	C5-C6-C1	-2.75	116.93	122.65
5	A	705	UQ0	C5-C6-C1	2.70	128.26	122.65
2	C	701	FAD	O2P-P-O1P	2.59	124.49	112.44
2	A	701	FAD	O3P-P-O1P	-2.52	103.11	110.70
2	A	701	FAD	C4B-O4B-C1B	-2.51	103.92	109.47
5	C	706	UQ0	C5-C6-C1	-2.48	117.49	122.65
5	D	706	UQ0	C6-C5-C4	2.44	121.60	119.56
2	B	701	FAD	C4B-O4B-C1B	-2.44	104.09	109.47
2	D	701	FAD	O5'-P-O1P	-2.43	99.32	108.94
5	B	705	UQ0	O3-C3-C2	-2.39	114.58	123.64
5	D	706	UQ0	C5-C6-C1	-2.35	117.75	122.65
5	B	705	UQ0	CM2-O2-C2	-2.30	108.40	116.47
5	B	705	UQ0	O1-C1-C2	-2.27	118.19	121.66
5	A	706	UQ0	O3-C3-C4	2.25	124.22	116.64
5	F	601	UQ0	C5-C6-C1	-2.23	118.02	122.65
5	B	706	UQ0	O1-C1-C2	-2.20	118.30	121.66
2	C	701	FAD	C4B-O4B-C1B	-2.15	104.72	109.47
5	E	601	UQ0	C6-C1-C2	2.08	121.44	115.39
3	B	702	TPP	O3B-PB-O2B	2.07	115.57	107.80
5	E	605	UQ0	O4-C4-C5	-2.04	118.82	120.91
3	B	702	TPP	O2A-PA-O1A	2.03	121.90	112.44
2	A	701	FAD	O2P-P-O1P	2.03	121.88	112.44
2	D	701	FAD	C4B-O4B-C1B	-2.00	105.05	109.47

There are no chirality outliers.

All (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
2	E	602	FAD	C5B-O5B-PA-O2A
2	E	602	FAD	C5B-O5B-PA-O3P
2	E	602	FAD	C5'-O5'-P-O1P
2	F	602	FAD	C5'-O5'-P-O1P
3	A	702	TPP	PA-O3A-PB-O2B
3	B	702	TPP	PA-O3A-PB-O2B
3	B	702	TPP	PA-O3A-PB-O3B
3	E	603	TPP	PA-O3A-PB-O2B
3	E	603	TPP	PA-O3A-PB-O3B
5	B	705	UQ0	C2-C3-O3-CM3
2	F	602	FAD	O4B-C4B-C5B-O5B
5	A	706	UQ0	C2-C3-O3-CM3
2	F	602	FAD	PA-O3P-P-O1P
3	D	702	TPP	C5-C6-C7-O7
3	F	603	TPP	C5-C6-C7-O7
2	F	602	FAD	C3B-C4B-C5B-O5B
2	E	602	FAD	C2B-C1B-N9A-C8A
2	C	701	FAD	PA-O3P-P-O2P
2	D	701	FAD	PA-O3P-P-O2P
2	A	701	FAD	C5B-O5B-PA-O2A
2	A	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	C5B-O5B-PA-O3P
2	C	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5'-O5'-P-O2P
2	D	701	FAD	C5'-O5'-P-O1P
2	D	701	FAD	C5'-O5'-P-O2P
2	D	701	FAD	C5'-O5'-P-O3P
2	E	602	FAD	C5'-O5'-P-O2P
2	E	602	FAD	C5'-O5'-P-O3P
2	F	602	FAD	C5B-O5B-PA-O1A
2	F	602	FAD	C5'-O5'-P-O2P
2	F	602	FAD	C5'-O5'-P-O3P
2	C	701	FAD	PA-O3P-P-O1P
2	D	701	FAD	PA-O3P-P-O1P
2	F	602	FAD	PA-O3P-P-O2P
2	D	701	FAD	C2B-C1B-N9A-C8A
3	F	603	TPP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	E	602	FAD	O4B-C4B-C5B-O5B
2	F	602	FAD	C2'-C3'-C4'-O4'
2	A	701	FAD	C2'-C3'-C4'-O4'
2	E	602	FAD	O4B-C1B-N9A-C8A
3	E	603	TPP	PA-O3A-PB-O1B
3	C	702	TPP	PA-O3A-PB-O2B
3	C	702	TPP	C5-C6-C7-O7
3	E	603	TPP	C5-C6-C7-O7
2	D	701	FAD	C2'-C3'-C4'-O4'
2	F	602	FAD	C2B-C1B-N9A-C8A
2	E	602	FAD	PA-O3P-P-O1P
2	C	701	FAD	C2B-C1B-N9A-C8A
2	E	602	FAD	C2B-C1B-N9A-C4A
2	A	701	FAD	C2B-C1B-N9A-C8A
2	B	701	FAD	C2B-C1B-N9A-C8A
2	C	701	FAD	C2'-C3'-C4'-O4'
5	D	704	UQ0	C4-C3-O3-CM3
2	A	701	FAD	P-O3P-PA-O2A
2	B	701	FAD	P-O3P-PA-O2A
2	E	602	FAD	PA-O3P-P-O2P
2	F	602	FAD	P-O3P-PA-O2A

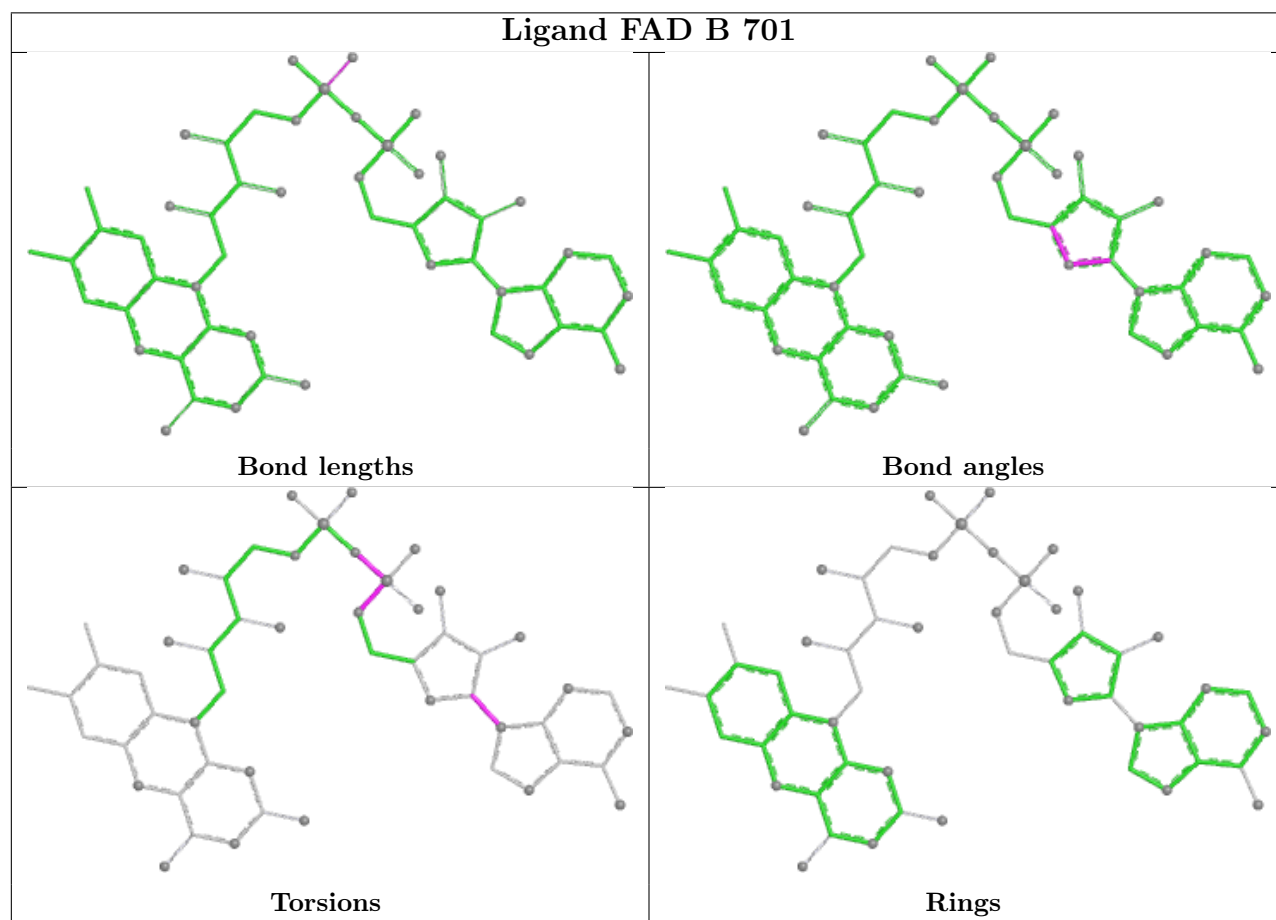
There are no ring outliers.

5 monomers are involved in 7 short contacts:

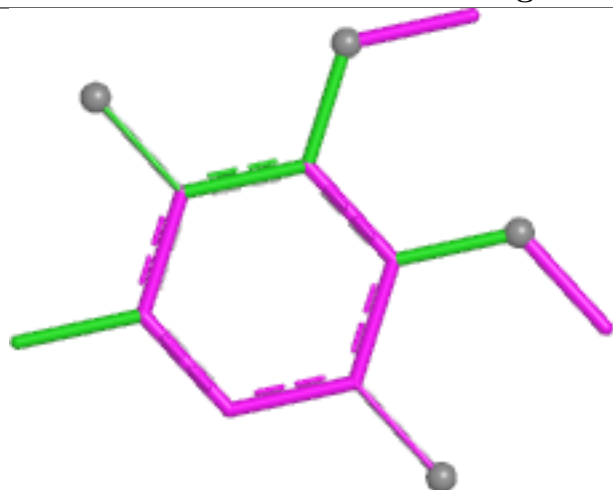
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	601	UQ0	1	0
5	F	601	UQ0	1	0
2	E	602	FAD	3	0
2	A	701	FAD	1	0
5	A	705	UQ0	1	0

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.

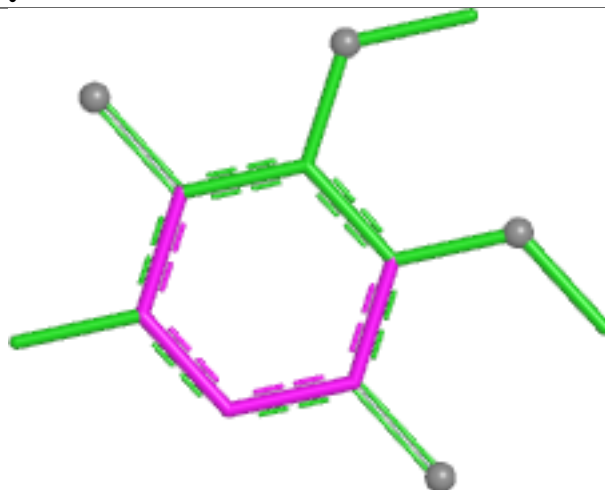
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



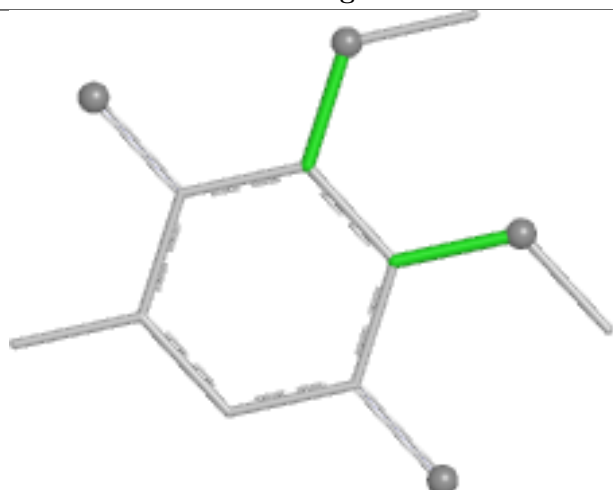
Ligand UQ0 E 601



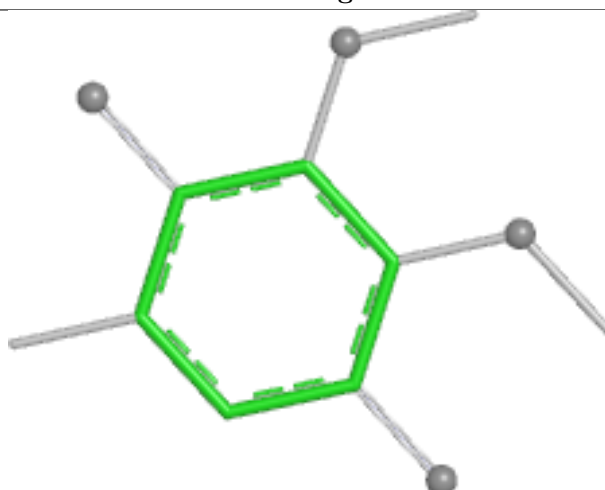
Bond lengths



Bond angles

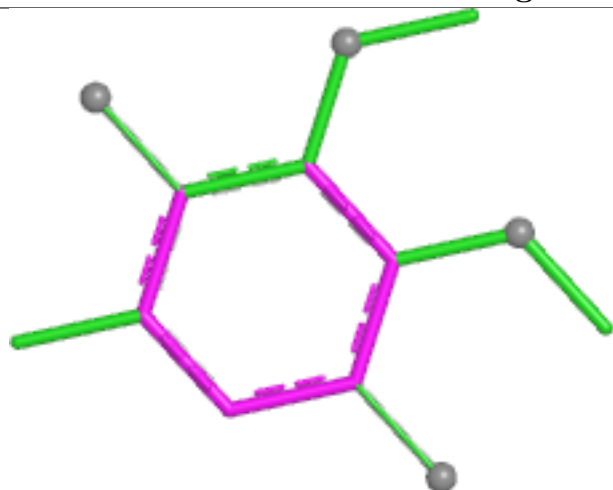


Torsions

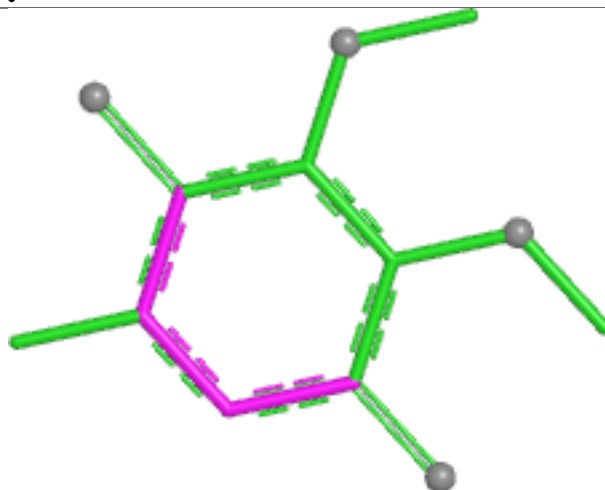


Rings

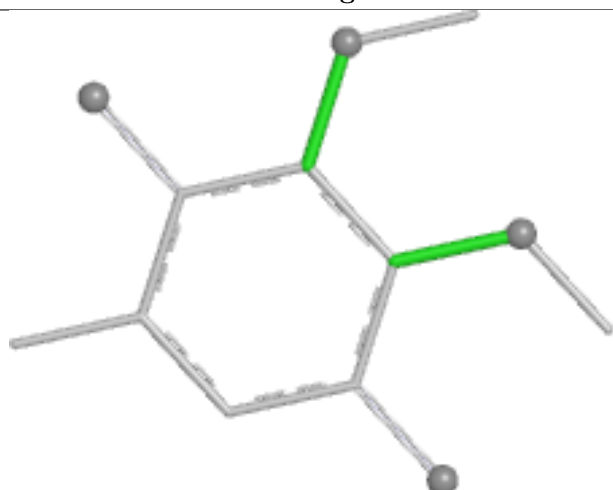
Ligand UQ0 C 706



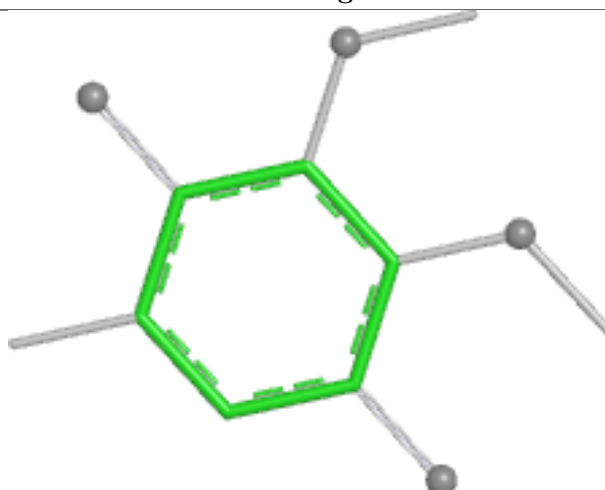
Bond lengths



Bond angles

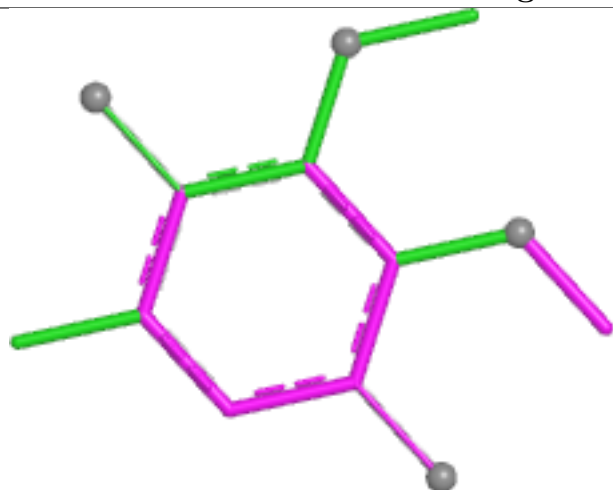


Torsions

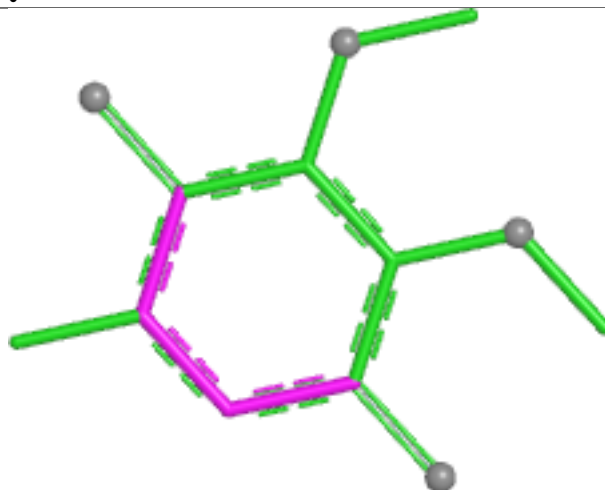


Rings

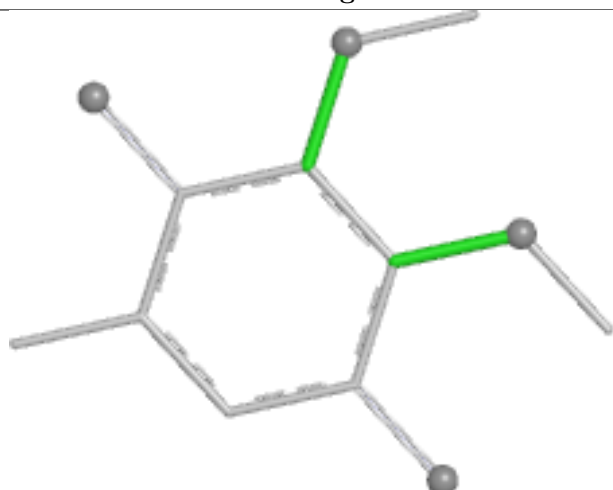
Ligand UQ0 F 601



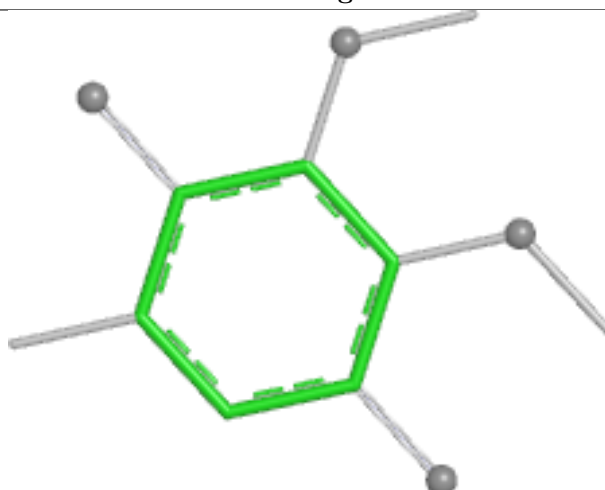
Bond lengths



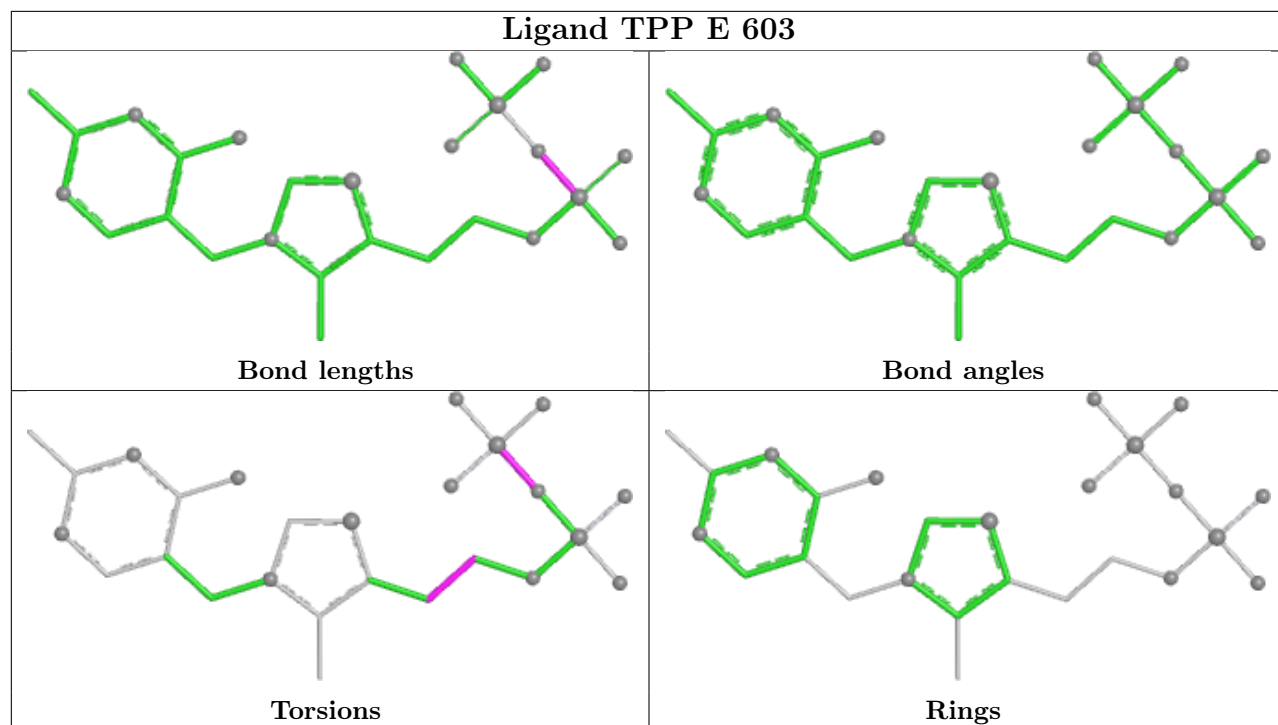
Bond angles



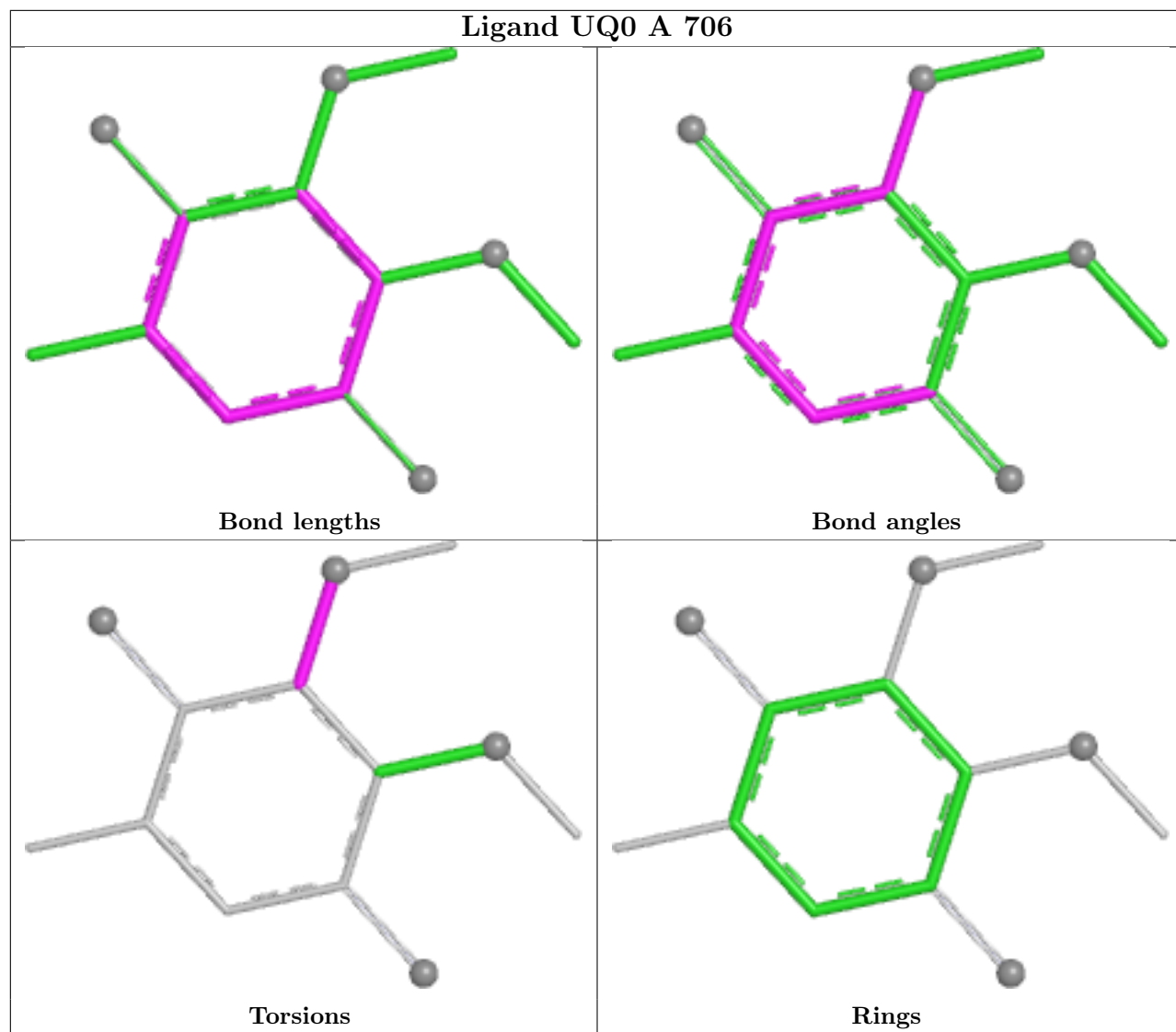
Torsions



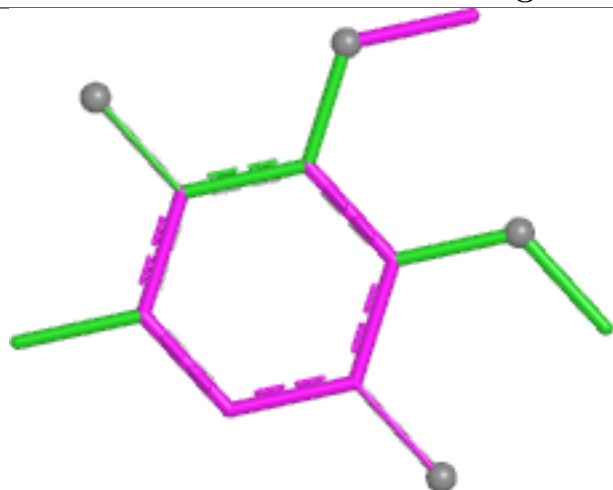
Rings



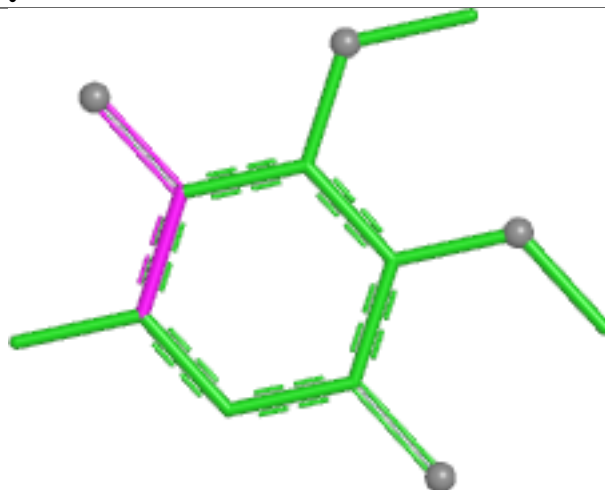
Ligand UQ0 A 706



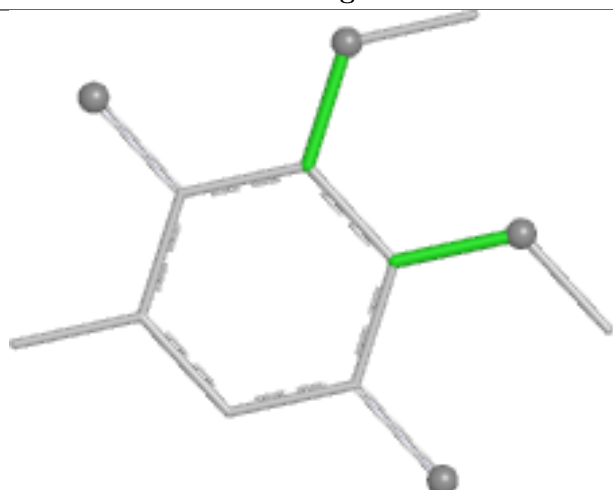
Ligand UQ0 E 605



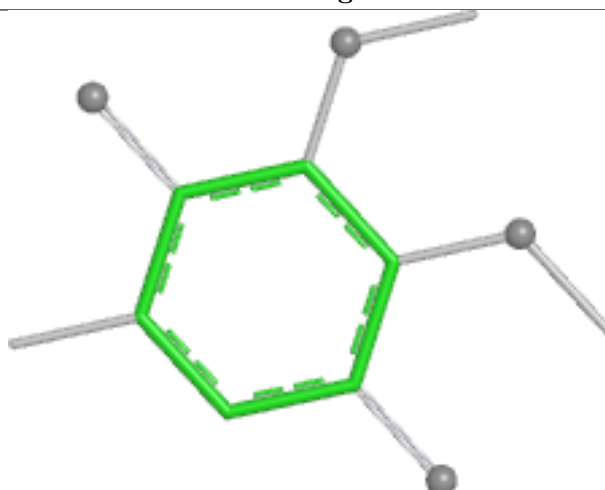
Bond lengths



Bond angles

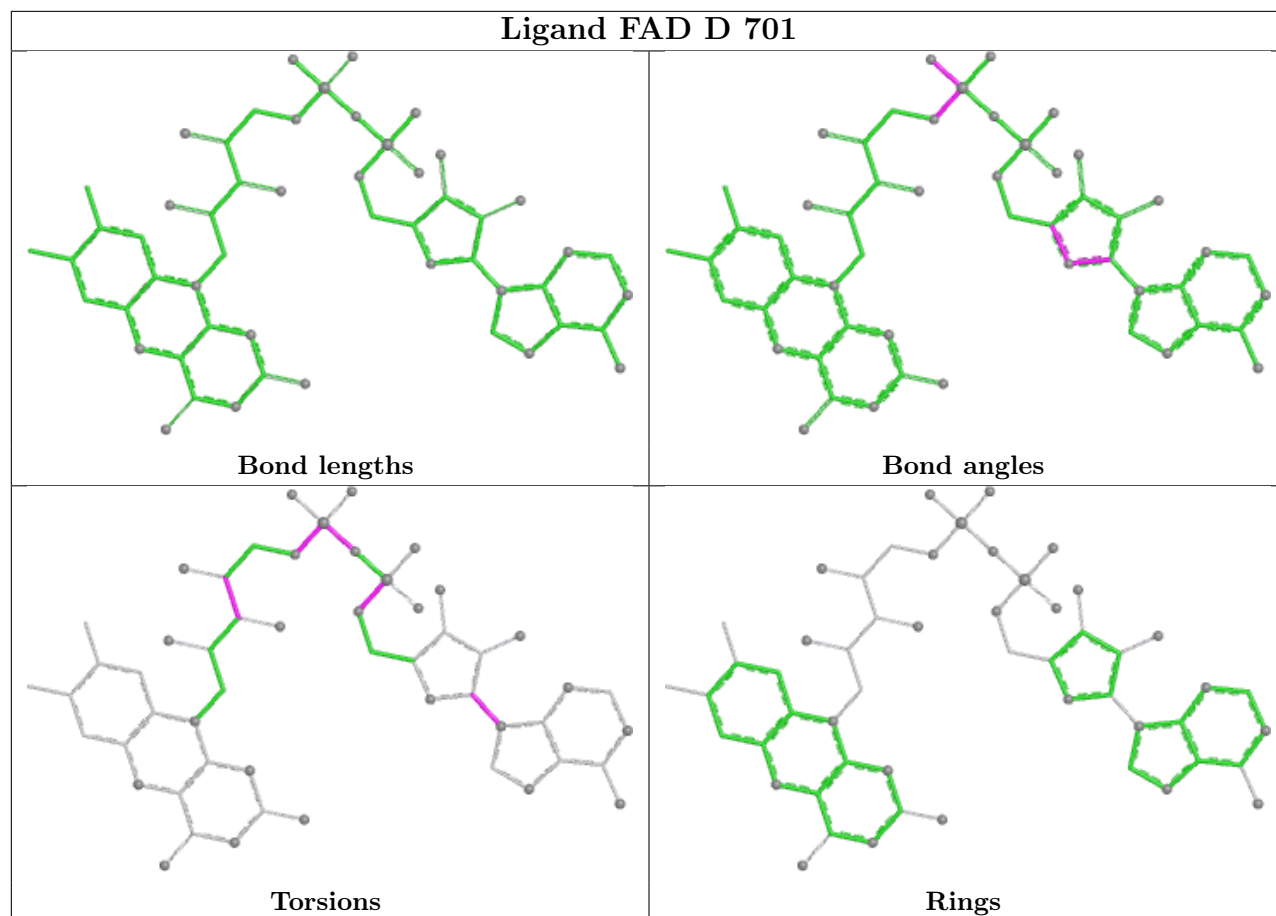


Torsions

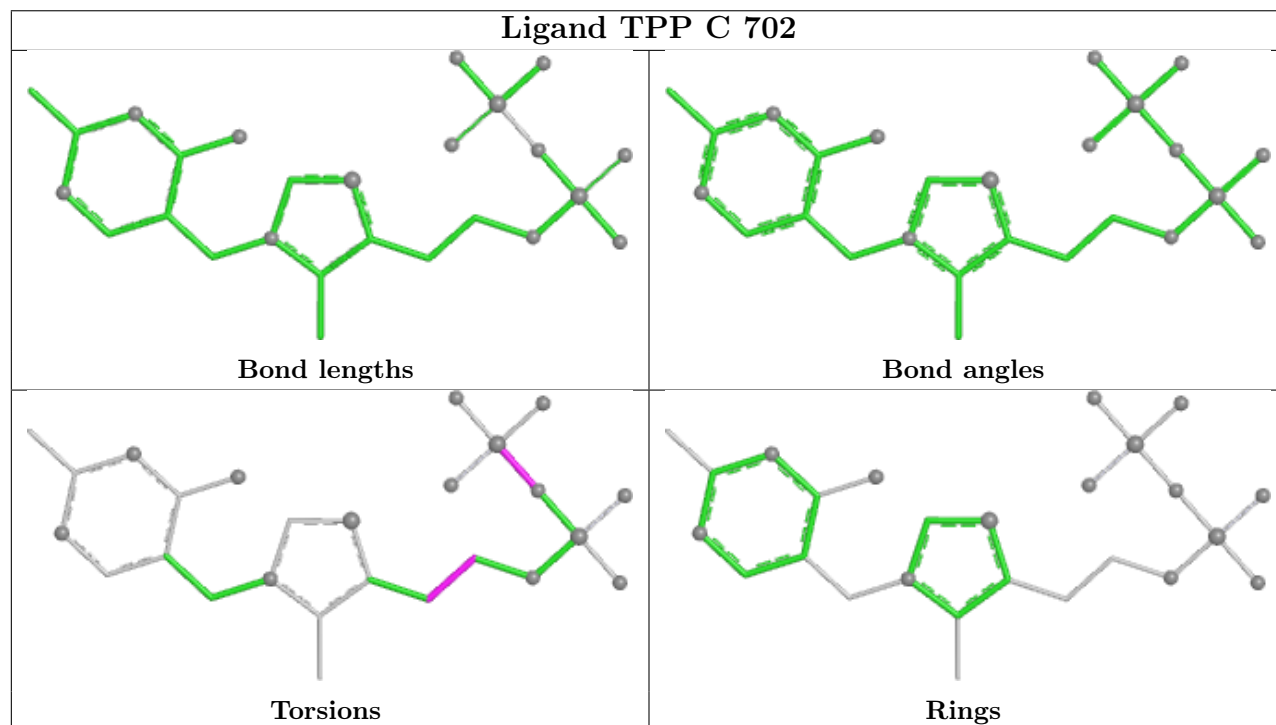


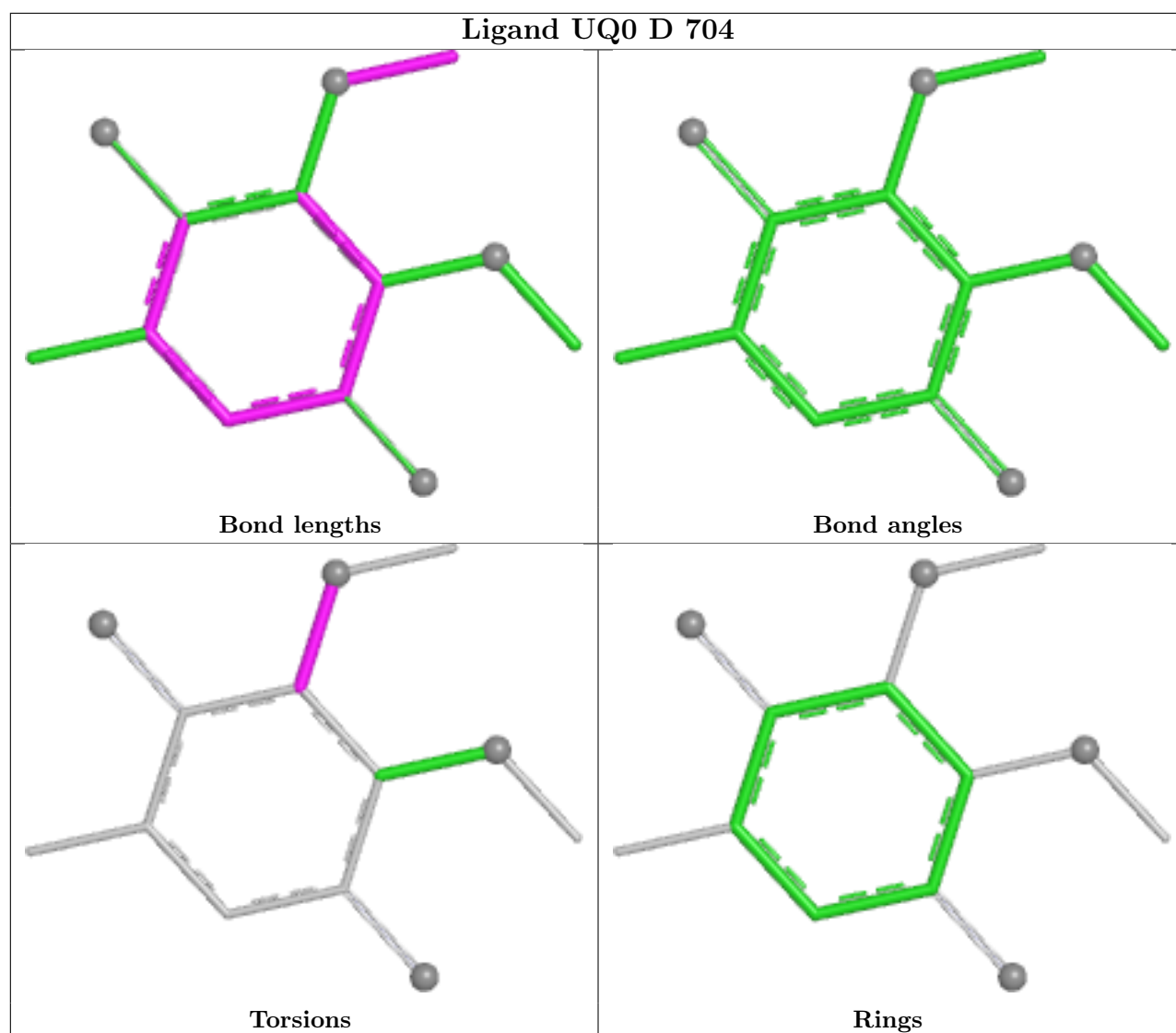
Rings

Ligand FAD D 701

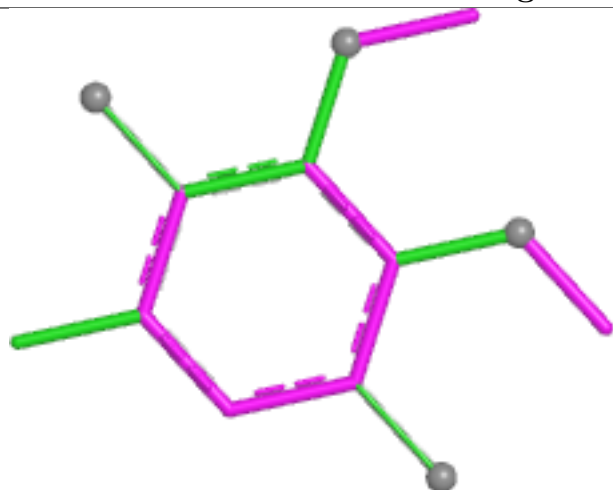


Ligand TPP C 702

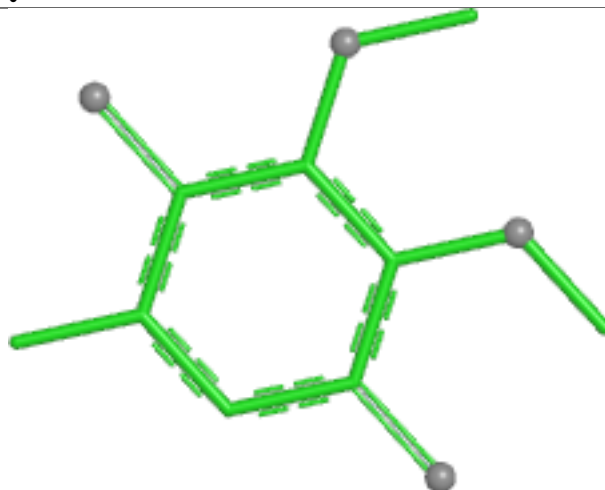




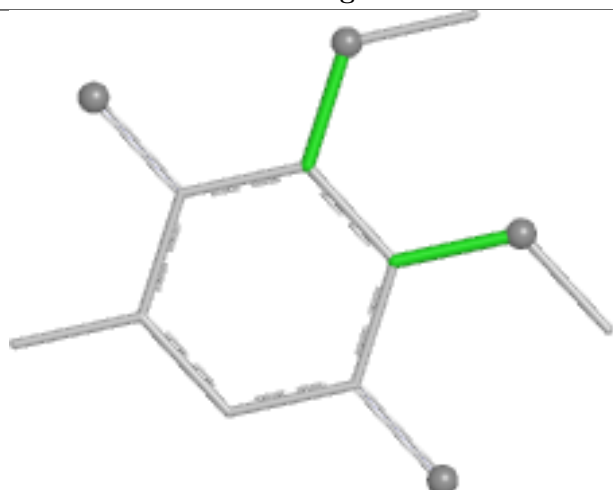
Ligand UQ0 F 605



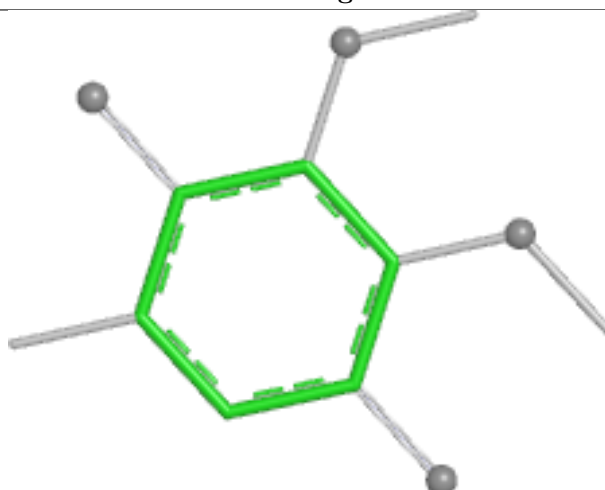
Bond lengths



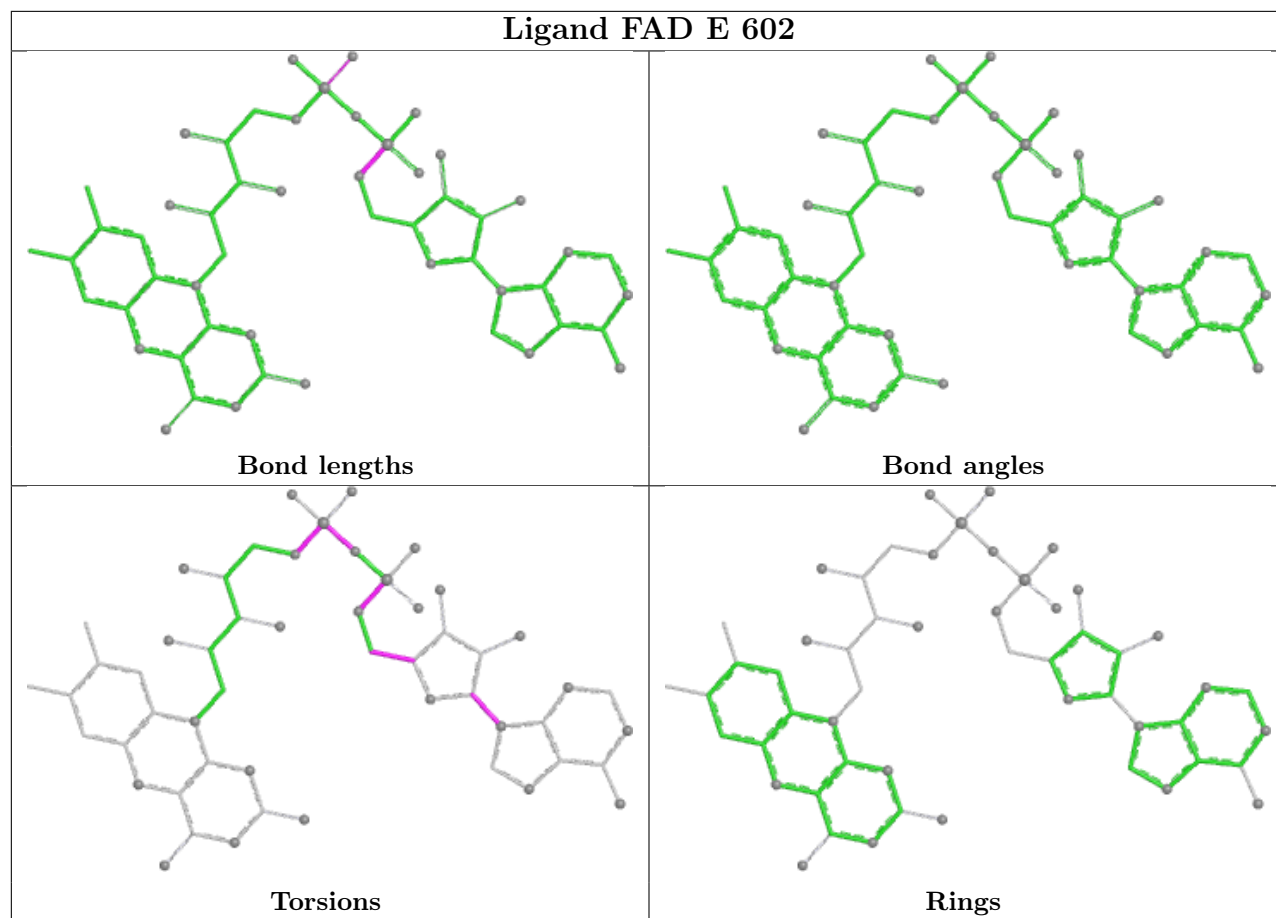
Bond angles

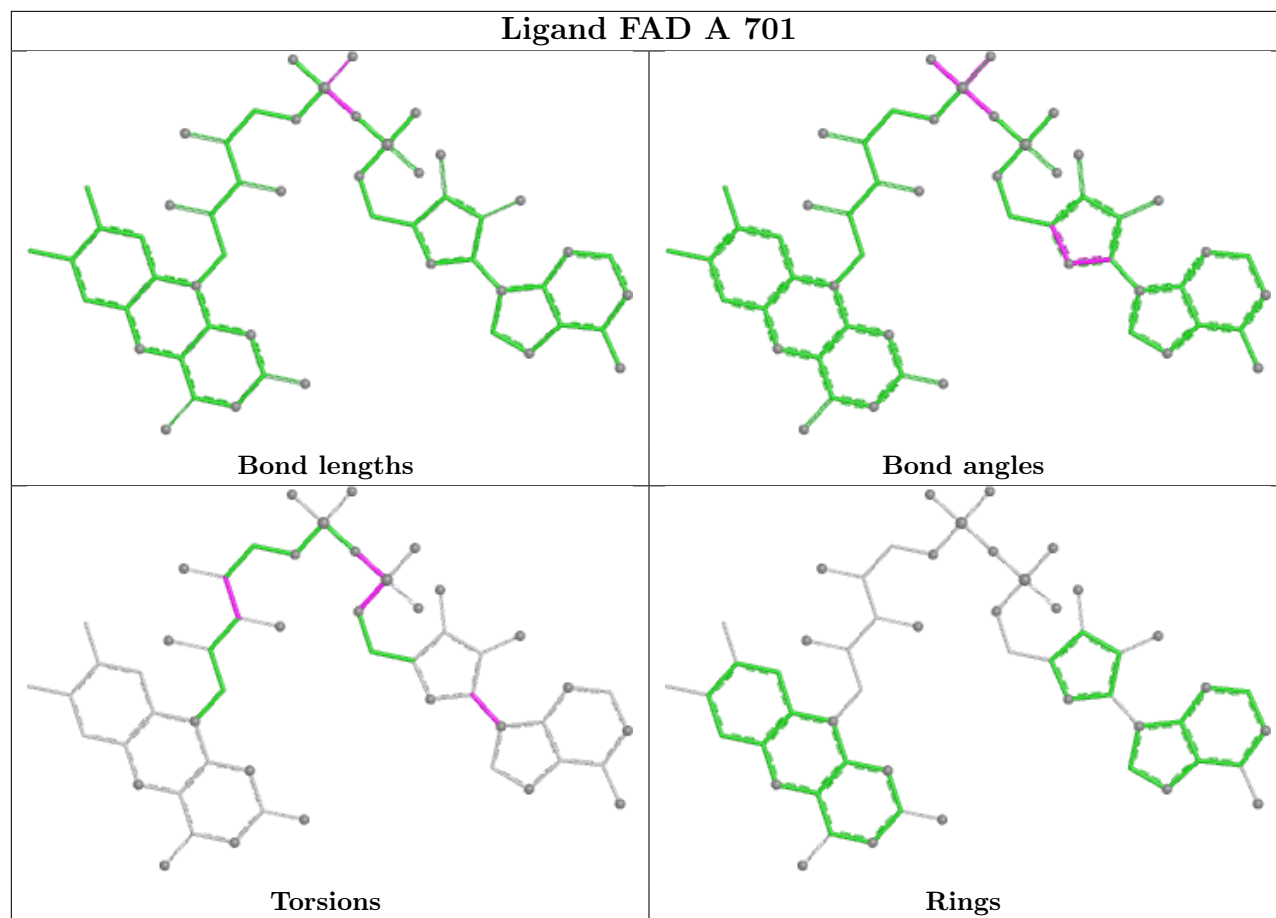


Torsions

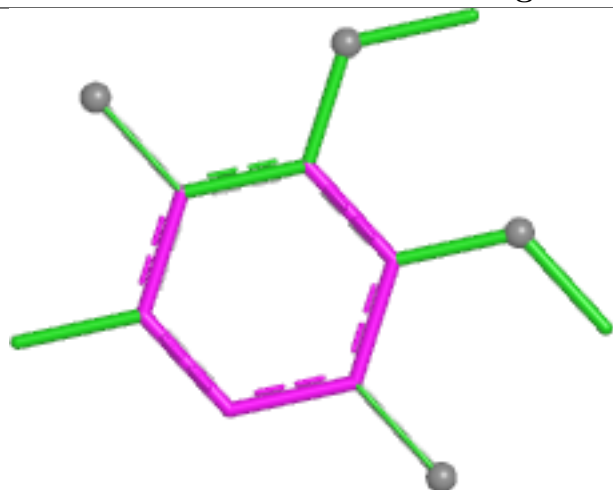


Rings

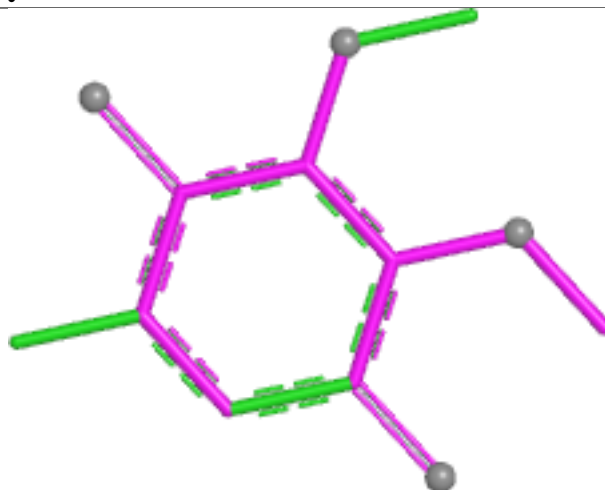




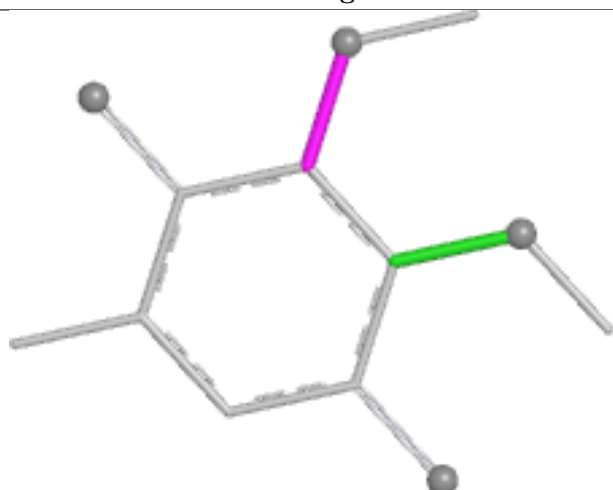
Ligand UQ0 B 705



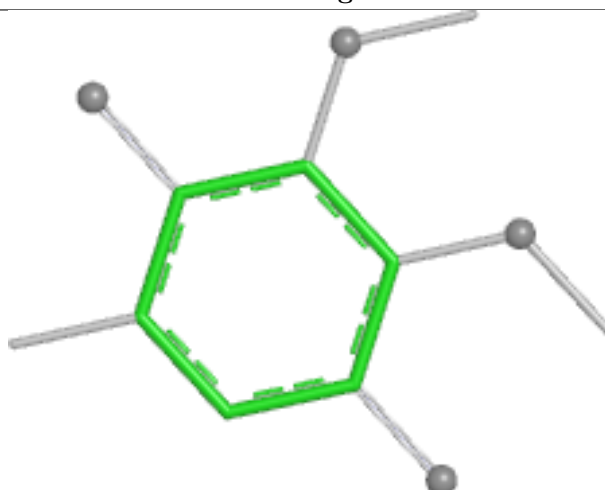
Bond lengths



Bond angles

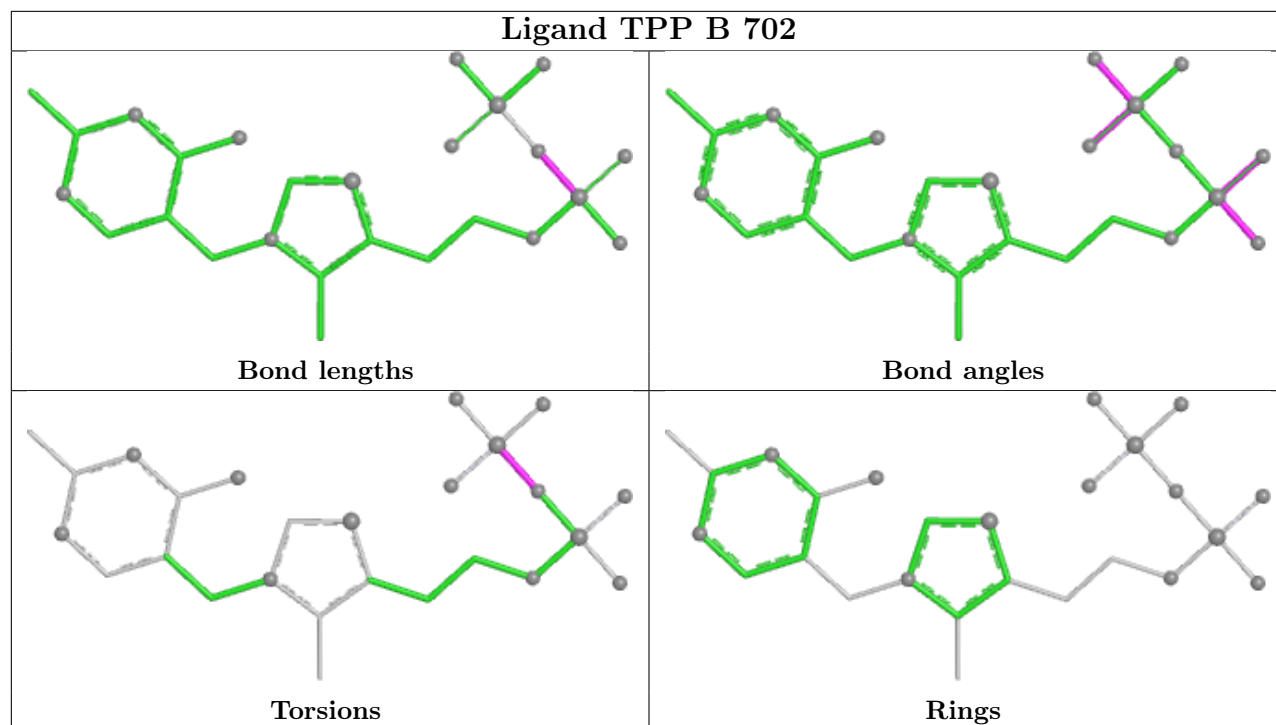


Torsions

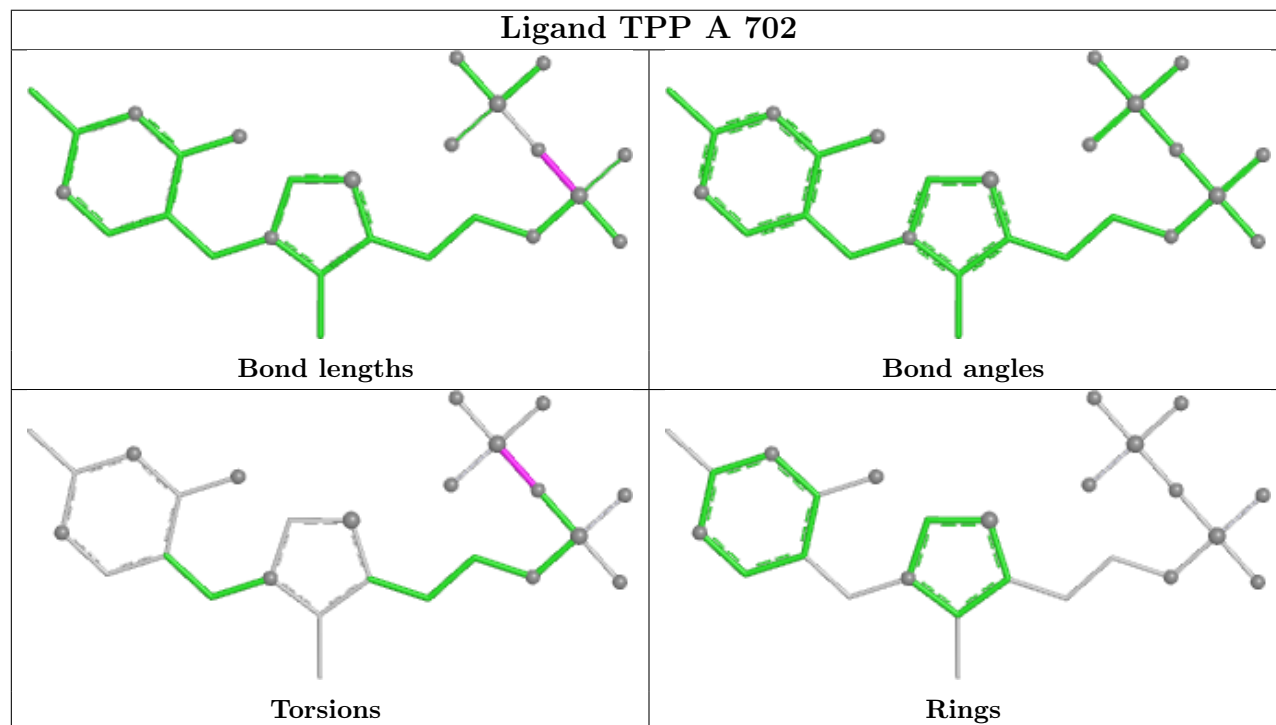


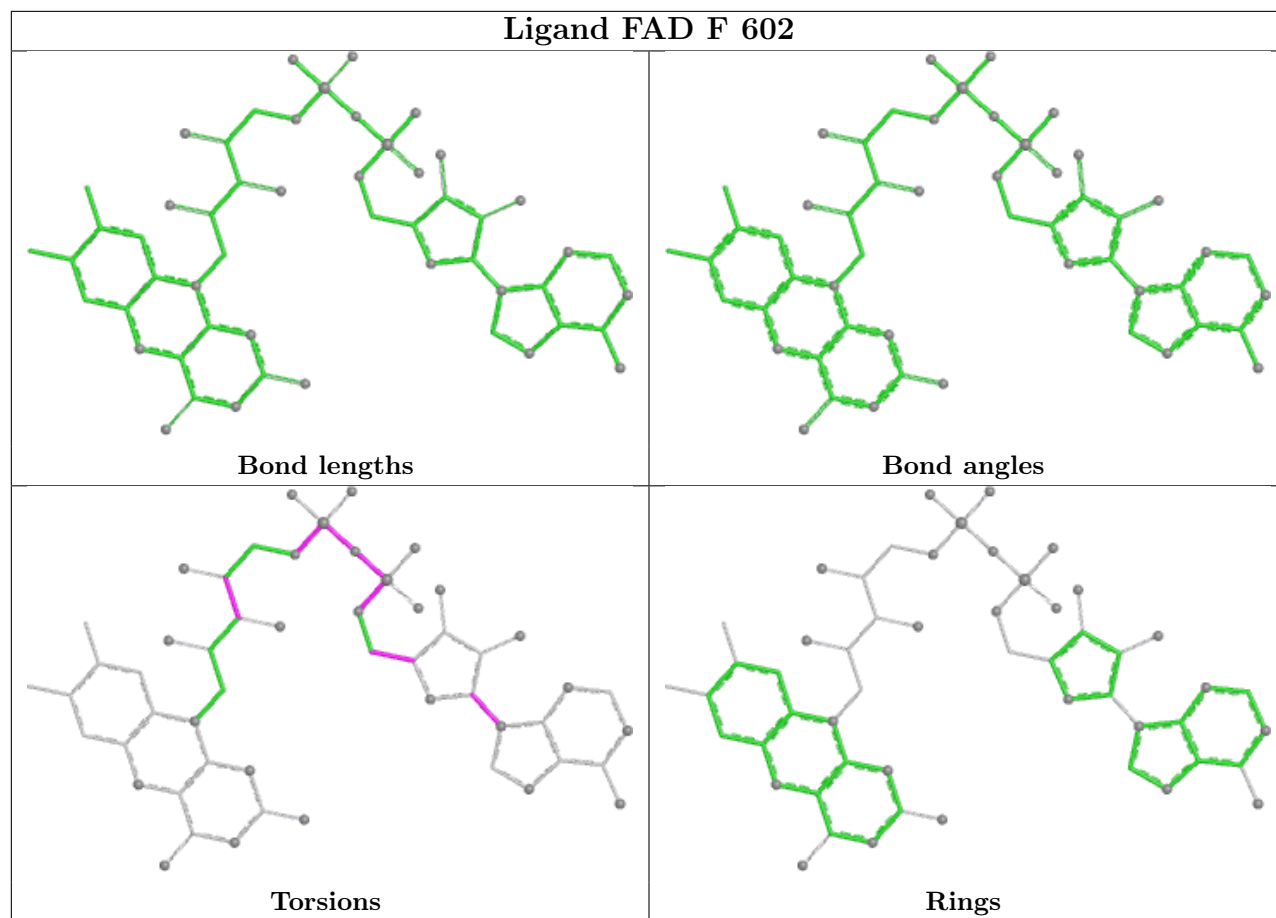
Rings

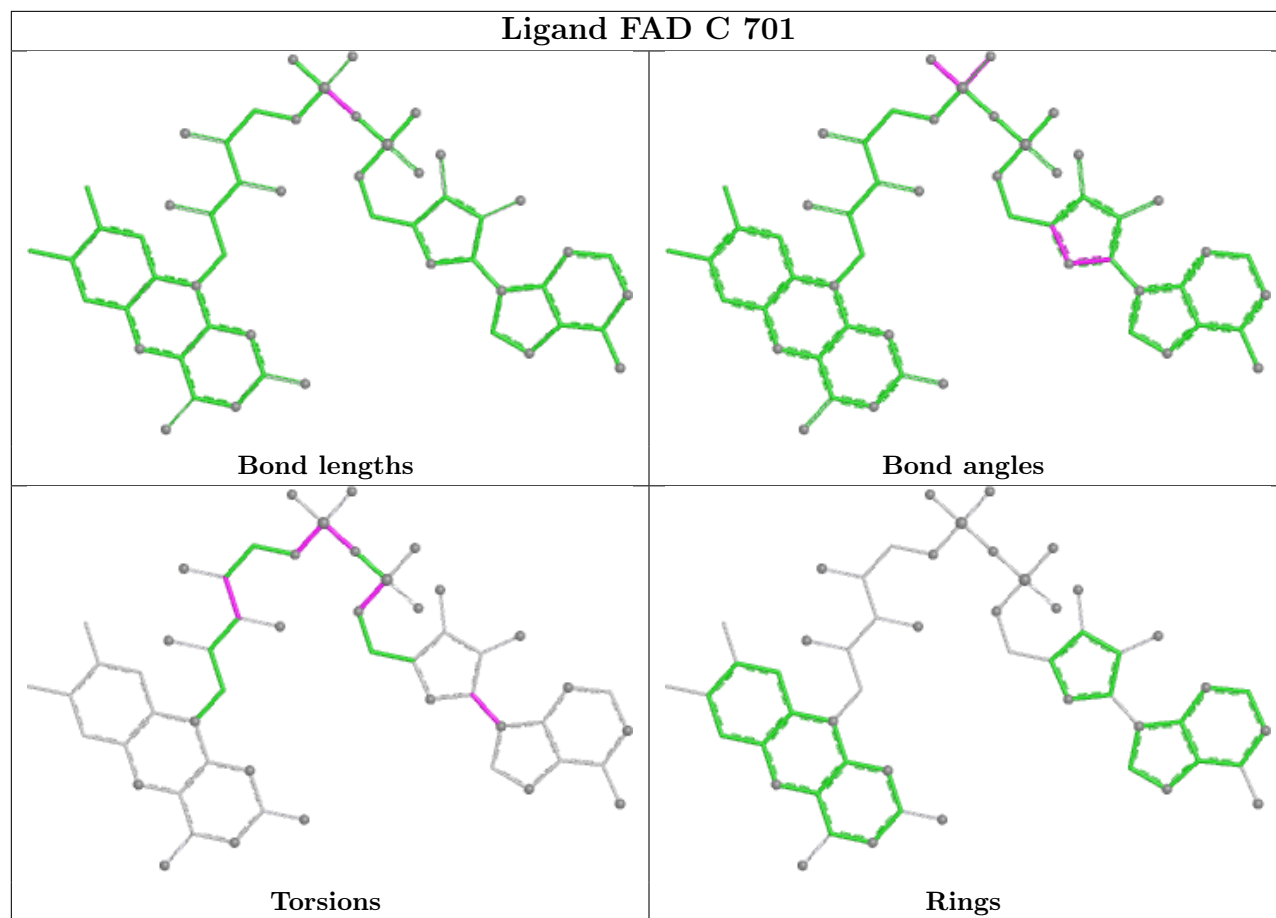
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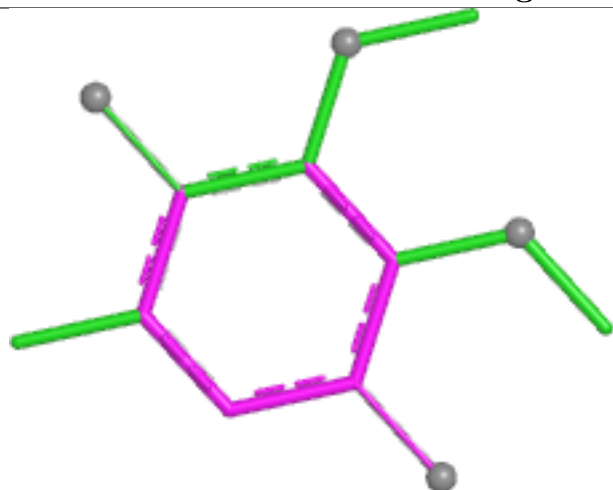
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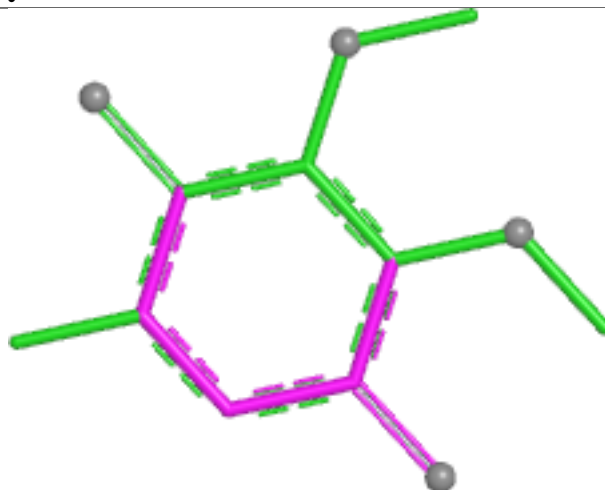




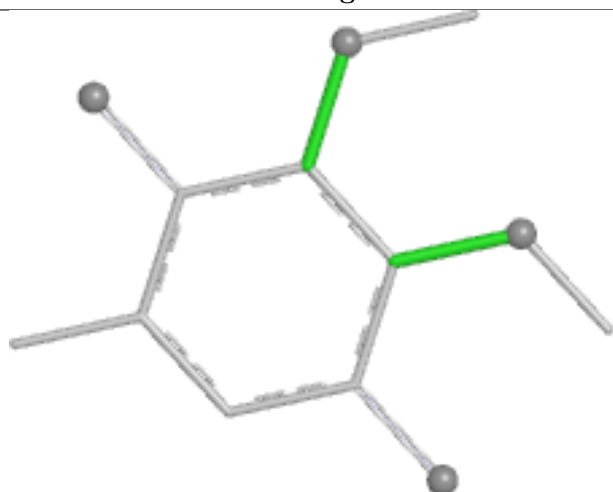
Ligand UQ0 B 706



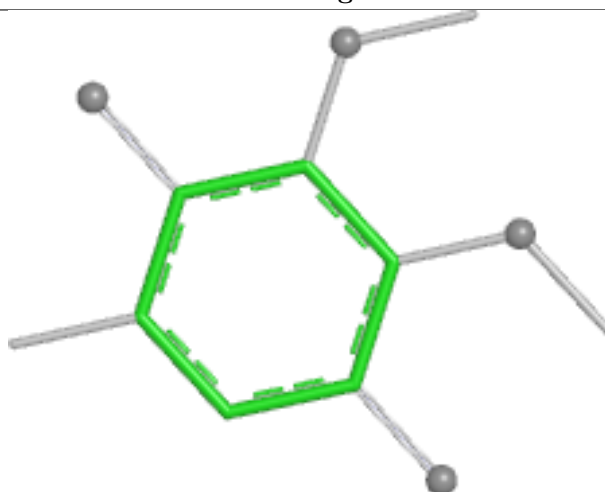
Bond lengths



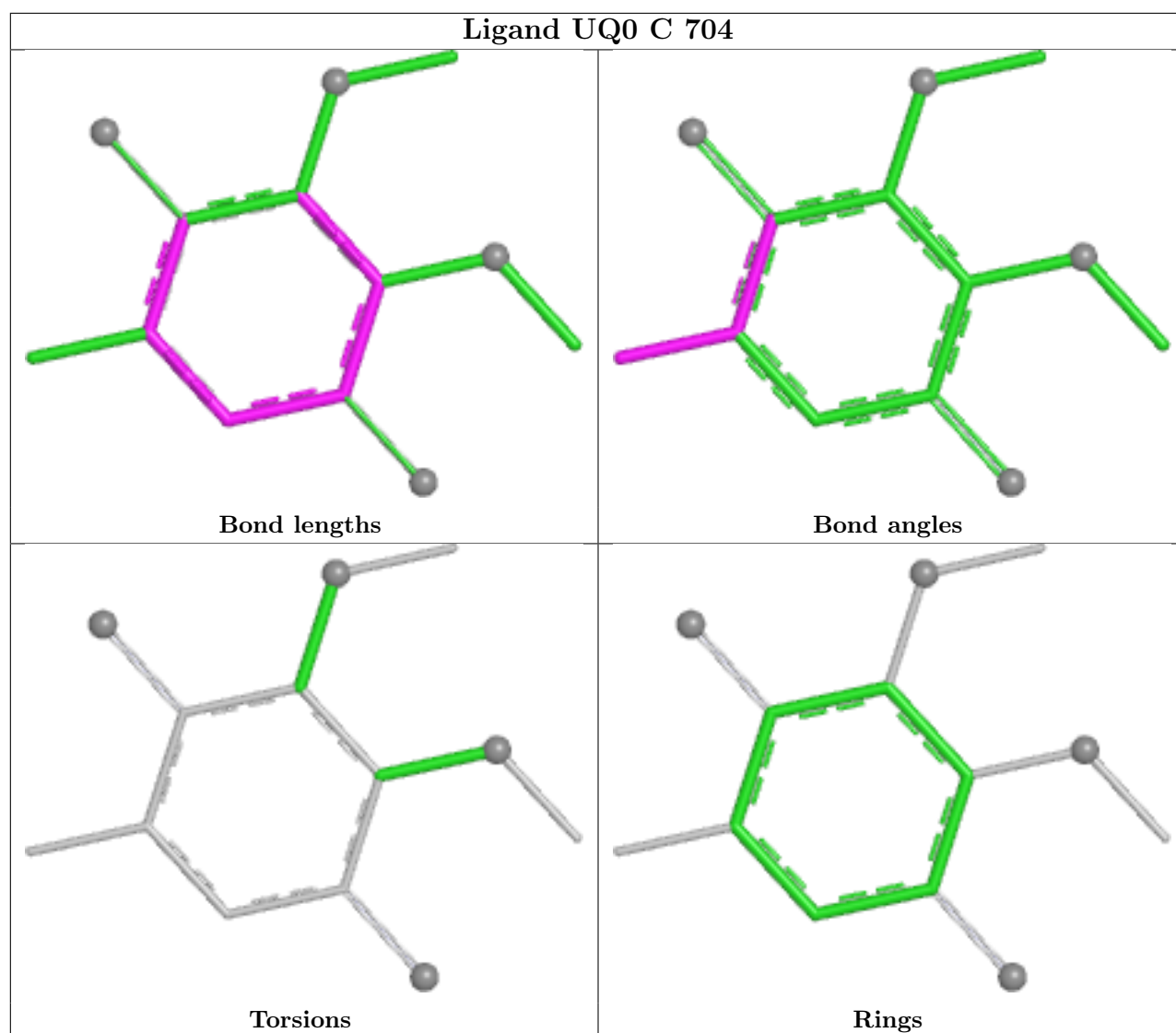
Bond angles



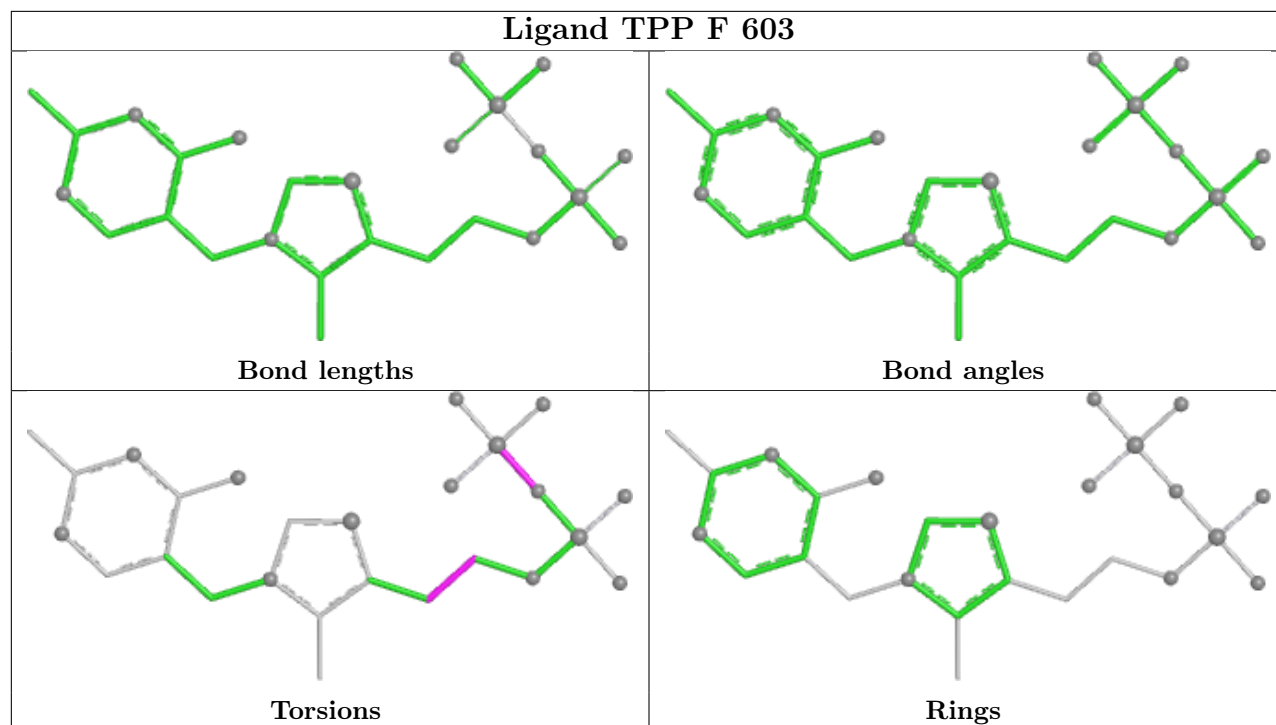
Torsions



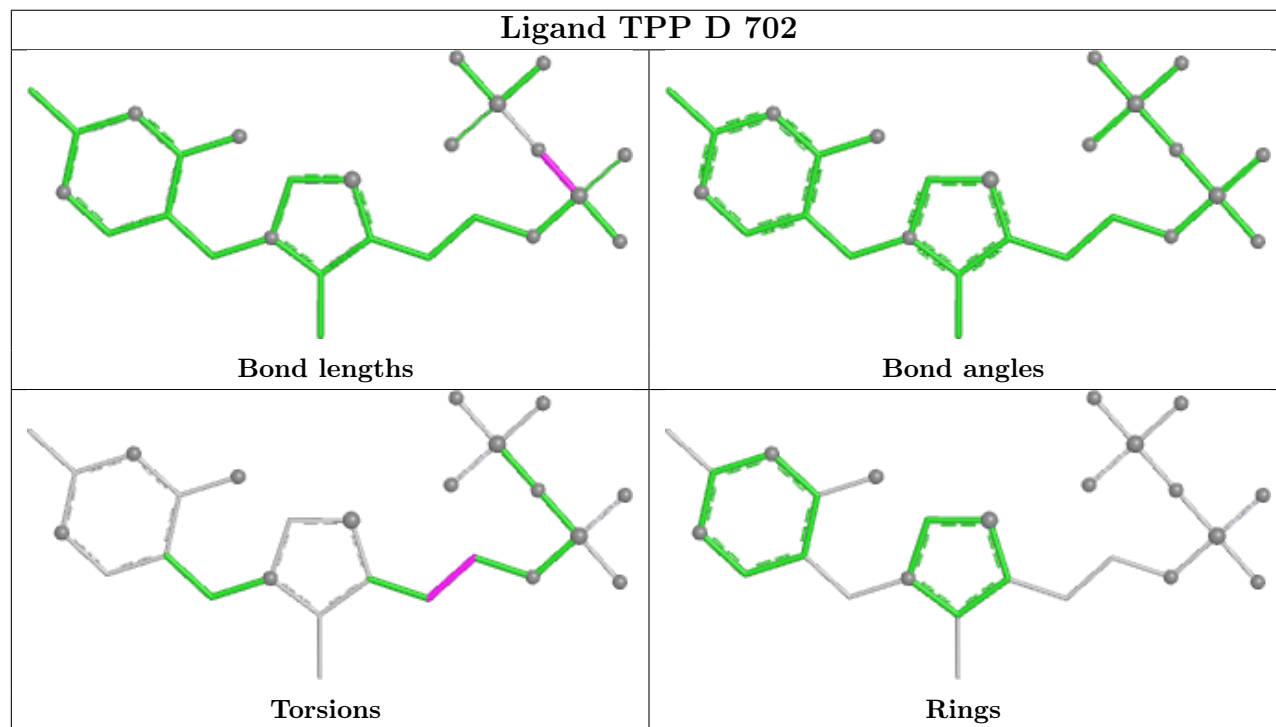
Rings



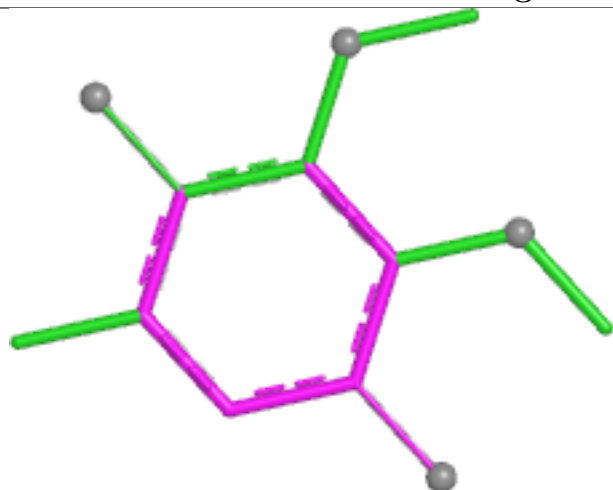
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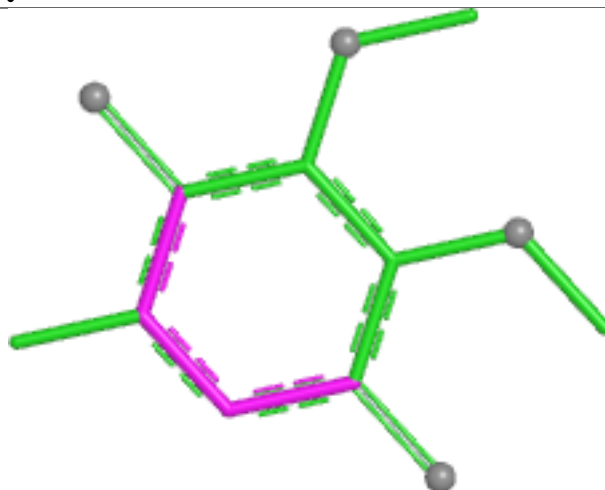
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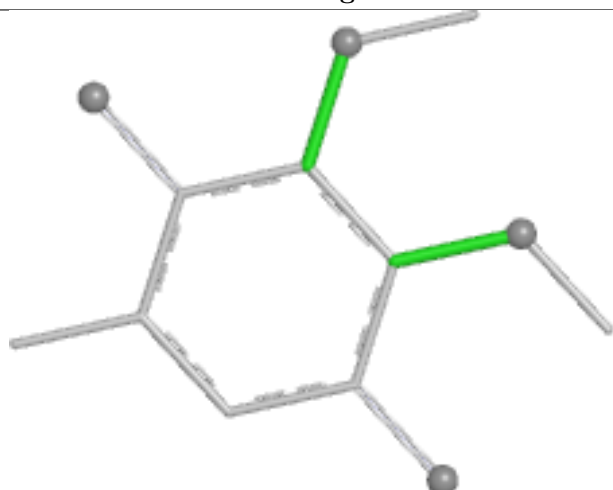
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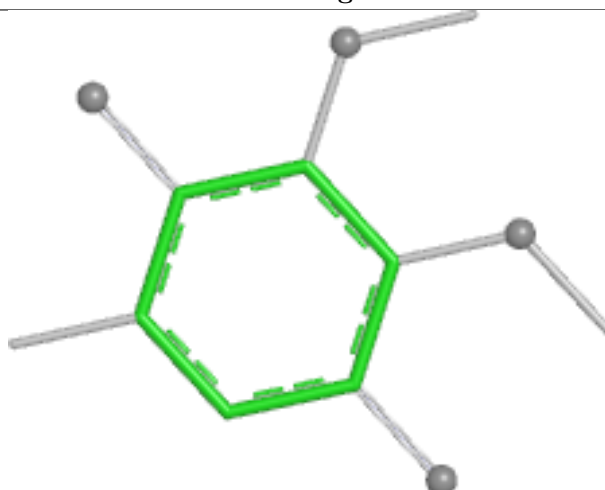
Bond lengths



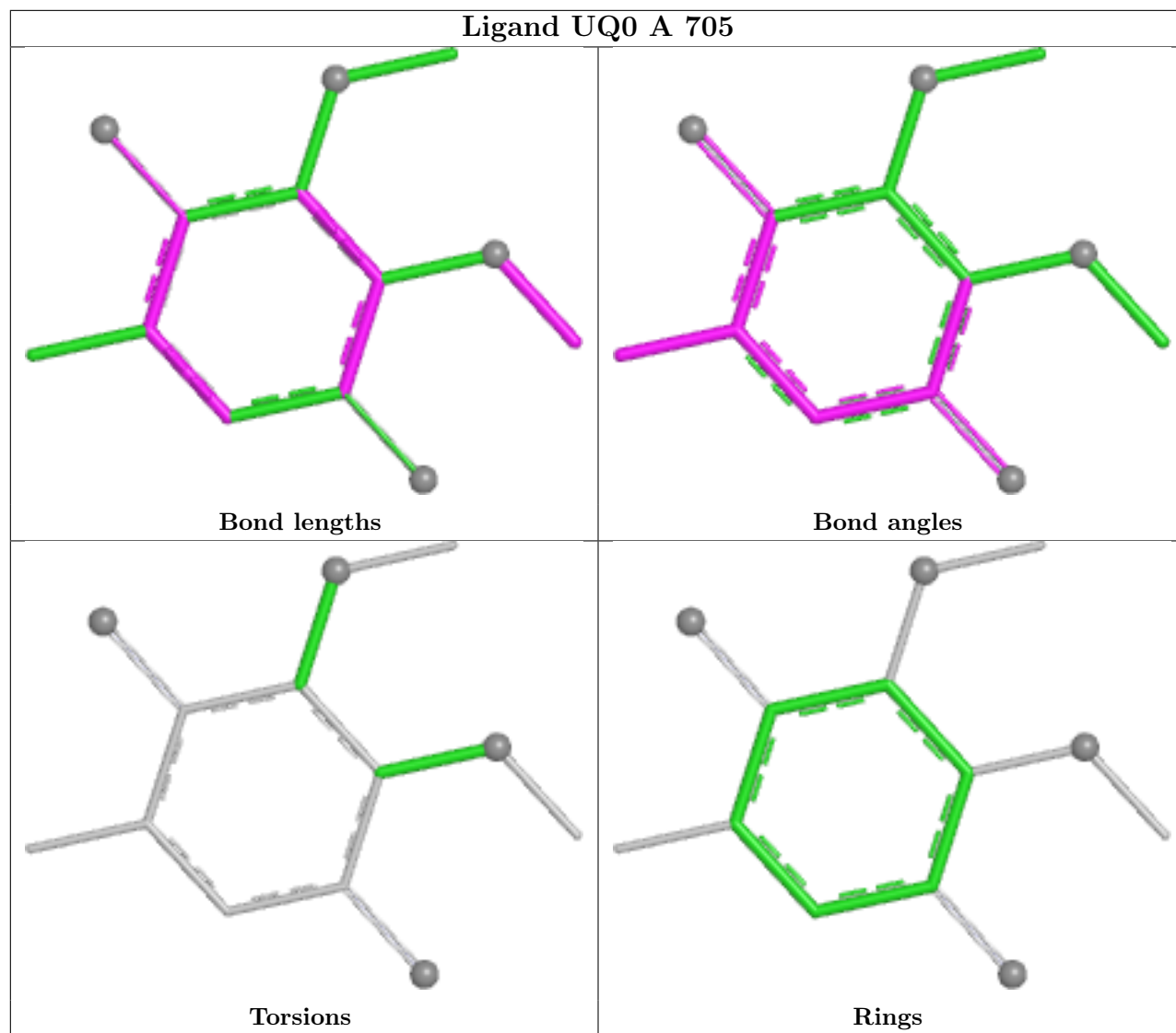
Bond angles



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%)	-0.73	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

All (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
1	C	110	HIS	3.1
1	F	107	ALA	3.0
1	C	339	ALA	3.0
1	D	485	ALA	2.9
1	F	109	LEU	2.9
1	A	593	GLU	2.9
1	E	38	ARG	2.8
1	E	593	GLU	2.8
1	F	111	LYS	2.8
1	C	202	GLN	2.7
1	F	110	HIS	2.5
1	F	313	CYS	2.5
1	C	108	ARG	2.5
1	C	340	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	0	GLY	2.4
1	B	593	GLU	2.4
1	A	110	HIS	2.4
1	C	1	MET	2.4
1	E	366	ASP	2.3
1	C	41	GLY	2.3
1	F	340	GLY	2.3
1	F	113	ASP	2.3
1	B	107	ALA	2.2
1	F	462	PHE	2.2
1	C	571	MET	2.2
1	E	110	HIS	2.2
1	F	108	ARG	2.2
1	F	569	ASN	2.2
1	D	109	LEU	2.2
1	D	1	MET	2.1
1	F	1	MET	2.1
1	C	107	ALA	2.1
1	F	593	GLU	2.1

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($\text{\AA}^2$)	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

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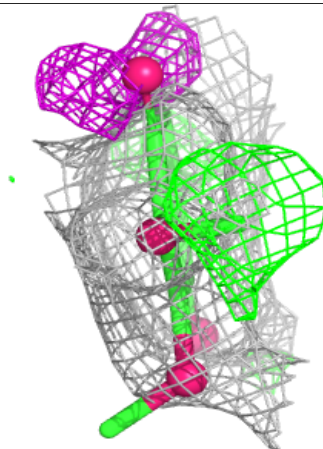
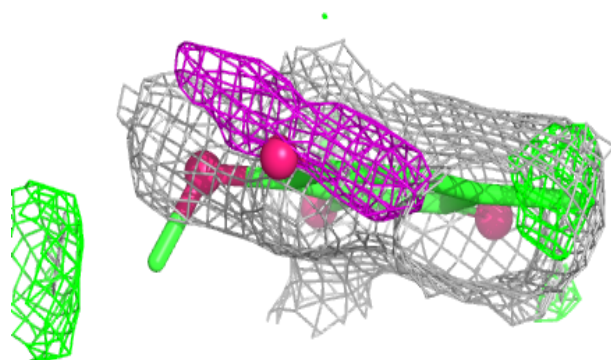
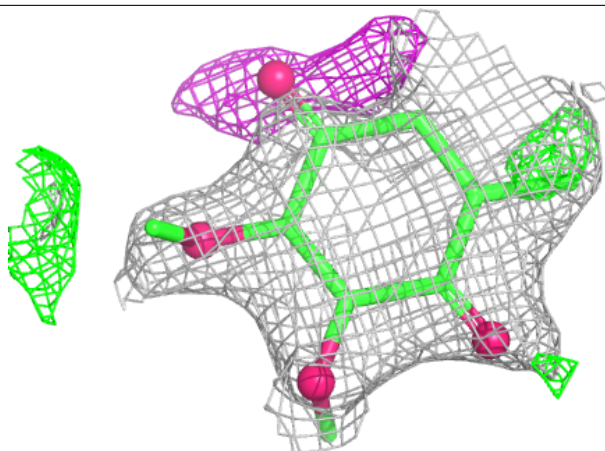
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	UQ0	D	706	13/13	0.84	0.14	55,59,62,62	0
5	UQ0	C	704	13/13	0.84	0.17	66,70,72,72	0
5	UQ0	A	705	13/13	0.87	0.11	26,33,36,36	0
5	UQ0	B	706	13/13	0.89	0.10	20,28,39,40	0
5	UQ0	A	706	13/13	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.

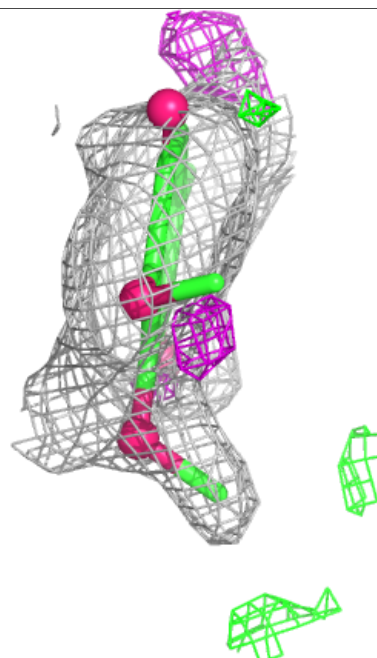
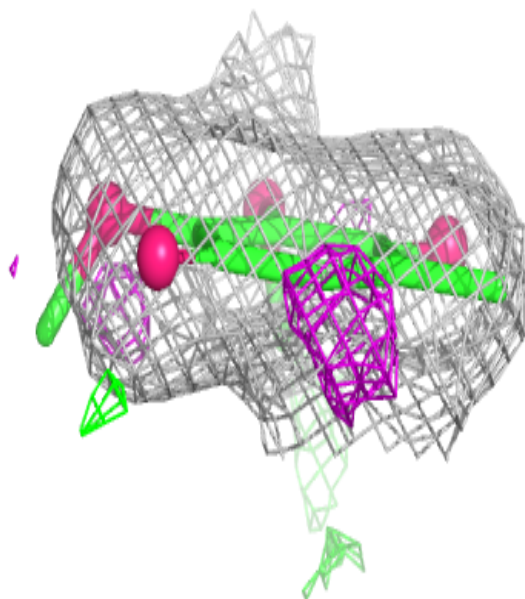
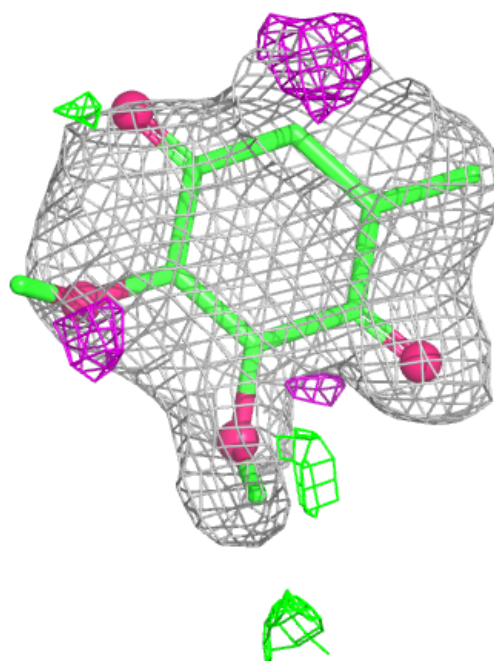
Electron density around UQ0 E 601:

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



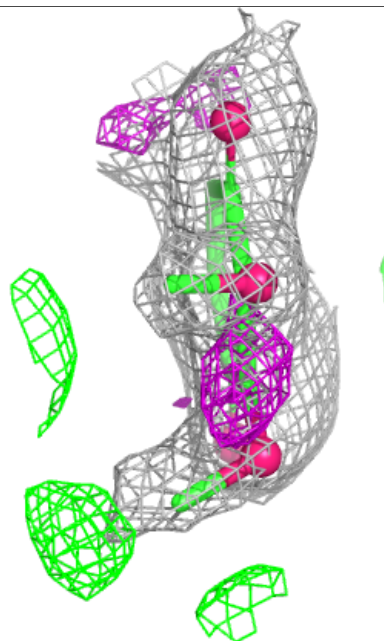
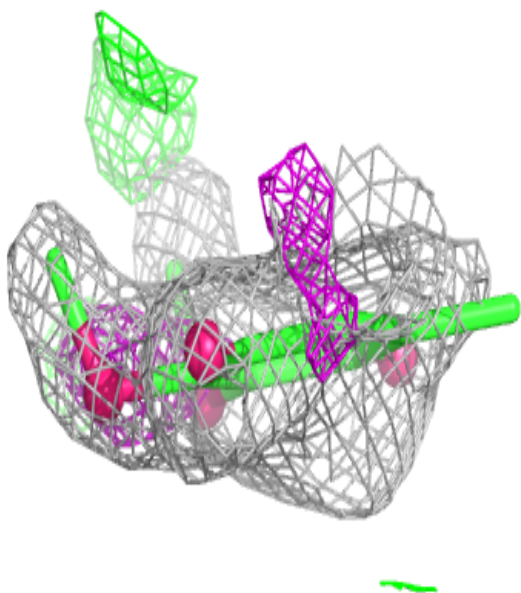
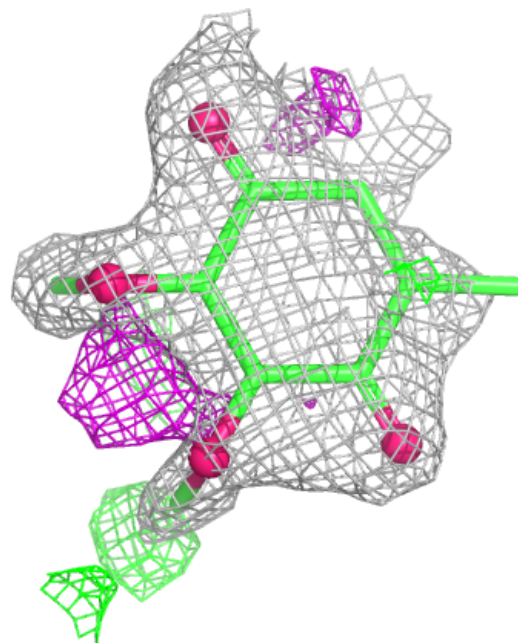
Electron density around UQ0 F 601:

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



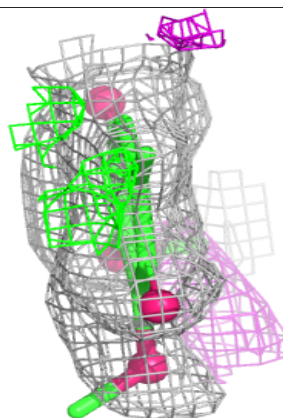
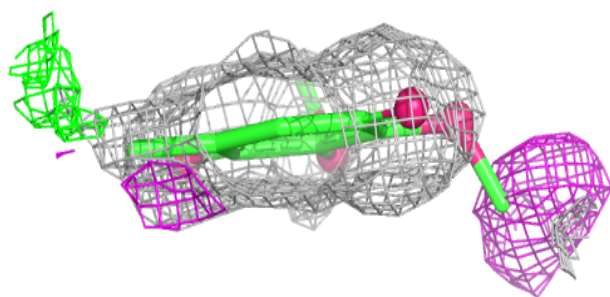
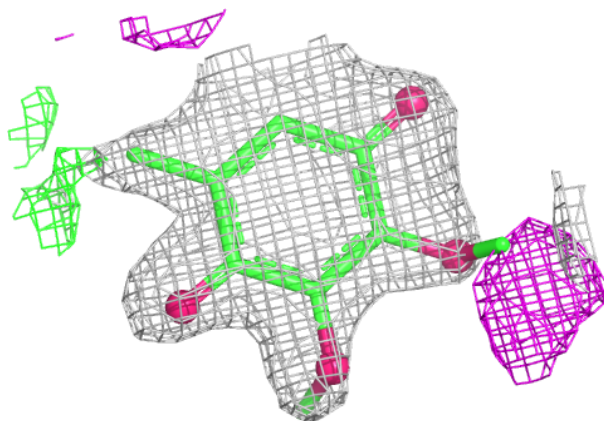
Electron density around UQ0 C 706:

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



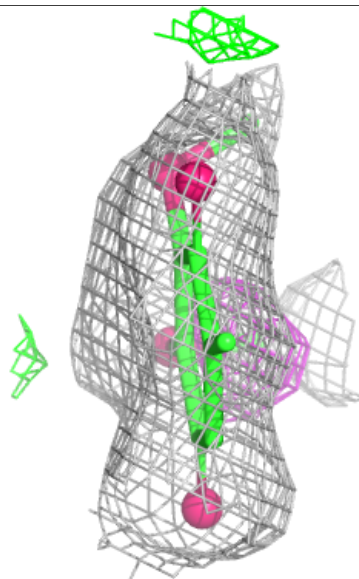
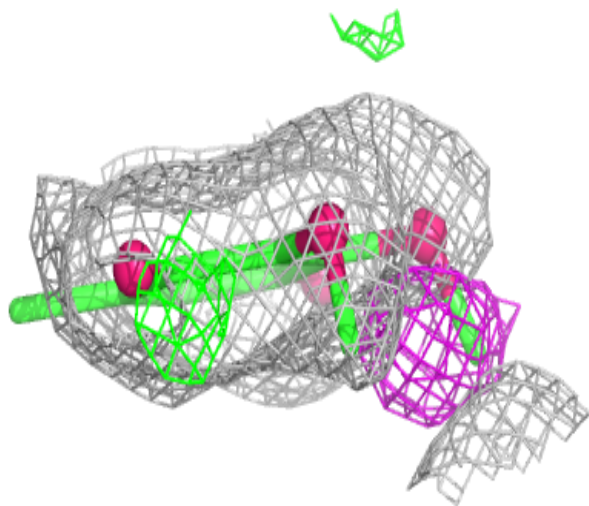
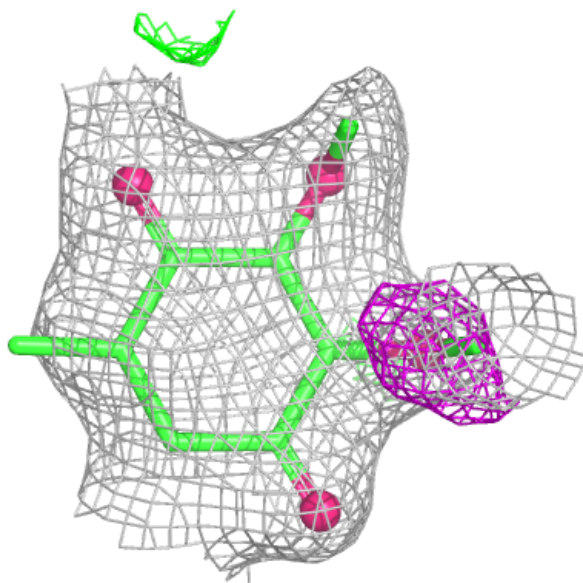
Electron density around UQ0 E 605:

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



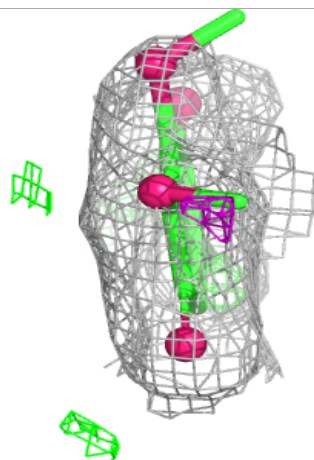
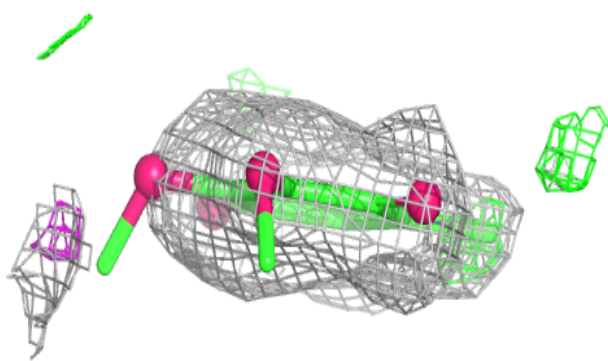
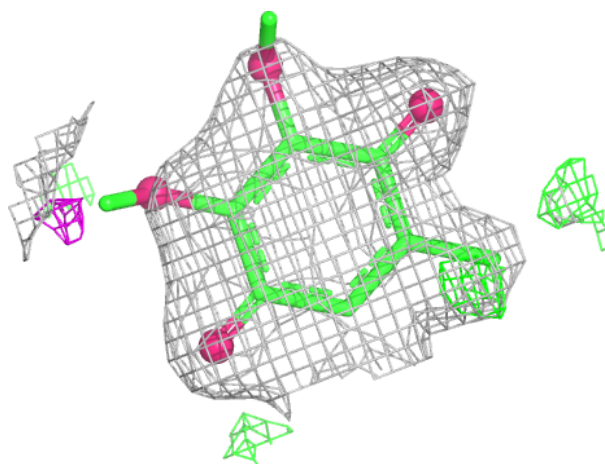
Electron density around UQ0 D 706:

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



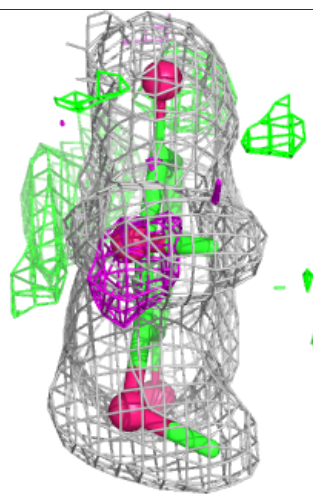
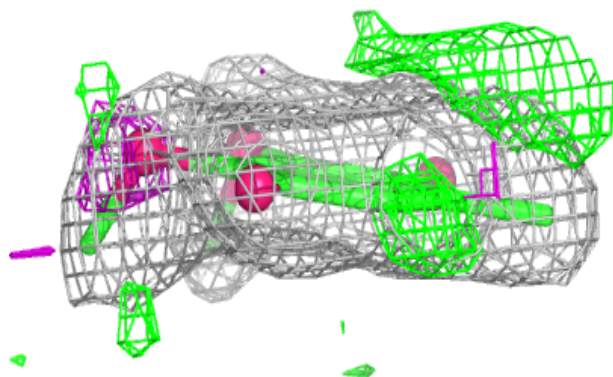
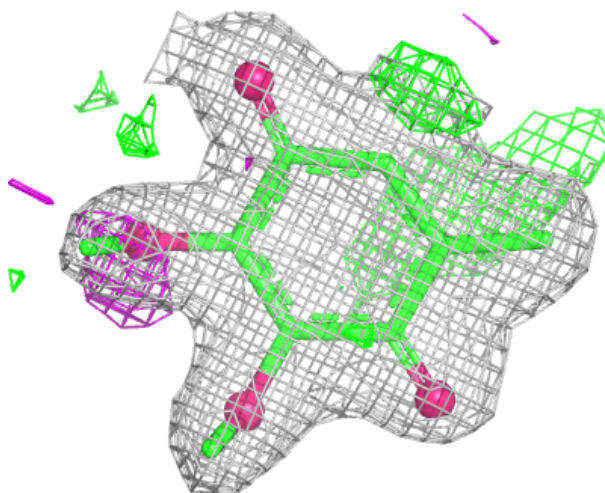
Electron density around UQ0 C 704:

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



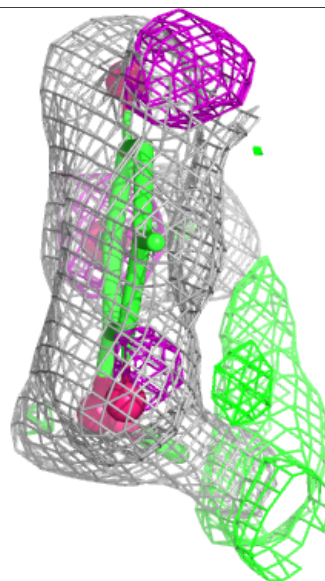
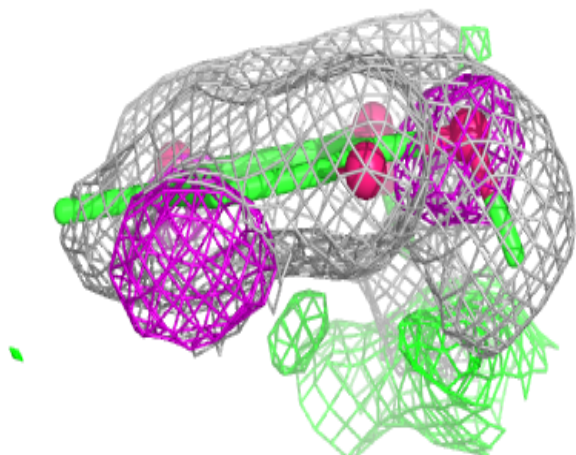
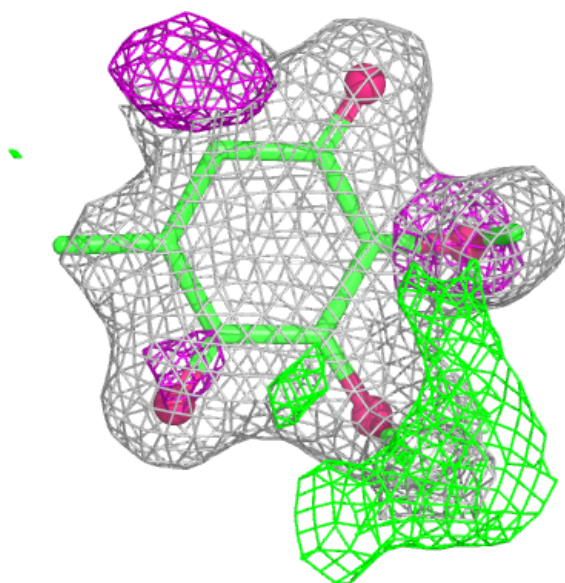
Electron density around UQ0 A 705:

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



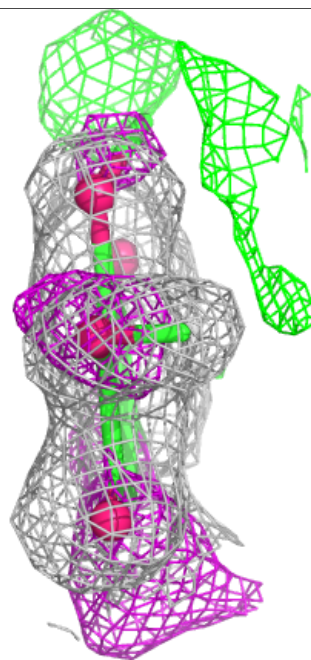
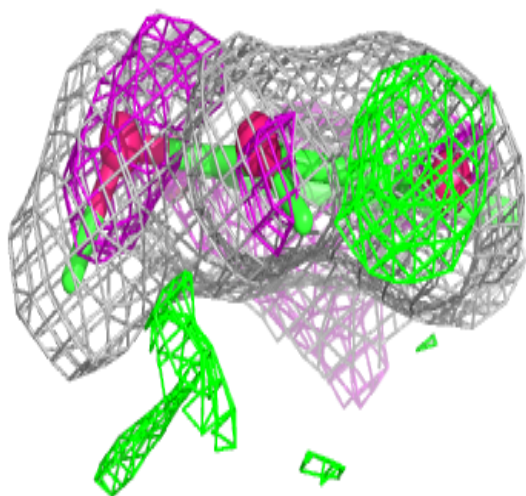
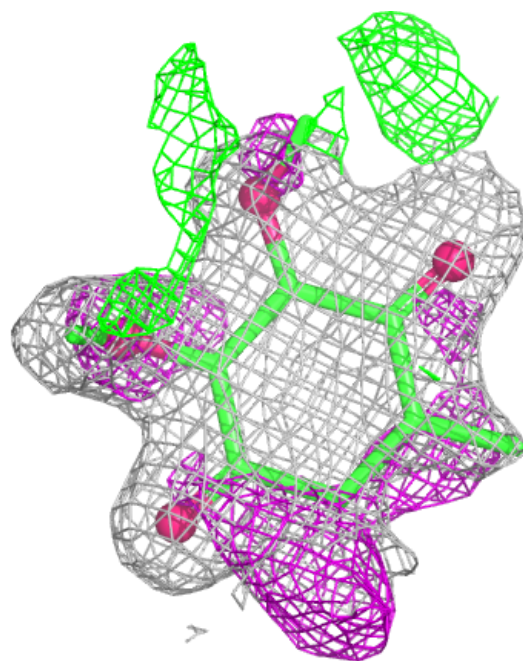
Electron density around UQ0 B 706:

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



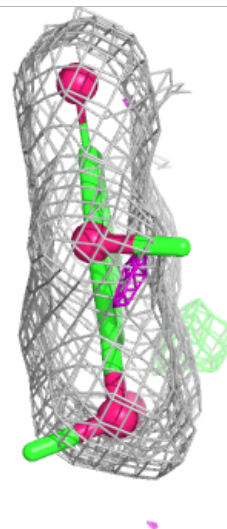
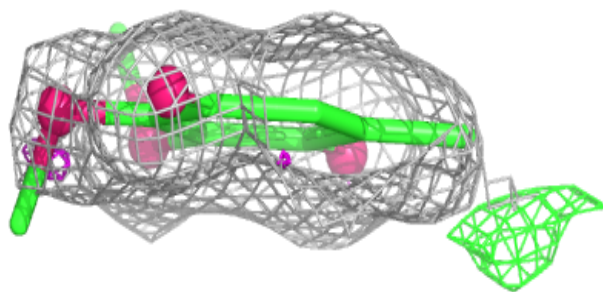
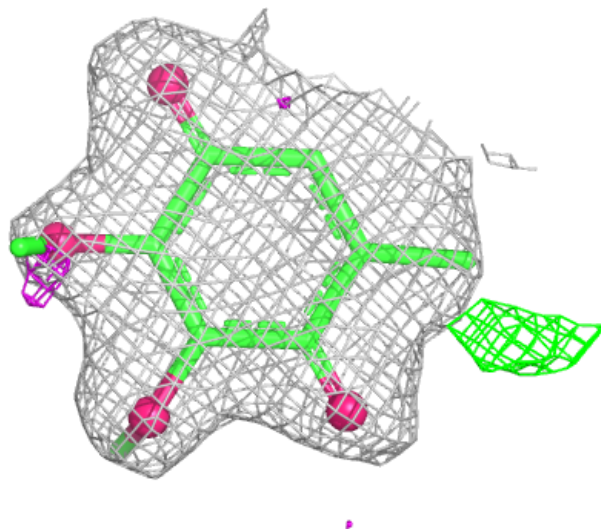
Electron density around UQ0 A 706:

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



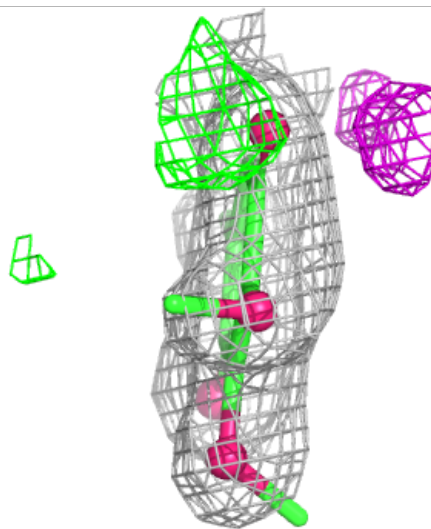
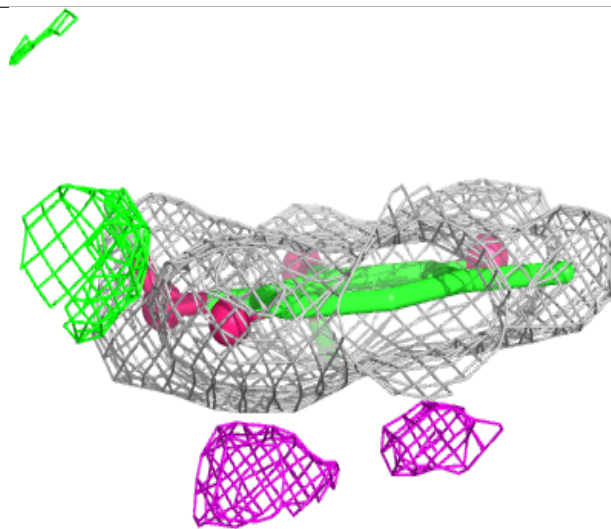
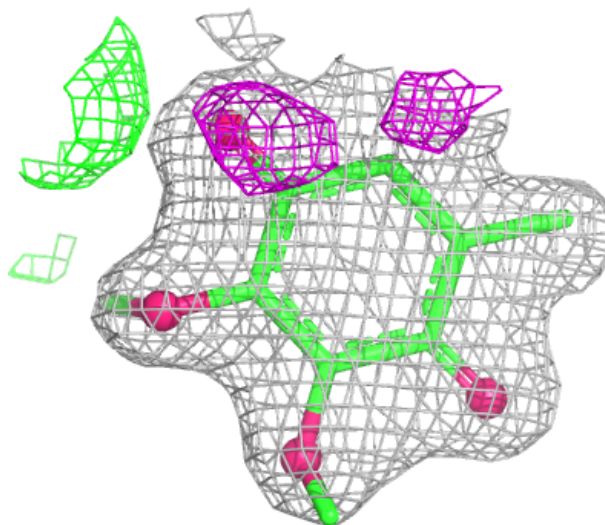
Electron density around UQ0 D 704:

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



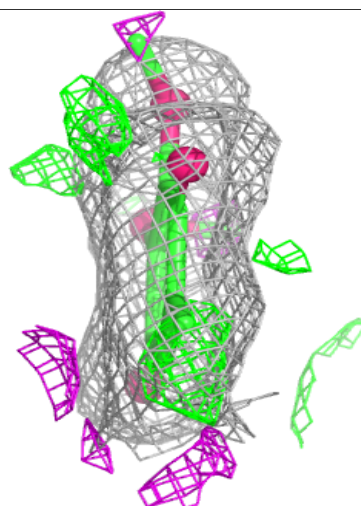
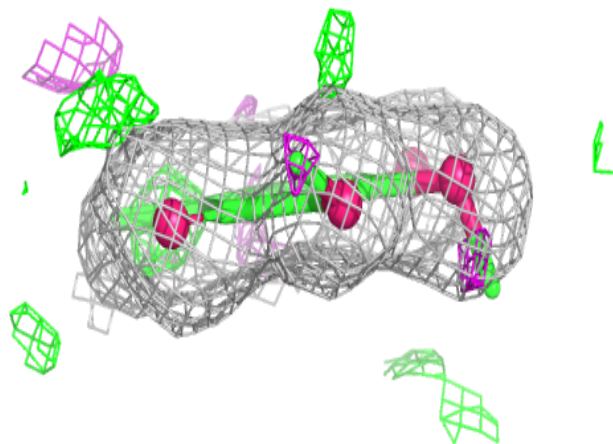
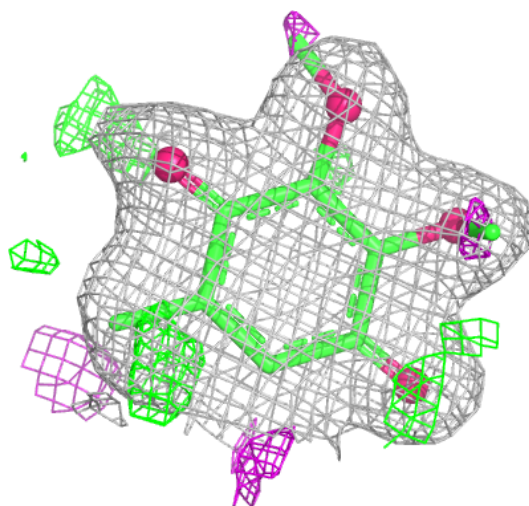
Electron density around UQ0 F 605:

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



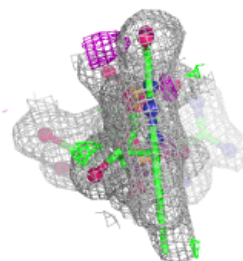
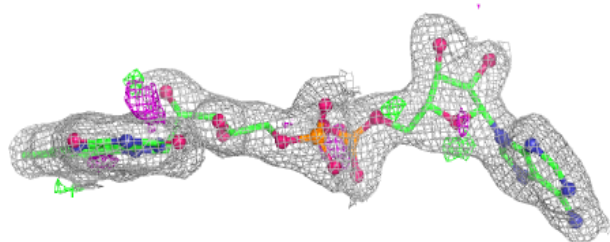
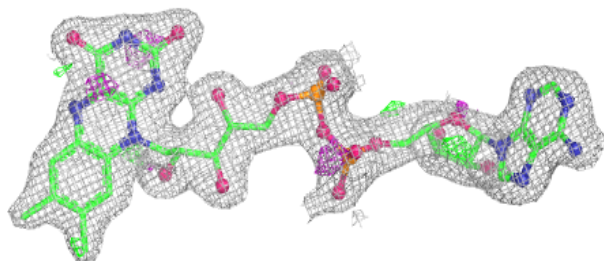
Electron density around UQ0 B 705:

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and green (positive)

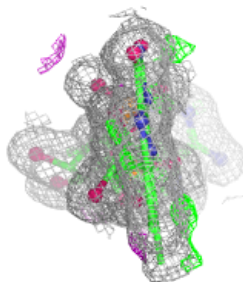
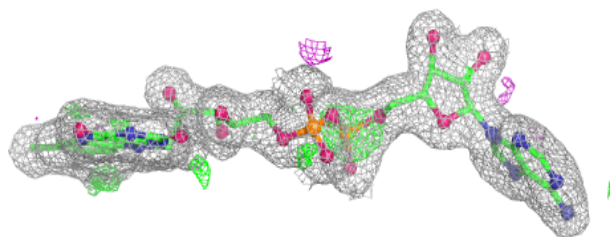
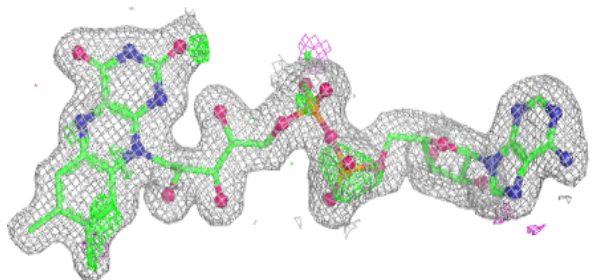


Electron density around FAD E 602:

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

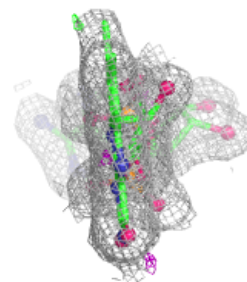
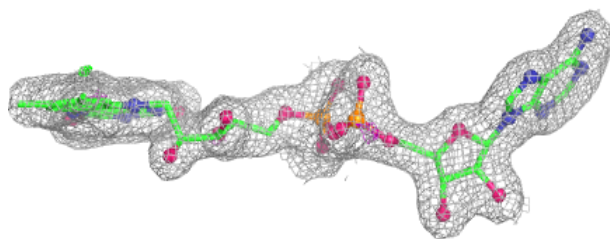
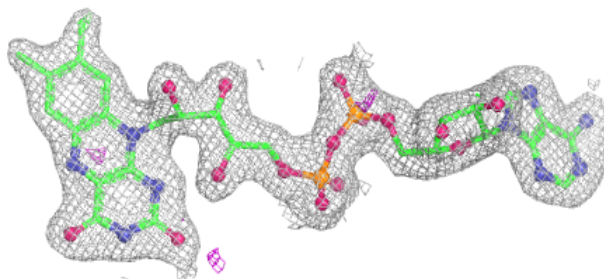
**Electron density around FAD B 701:**

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

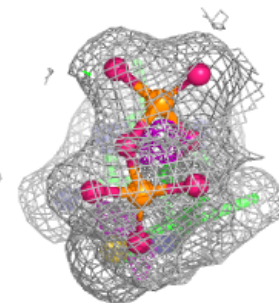
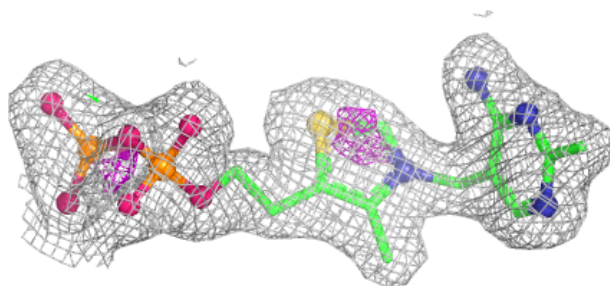
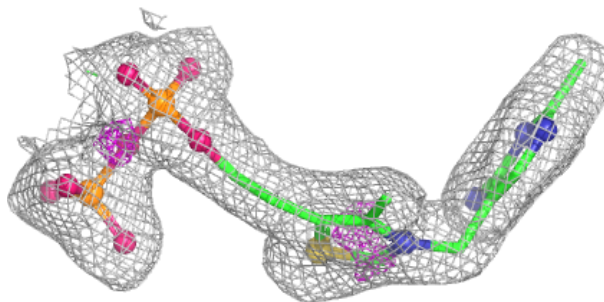


Electron density around FAD F 602:

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and green (positive)

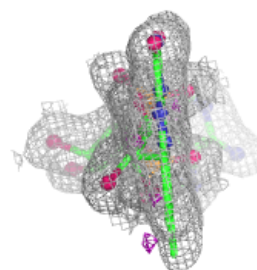
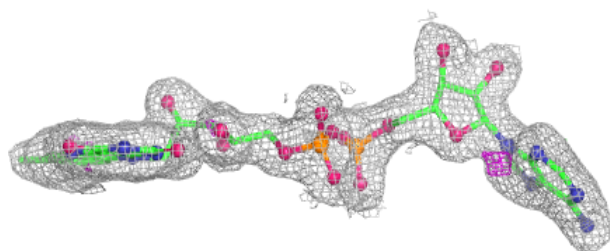
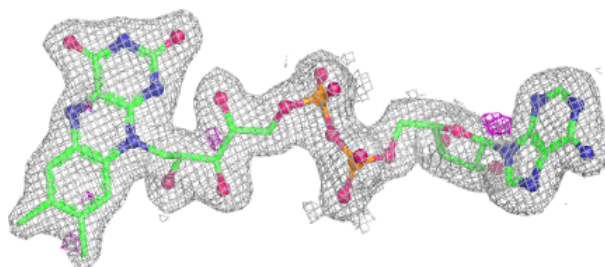
**Electron density around TPP F 603:**

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

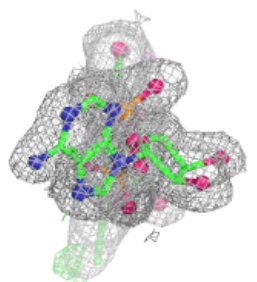
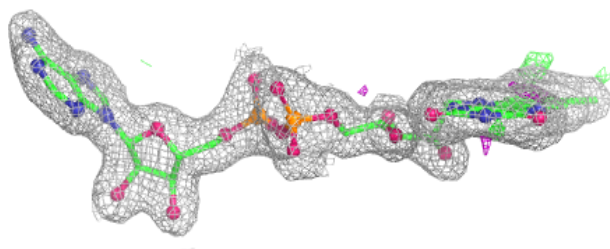
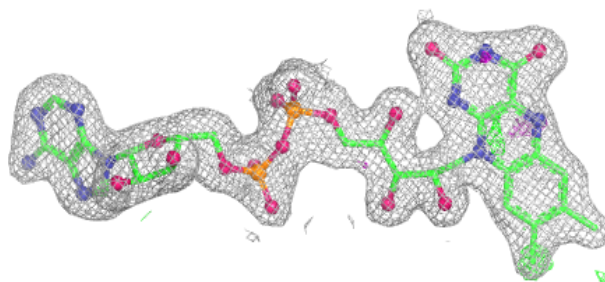


Electron density around FAD C 701:

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

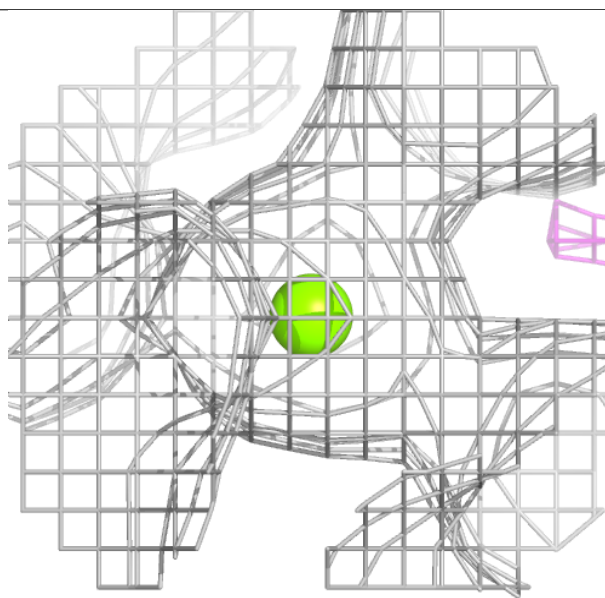
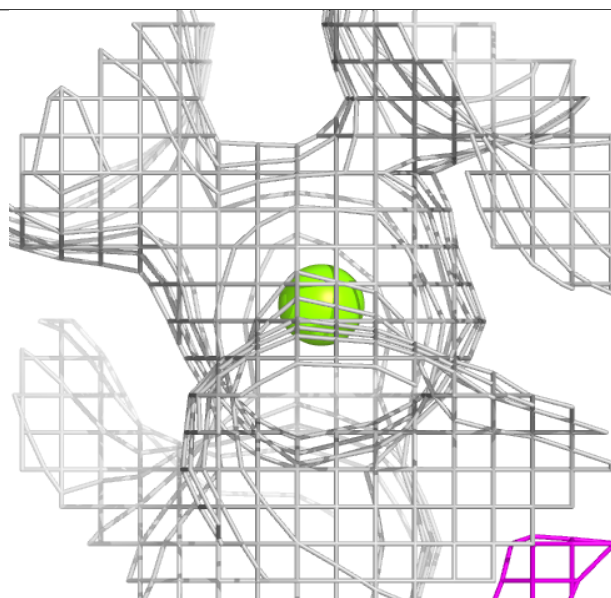
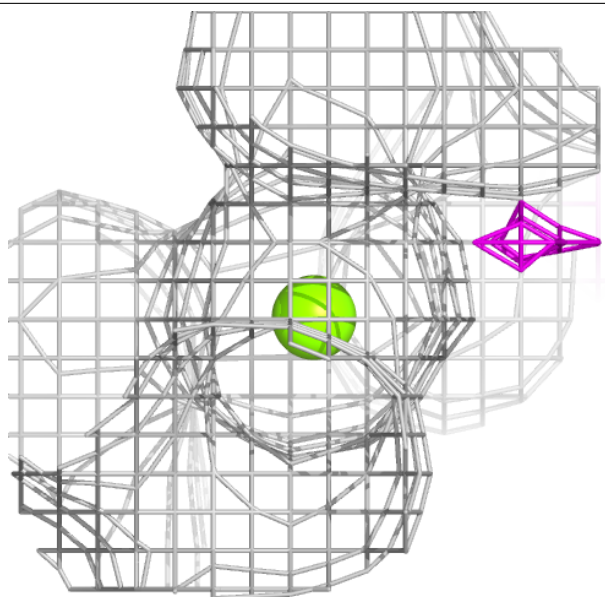
**Electron density around FAD D 701:**

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



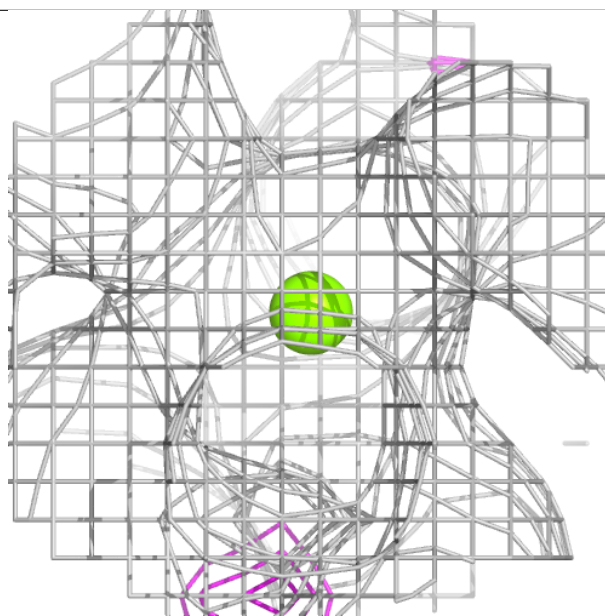
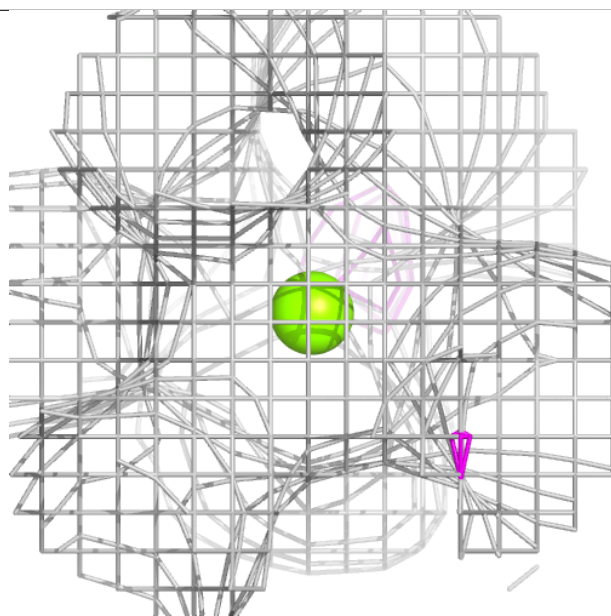
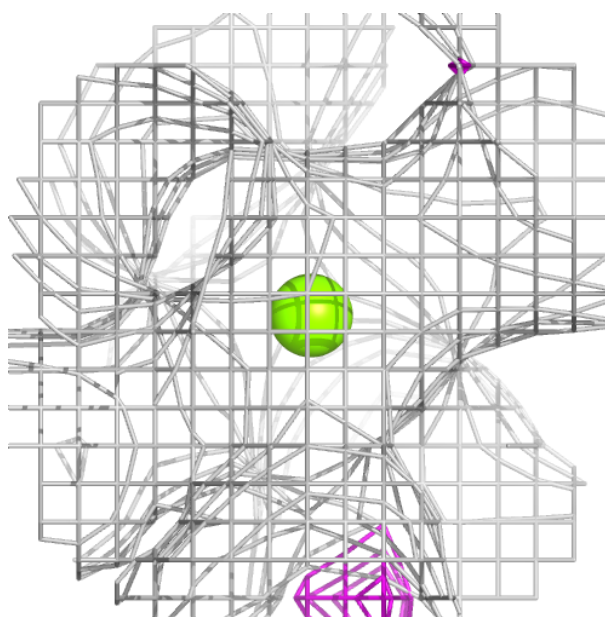
Electron density around MG D 705:

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



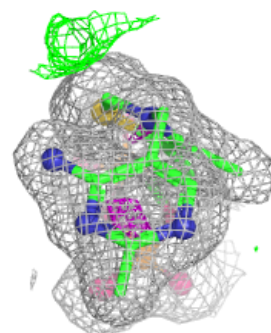
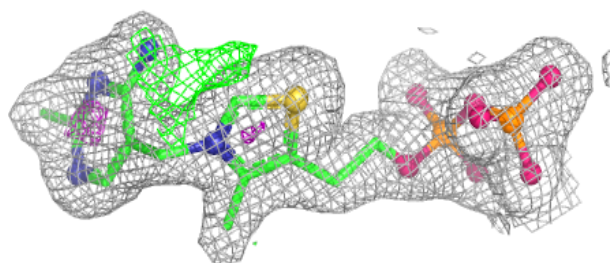
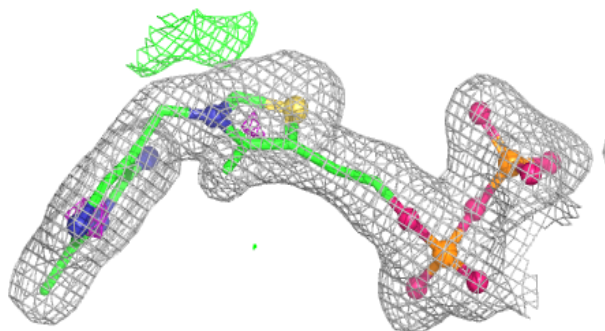
Electron density around MG F 604:

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and green (positive)

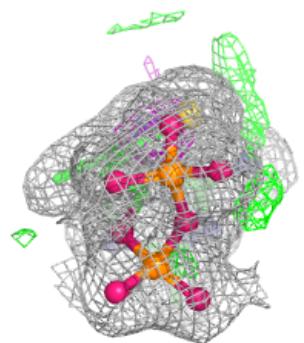
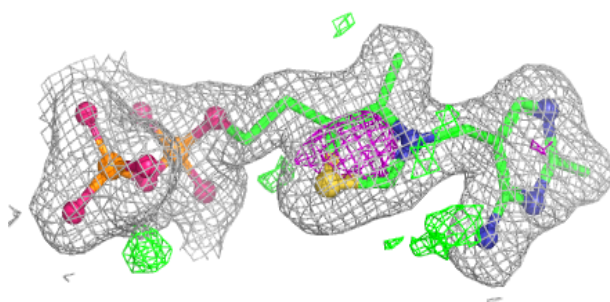
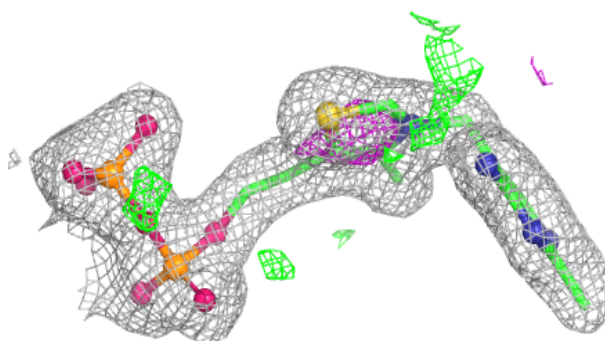


Electron density around TPP C 702:

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

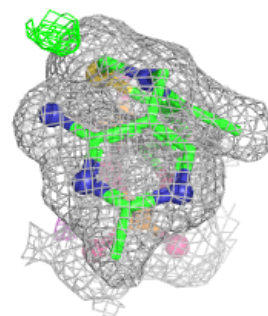
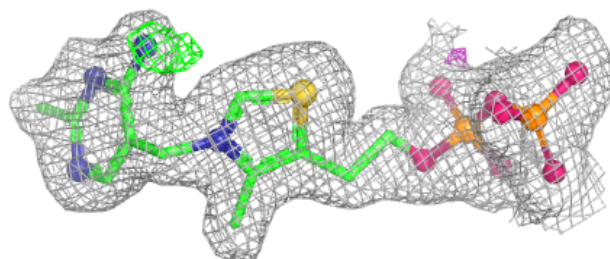
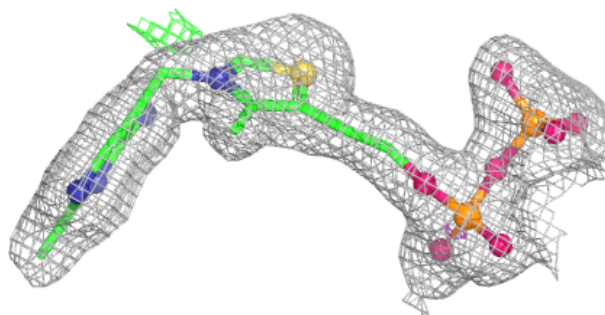
**Electron density around TPP D 702:**

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and green (positive)

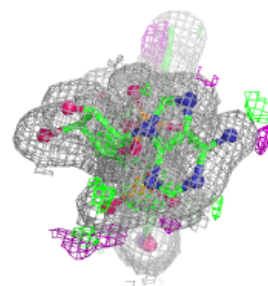
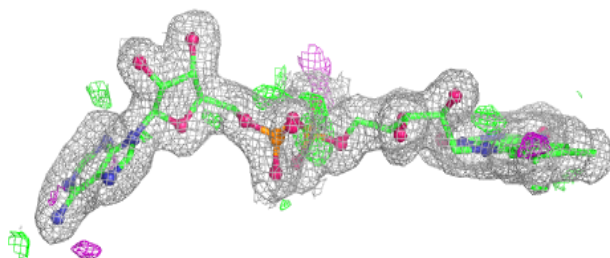
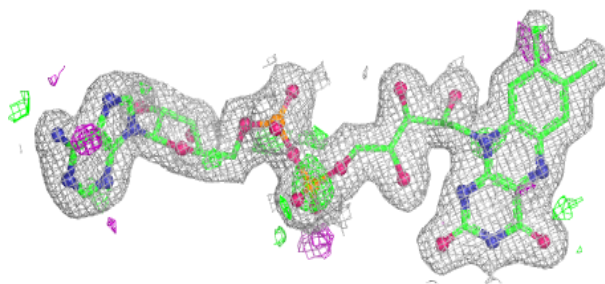


Electron density around TPP E 603:

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and green (positive)

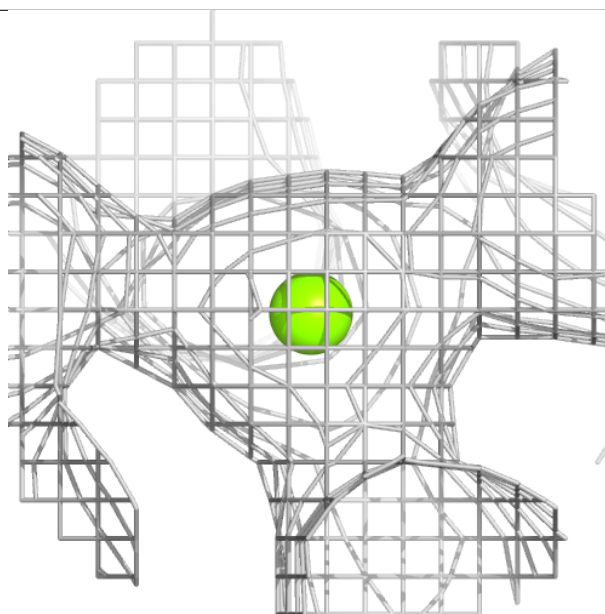
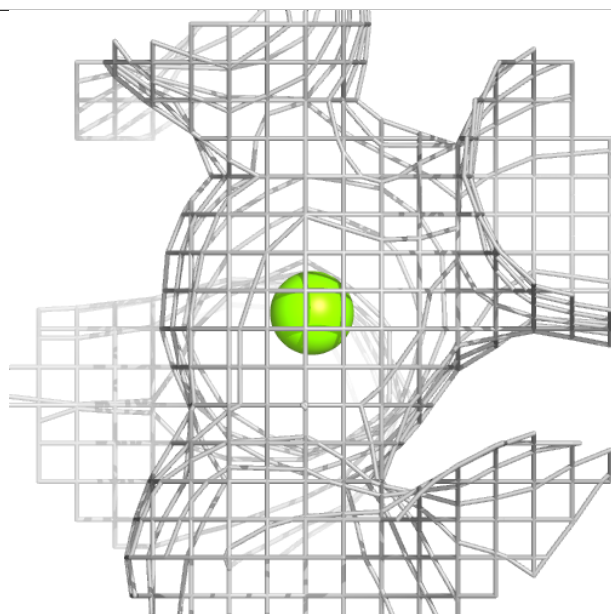
**Electron density around FAD A 701:**

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



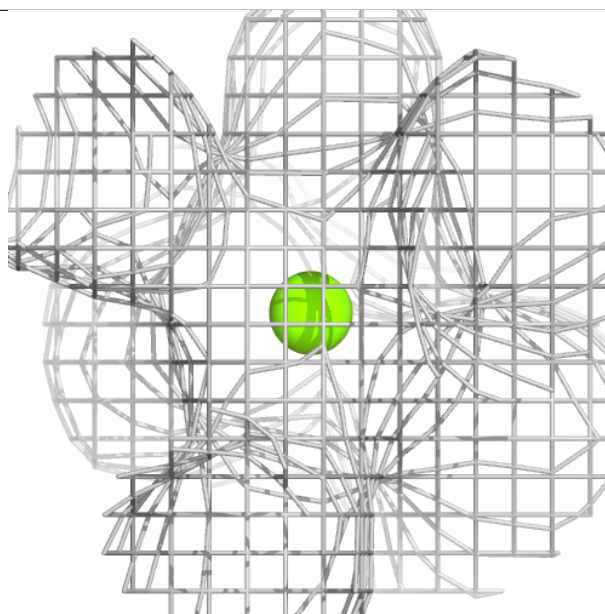
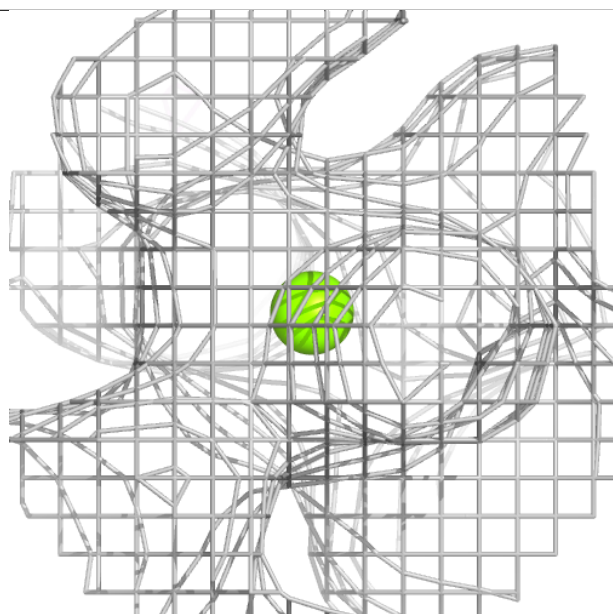
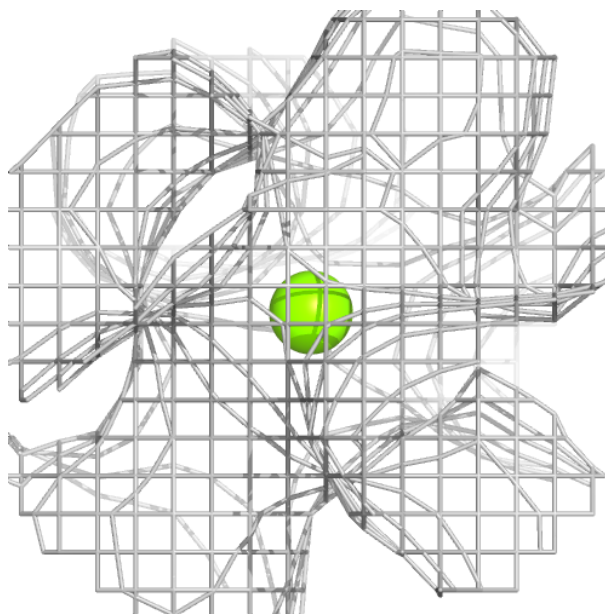
Electron density around MG C 705:

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



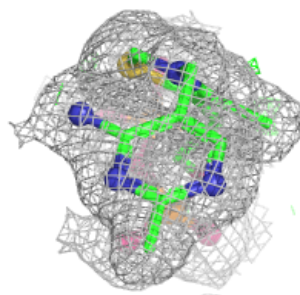
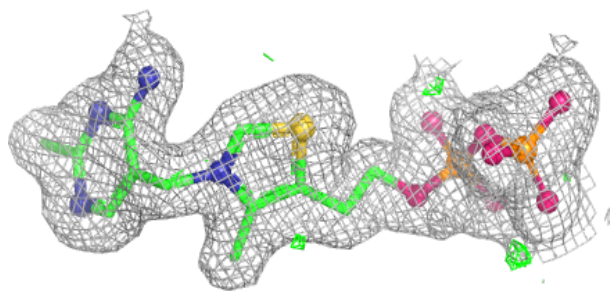
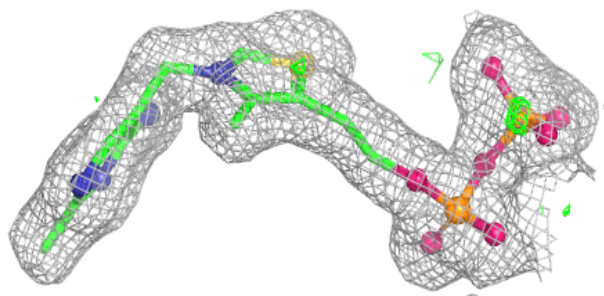
Electron density around MG D 703:

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



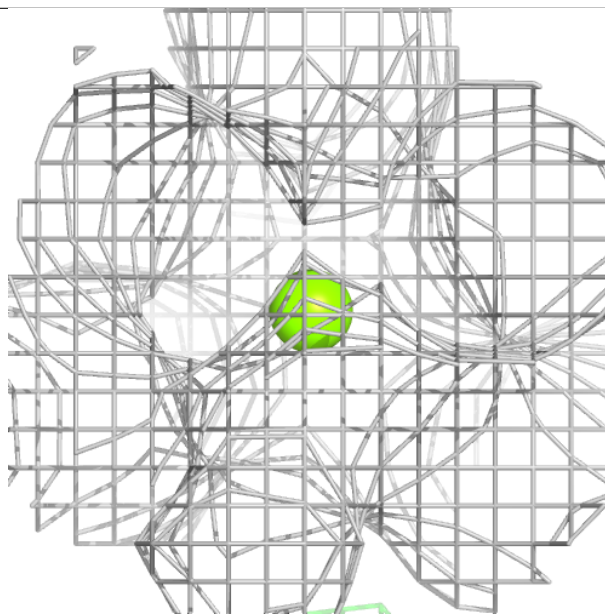
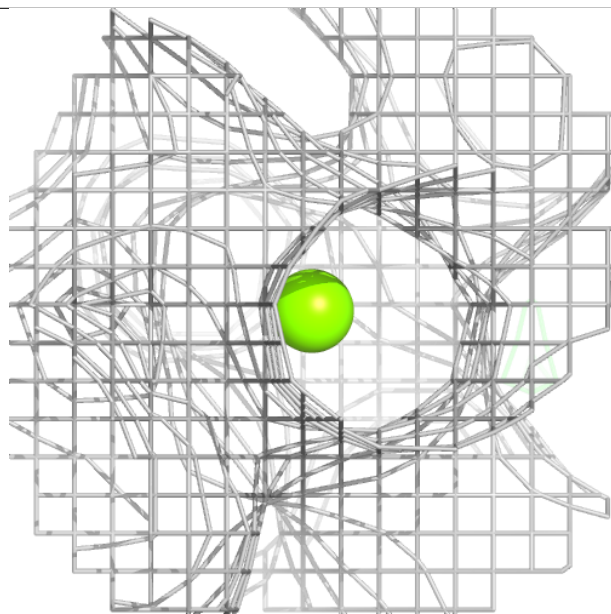
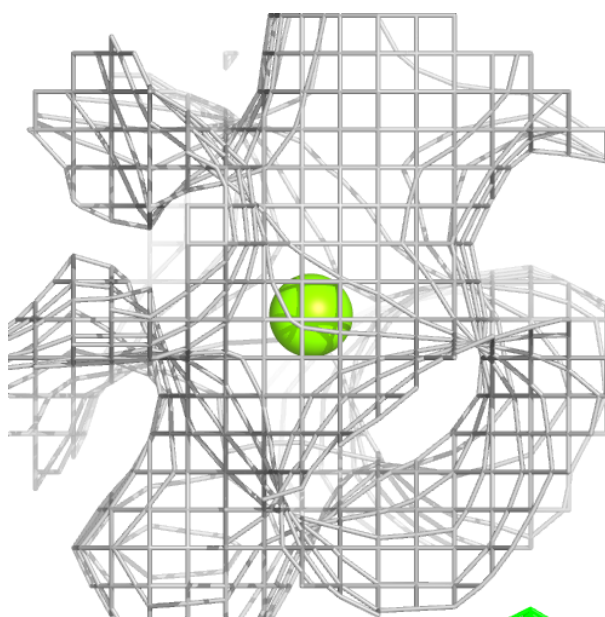
Electron density around TPP B 702:

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



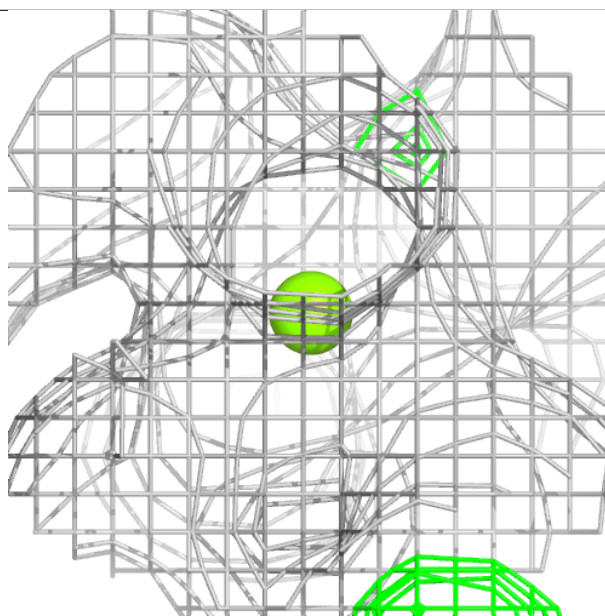
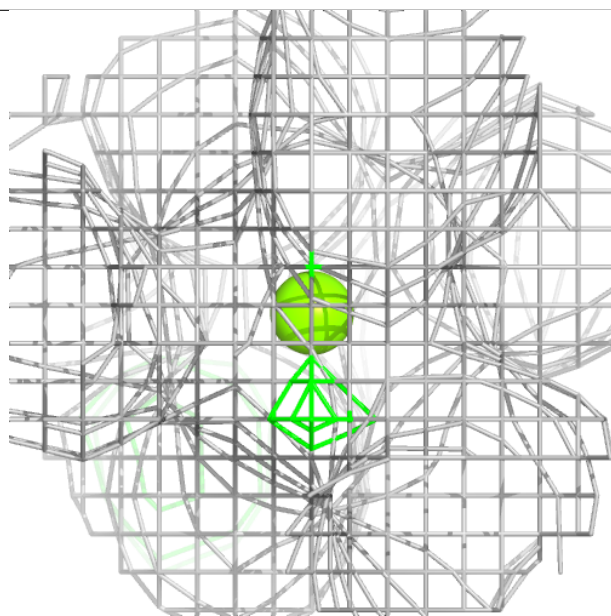
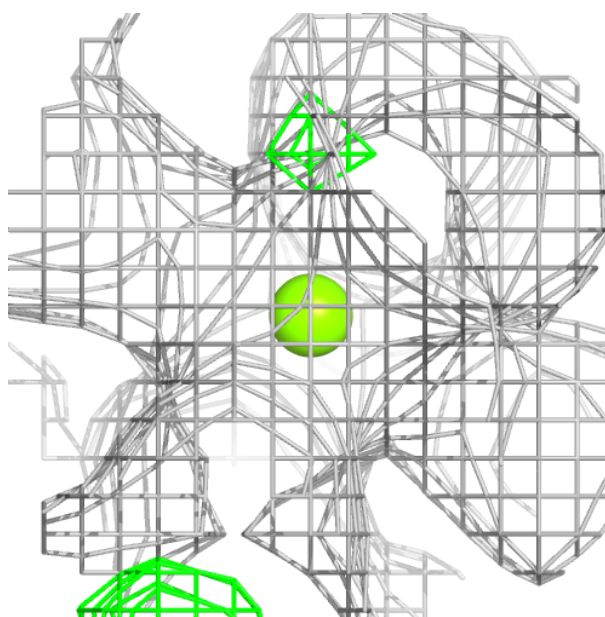
Electron density around MG E 604:

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



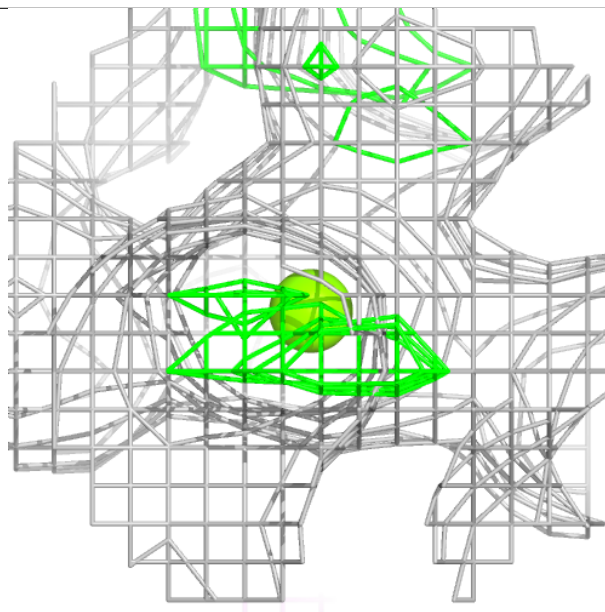
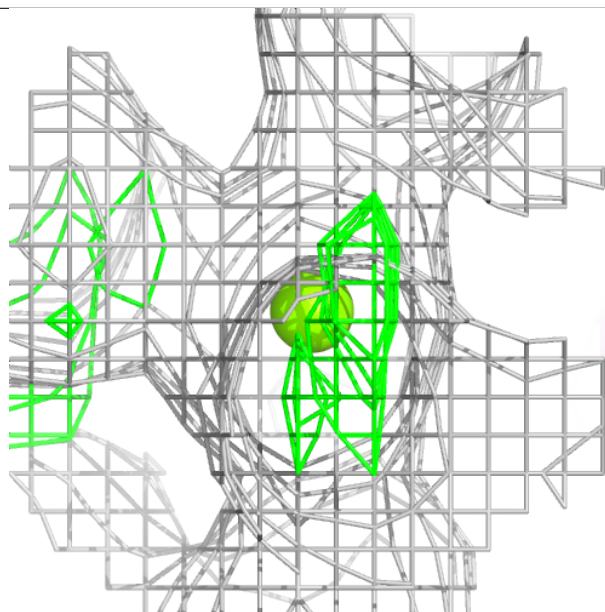
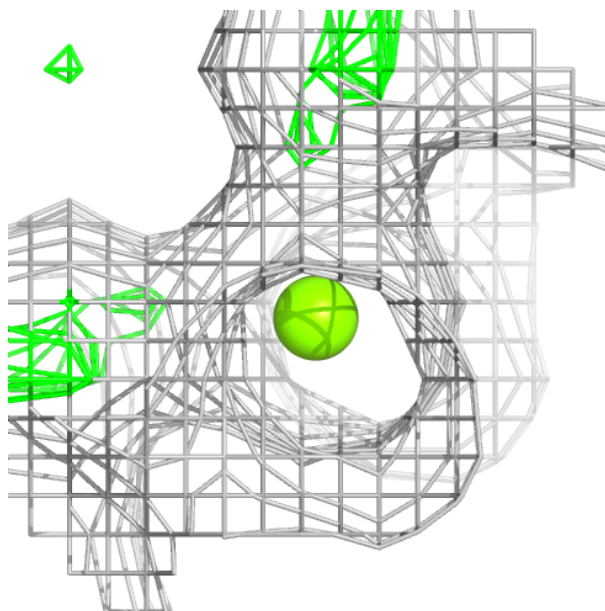
Electron density around MG A 703:

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



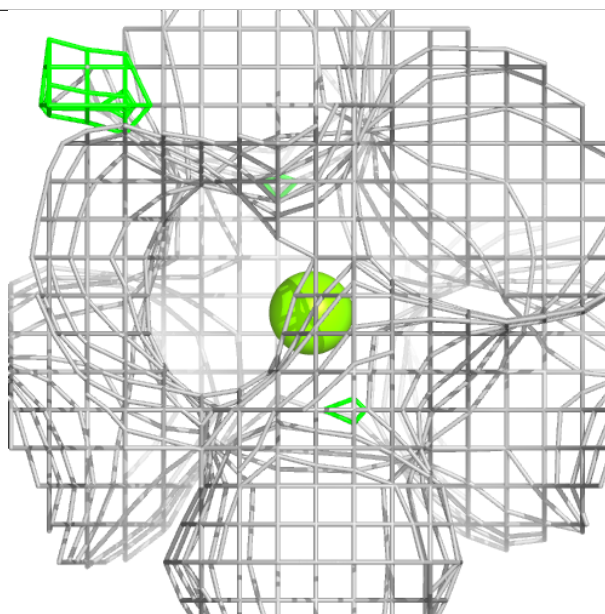
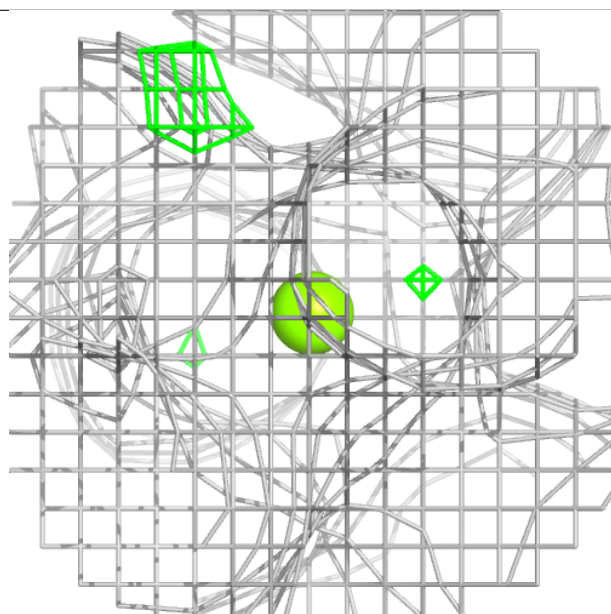
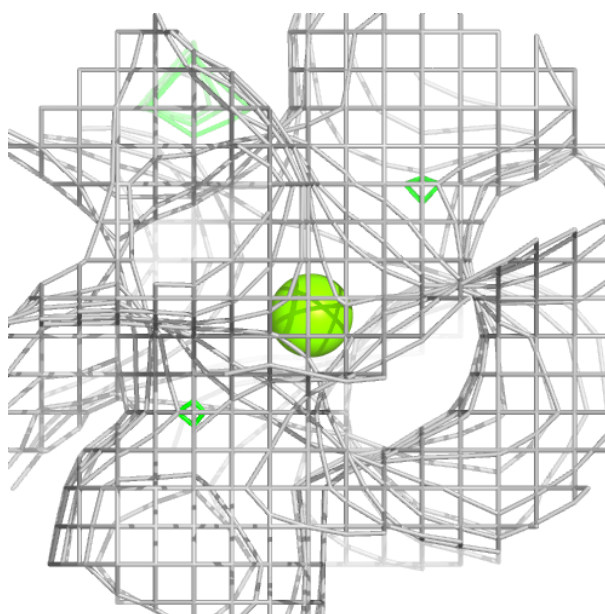
Electron density around MG A 704:

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



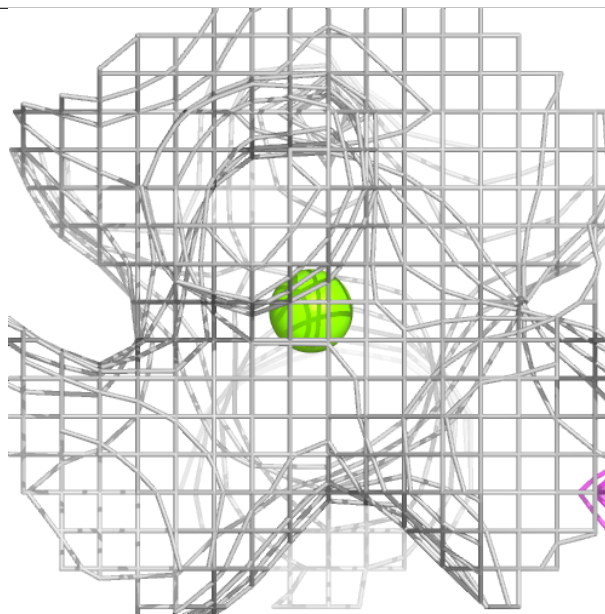
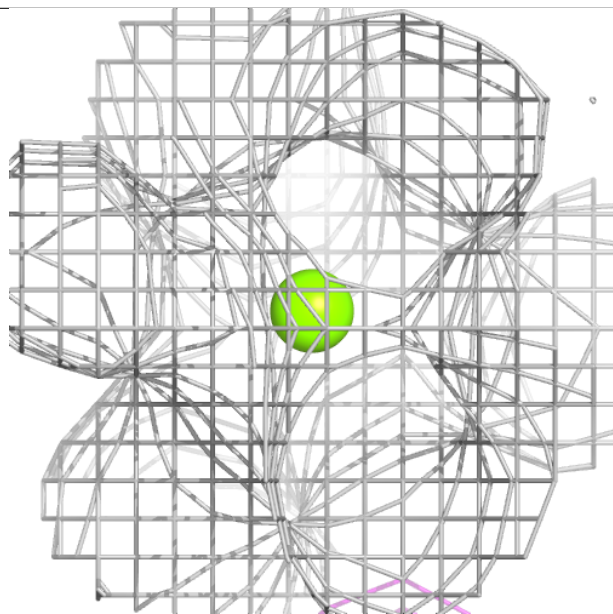
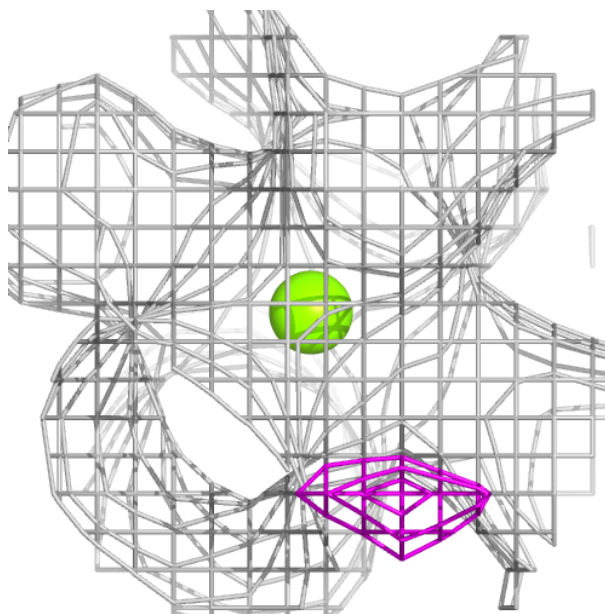
Electron density around MG B 703:

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



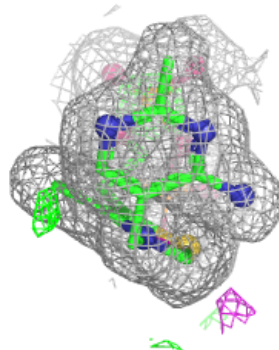
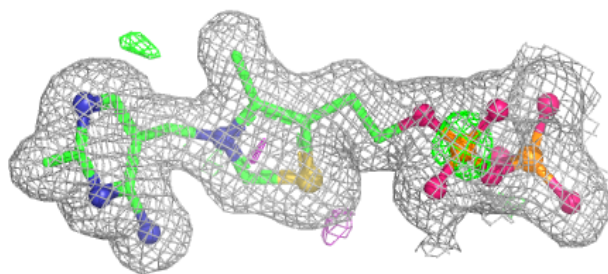
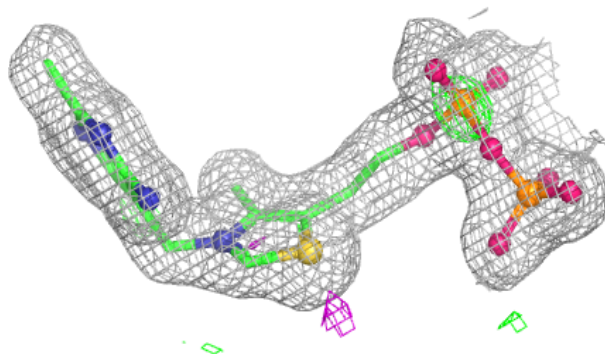
Electron density around MG C 703:

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



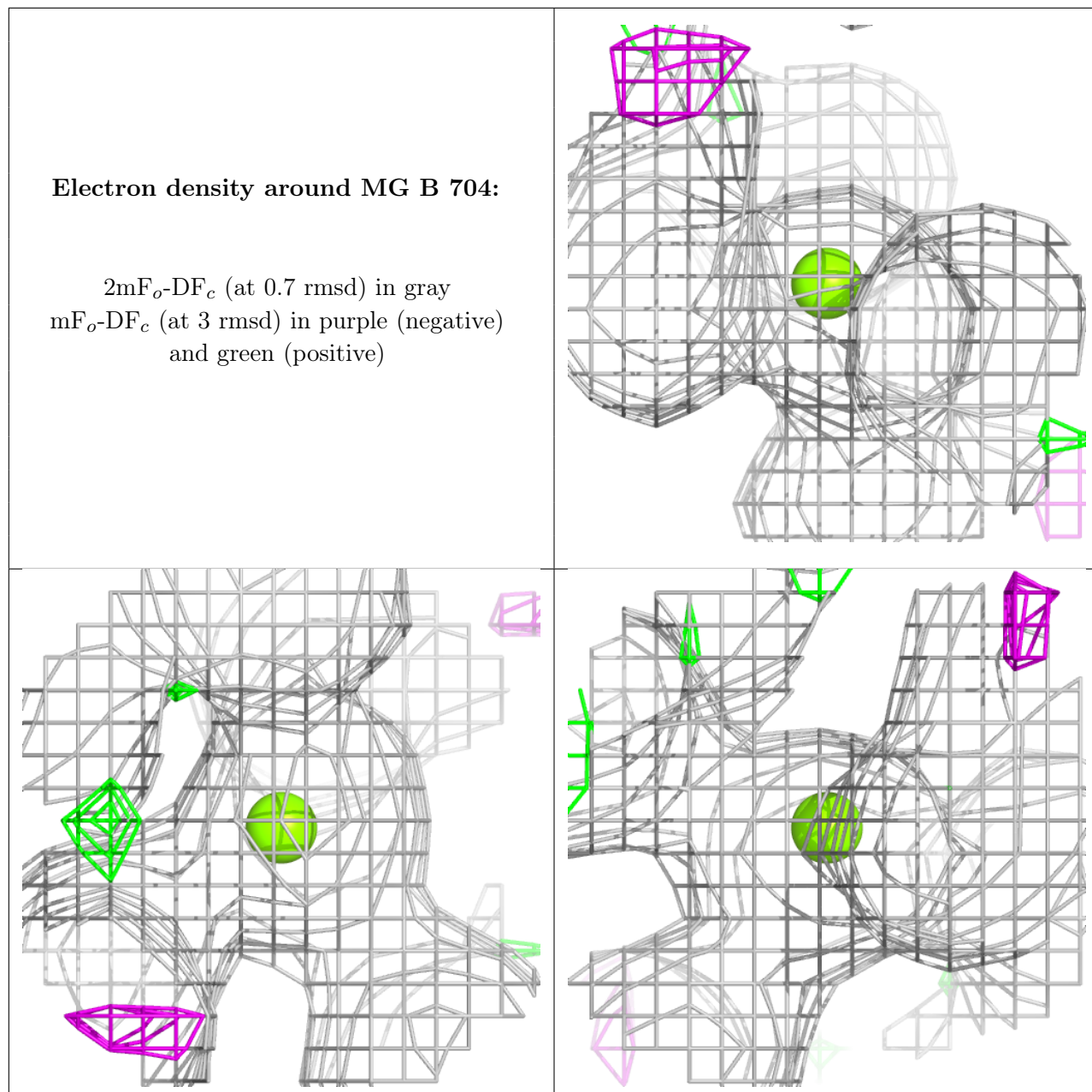
Electron density around TPP A 702:

$2mF_o-DF_c$ (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.