



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:44 AM UTC

PDB ID : 7XXM / pdb_00007xxm
Title : Orf1-glycine-4-aminobutylthricin complex
Authors : Wang, Y.L.; Li, T.L.
Deposited on : 2022-05-30
Resolution : 2.12 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

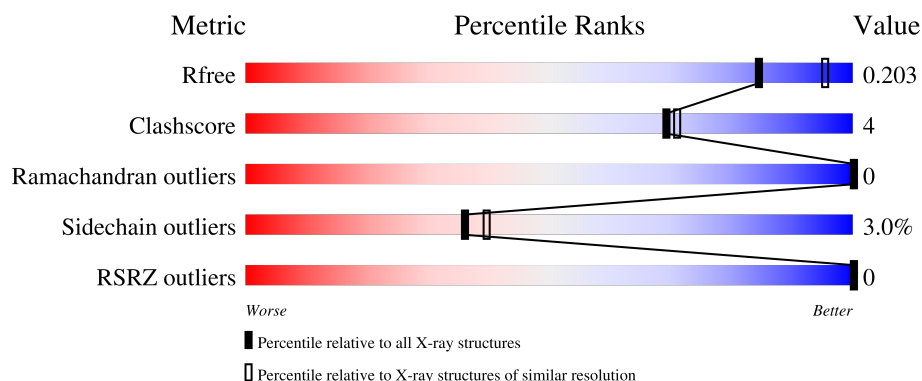
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	512	 87% 6% • 6%
1	B	512	 87% 7% • 6%
1	C	512	 83% 9% • 8%
1	D	512	 81% 9% • 9%
1	E	512	 87% 6% • 6%

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Mol	Chain	Length	Quality of chain
1	F	512	 87% 6% • 6%
1	G	512	 83% 9% • 8%
1	H	512	 81% 8% • 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLY	G	702	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32019 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 N-formimidoyl fortimicin A synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3654	2293	660	689	12			
1	B	482	Total	C	N	O	S	0	1	0
			3660	2296	661	690	13			
1	C	472	Total	C	N	O	S	0	1	0
			3590	2253	647	677	13			
1	D	466	Total	C	N	O	S	0	1	0
			3542	2228	636	665	13			
1	E	482	Total	C	N	O	S	0	0	0
			3654	2293	660	689	12			
1	F	482	Total	C	N	O	S	0	1	0
			3660	2296	661	690	13			
1	G	472	Total	C	N	O	S	0	1	0
			3590	2253	647	677	13			
1	H	465	Total	C	N	O	S	0	1	0
			3525	2219	629	664	13			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A125SZC1
A	-19	GLY	-	expression tag	UNP A0A125SZC1
A	-18	SER	-	expression tag	UNP A0A125SZC1
A	-17	SER	-	expression tag	UNP A0A125SZC1
A	-16	HIS	-	expression tag	UNP A0A125SZC1
A	-15	HIS	-	expression tag	UNP A0A125SZC1
A	-14	HIS	-	expression tag	UNP A0A125SZC1
A	-13	HIS	-	expression tag	UNP A0A125SZC1
A	-12	HIS	-	expression tag	UNP A0A125SZC1
A	-11	HIS	-	expression tag	UNP A0A125SZC1
A	-10	SER	-	expression tag	UNP A0A125SZC1
A	-9	SER	-	expression tag	UNP A0A125SZC1
A	-8	GLY	-	expression tag	UNP A0A125SZC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	LEU	-	expression tag	UNP A0A125SZC1
A	-6	VAL	-	expression tag	UNP A0A125SZC1
A	-5	PRO	-	expression tag	UNP A0A125SZC1
A	-4	ARG	-	expression tag	UNP A0A125SZC1
A	-3	GLY	-	expression tag	UNP A0A125SZC1
A	-2	SER	-	expression tag	UNP A0A125SZC1
A	-1	HIS	-	expression tag	UNP A0A125SZC1
A	0	MET	-	expression tag	UNP A0A125SZC1
B	-20	MET	-	initiating methionine	UNP A0A125SZC1
B	-19	GLY	-	expression tag	UNP A0A125SZC1
B	-18	SER	-	expression tag	UNP A0A125SZC1
B	-17	SER	-	expression tag	UNP A0A125SZC1
B	-16	HIS	-	expression tag	UNP A0A125SZC1
B	-15	HIS	-	expression tag	UNP A0A125SZC1
B	-14	HIS	-	expression tag	UNP A0A125SZC1
B	-13	HIS	-	expression tag	UNP A0A125SZC1
B	-12	HIS	-	expression tag	UNP A0A125SZC1
B	-11	HIS	-	expression tag	UNP A0A125SZC1
B	-10	SER	-	expression tag	UNP A0A125SZC1
B	-9	SER	-	expression tag	UNP A0A125SZC1
B	-8	GLY	-	expression tag	UNP A0A125SZC1
B	-7	LEU	-	expression tag	UNP A0A125SZC1
B	-6	VAL	-	expression tag	UNP A0A125SZC1
B	-5	PRO	-	expression tag	UNP A0A125SZC1
B	-4	ARG	-	expression tag	UNP A0A125SZC1
B	-3	GLY	-	expression tag	UNP A0A125SZC1
B	-2	SER	-	expression tag	UNP A0A125SZC1
B	-1	HIS	-	expression tag	UNP A0A125SZC1
B	0	MET	-	expression tag	UNP A0A125SZC1
C	-20	MET	-	initiating methionine	UNP A0A125SZC1
C	-19	GLY	-	expression tag	UNP A0A125SZC1
C	-18	SER	-	expression tag	UNP A0A125SZC1
C	-17	SER	-	expression tag	UNP A0A125SZC1
C	-16	HIS	-	expression tag	UNP A0A125SZC1
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C	-14	HIS	-	expression tag	UNP A0A125SZC1
C	-13	HIS	-	expression tag	UNP A0A125SZC1
C	-12	HIS	-	expression tag	UNP A0A125SZC1
C	-11	HIS	-	expression tag	UNP A0A125SZC1
C	-10	SER	-	expression tag	UNP A0A125SZC1
C	-9	SER	-	expression tag	UNP A0A125SZC1
C	-8	GLY	-	expression tag	UNP A0A125SZC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	expression tag	UNP A0A125SZC1
C	-6	VAL	-	expression tag	UNP A0A125SZC1
C	-5	PRO	-	expression tag	UNP A0A125SZC1
C	-4	ARG	-	expression tag	UNP A0A125SZC1
C	-3	GLY	-	expression tag	UNP A0A125SZC1
C	-2	SER	-	expression tag	UNP A0A125SZC1
C	-1	HIS	-	expression tag	UNP A0A125SZC1
C	0	MET	-	expression tag	UNP A0A125SZC1
D	-20	MET	-	initiating methionine	UNP A0A125SZC1
D	-19	GLY	-	expression tag	UNP A0A125SZC1
D	-18	SER	-	expression tag	UNP A0A125SZC1
D	-17	SER	-	expression tag	UNP A0A125SZC1
D	-16	HIS	-	expression tag	UNP A0A125SZC1
D	-15	HIS	-	expression tag	UNP A0A125SZC1
D	-14	HIS	-	expression tag	UNP A0A125SZC1
D	-13	HIS	-	expression tag	UNP A0A125SZC1
D	-12	HIS	-	expression tag	UNP A0A125SZC1
D	-11	HIS	-	expression tag	UNP A0A125SZC1
D	-10	SER	-	expression tag	UNP A0A125SZC1
D	-9	SER	-	expression tag	UNP A0A125SZC1
D	-8	GLY	-	expression tag	UNP A0A125SZC1
D	-7	LEU	-	expression tag	UNP A0A125SZC1
D	-6	VAL	-	expression tag	UNP A0A125SZC1
D	-5	PRO	-	expression tag	UNP A0A125SZC1
D	-4	ARG	-	expression tag	UNP A0A125SZC1
D	-3	GLY	-	expression tag	UNP A0A125SZC1
D	-2	SER	-	expression tag	UNP A0A125SZC1
D	-1	HIS	-	expression tag	UNP A0A125SZC1
D	0	MET	-	expression tag	UNP A0A125SZC1
E	-20	MET	-	initiating methionine	UNP A0A125SZC1
E	-19	GLY	-	expression tag	UNP A0A125SZC1
E	-18	SER	-	expression tag	UNP A0A125SZC1
E	-17	SER	-	expression tag	UNP A0A125SZC1
E	-16	HIS	-	expression tag	UNP A0A125SZC1
E	-15	HIS	-	expression tag	UNP A0A125SZC1
E	-14	HIS	-	expression tag	UNP A0A125SZC1
E	-13	HIS	-	expression tag	UNP A0A125SZC1
E	-12	HIS	-	expression tag	UNP A0A125SZC1
E	-11	HIS	-	expression tag	UNP A0A125SZC1
E	-10	SER	-	expression tag	UNP A0A125SZC1
E	-9	SER	-	expression tag	UNP A0A125SZC1
E	-8	GLY	-	expression tag	UNP A0A125SZC1

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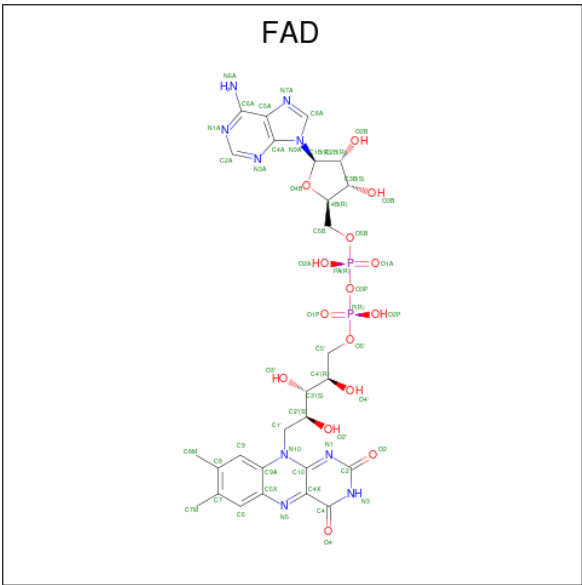
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E	-6	VAL	-	expression tag	UNP A0A125SZC1
E	-5	PRO	-	expression tag	UNP A0A125SZC1
E	-4	ARG	-	expression tag	UNP A0A125SZC1
E	-3	GLY	-	expression tag	UNP A0A125SZC1
E	-2	SER	-	expression tag	UNP A0A125SZC1
E	-1	HIS	-	expression tag	UNP A0A125SZC1
E	0	MET	-	expression tag	UNP A0A125SZC1
F	-20	MET	-	initiating methionine	UNP A0A125SZC1
F	-19	GLY	-	expression tag	UNP A0A125SZC1
F	-18	SER	-	expression tag	UNP A0A125SZC1
F	-17	SER	-	expression tag	UNP A0A125SZC1
F	-16	HIS	-	expression tag	UNP A0A125SZC1
F	-15	HIS	-	expression tag	UNP A0A125SZC1
F	-14	HIS	-	expression tag	UNP A0A125SZC1
F	-13	HIS	-	expression tag	UNP A0A125SZC1
F	-12	HIS	-	expression tag	UNP A0A125SZC1
F	-11	HIS	-	expression tag	UNP A0A125SZC1
F	-10	SER	-	expression tag	UNP A0A125SZC1
F	-9	SER	-	expression tag	UNP A0A125SZC1
F	-8	GLY	-	expression tag	UNP A0A125SZC1
F	-7	LEU	-	expression tag	UNP A0A125SZC1
F	-6	VAL	-	expression tag	UNP A0A125SZC1
F	-5	PRO	-	expression tag	UNP A0A125SZC1
F	-4	ARG	-	expression tag	UNP A0A125SZC1
F	-3	GLY	-	expression tag	UNP A0A125SZC1
F	-2	SER	-	expression tag	UNP A0A125SZC1
F	-1	HIS	-	expression tag	UNP A0A125SZC1
F	0	MET	-	expression tag	UNP A0A125SZC1
G	-20	MET	-	initiating methionine	UNP A0A125SZC1
G	-19	GLY	-	expression tag	UNP A0A125SZC1
G	-18	SER	-	expression tag	UNP A0A125SZC1
G	-17	SER	-	expression tag	UNP A0A125SZC1
G	-16	HIS	-	expression tag	UNP A0A125SZC1
G	-15	HIS	-	expression tag	UNP A0A125SZC1
G	-14	HIS	-	expression tag	UNP A0A125SZC1
G	-13	HIS	-	expression tag	UNP A0A125SZC1
G	-12	HIS	-	expression tag	UNP A0A125SZC1
G	-11	HIS	-	expression tag	UNP A0A125SZC1
G	-10	SER	-	expression tag	UNP A0A125SZC1
G	-9	SER	-	expression tag	UNP A0A125SZC1
G	-8	GLY	-	expression tag	UNP A0A125SZC1

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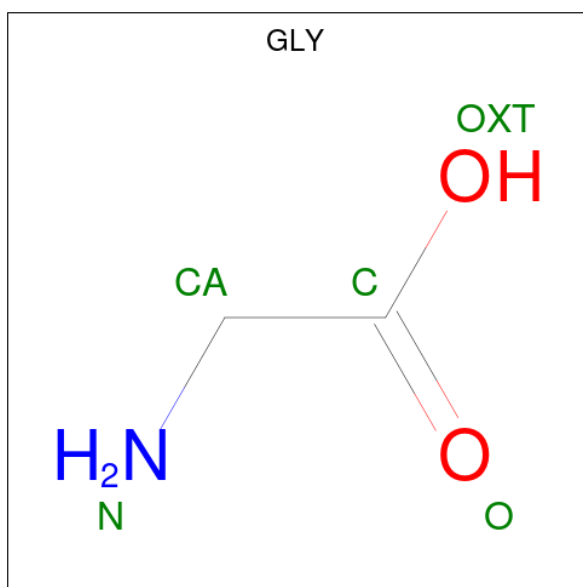
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	LEU	-	expression tag	UNP A0A125SZC1
G	-6	VAL	-	expression tag	UNP A0A125SZC1
G	-5	PRO	-	expression tag	UNP A0A125SZC1
G	-4	ARG	-	expression tag	UNP A0A125SZC1
G	-3	GLY	-	expression tag	UNP A0A125SZC1
G	-2	SER	-	expression tag	UNP A0A125SZC1
G	-1	HIS	-	expression tag	UNP A0A125SZC1
G	0	MET	-	expression tag	UNP A0A125SZC1
H	-20	MET	-	initiating methionine	UNP A0A125SZC1
H	-19	GLY	-	expression tag	UNP A0A125SZC1
H	-18	SER	-	expression tag	UNP A0A125SZC1
H	-17	SER	-	expression tag	UNP A0A125SZC1
H	-16	HIS	-	expression tag	UNP A0A125SZC1
H	-15	HIS	-	expression tag	UNP A0A125SZC1
H	-14	HIS	-	expression tag	UNP A0A125SZC1
H	-13	HIS	-	expression tag	UNP A0A125SZC1
H	-12	HIS	-	expression tag	UNP A0A125SZC1
H	-11	HIS	-	expression tag	UNP A0A125SZC1
H	-10	SER	-	expression tag	UNP A0A125SZC1
H	-9	SER	-	expression tag	UNP A0A125SZC1
H	-8	GLY	-	expression tag	UNP A0A125SZC1
H	-7	LEU	-	expression tag	UNP A0A125SZC1
H	-6	VAL	-	expression tag	UNP A0A125SZC1
H	-5	PRO	-	expression tag	UNP A0A125SZC1
H	-4	ARG	-	expression tag	UNP A0A125SZC1
H	-3	GLY	-	expression tag	UNP A0A125SZC1
H	-2	SER	-	expression tag	UNP A0A125SZC1
H	-1	HIS	-	expression tag	UNP A0A125SZC1
H	0	MET	-	expression tag	UNP A0A125SZC1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



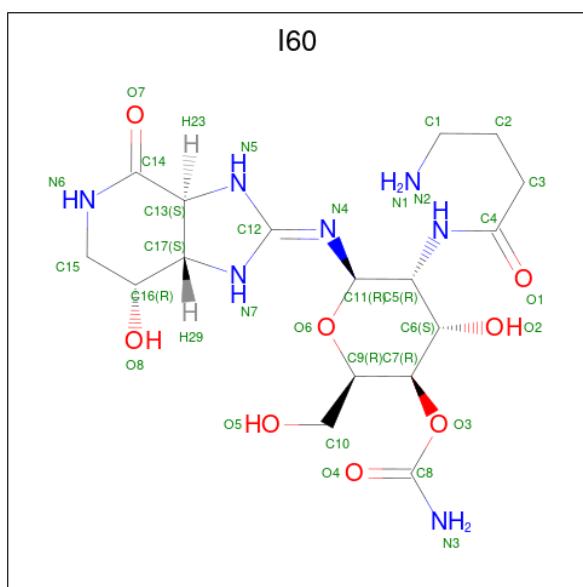
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G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

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	B	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		
3	D	1	Total	C	N	O	0	0
			5	2	1	2		
3	E	1	Total	C	N	O	0	0
			5	2	1	2		
3	F	1	Total	C	N	O	0	0
			5	2	1	2		
3	G	1	Total	C	N	O	0	0
			5	2	1	2		
3	H	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is [(2 {R},3 {R},4 {S},5 {R},6 {R})-6-[({E})-(3 {a} {S},7 {R},7 {a} {S})-7-oxidanyl-4-oxidanylidene-3,3 {a},5,6,7,7 {a}-hexahydro-1 {H}-imidazo[4,5-c]pyridin-2-ylidene]amino]-5-(4-azanylbutanoylamino)-2-(hydroxymethyl)-4-oxidanyl-oxan-3-yl] carbamate (CCD ID: I60) (formula: C₁₇H₂₉N₇O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	17	7	8		
4	B	1	Total	C	N	O	0	0
			32	17	7	8		
4	C	1	Total	C	N	O	0	0
			32	17	7	8		
4	D	1	Total	C	N	O	0	0
			32	17	7	8		
4	E	1	Total	C	N	O	0	0
			32	17	7	8		
4	F	1	Total	C	N	O	0	0
			32	17	7	8		
4	G	1	Total	C	N	O	0	0
			32	17	7	8		
4	H	1	Total	C	N	O	0	0
			32	17	7	8		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	368	Total	O	0	0
			368	368		
5	B	359	Total	O	0	0
			359	359		
5	C	312	Total	O	0	0
			312	312		
5	D	200	Total	O	0	0
			200	200		

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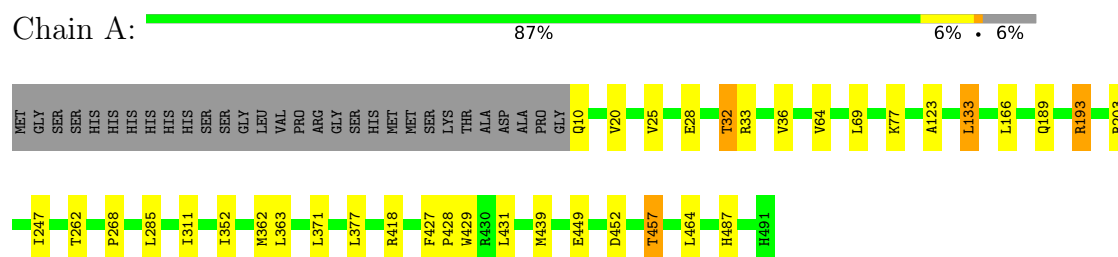
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	330	Total 330	O 330	0	0
5	F	352	Total 352	O 352	0	0
5	G	310	Total 310	O 310	0	0
5	H	193	Total 193	O 193	0	0

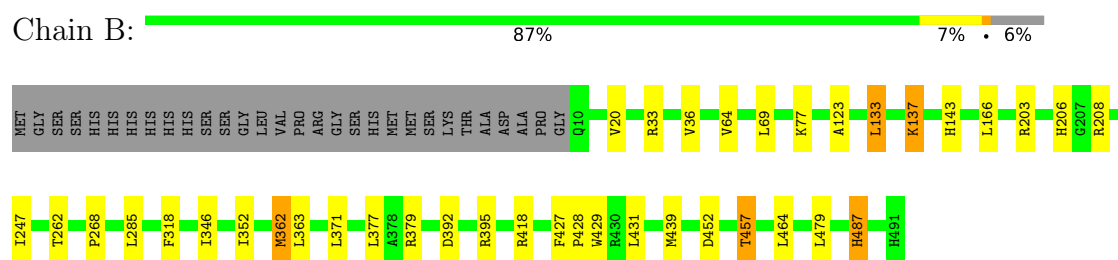
3 Residue-property plots [i](#)

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.

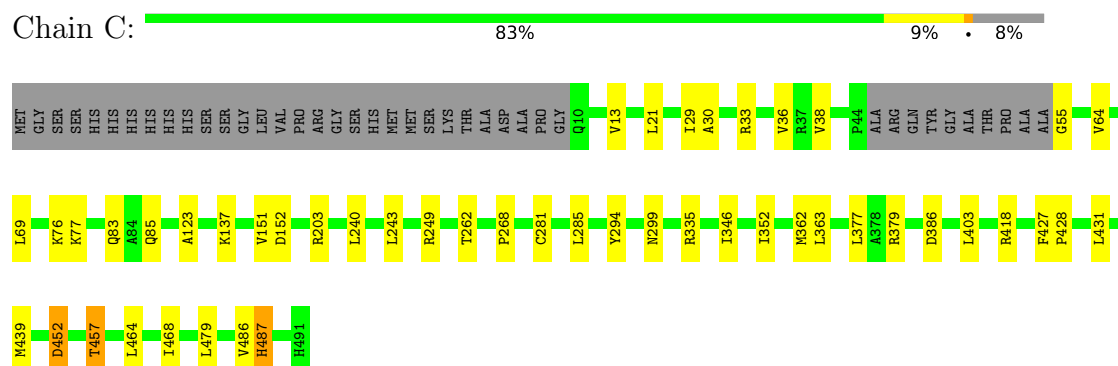
- Molecule 1: N-formimidoyl fortimicin A synthase



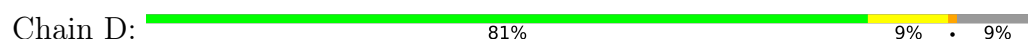
- Molecule 1: N-formimidoyl fortimicin A synthase

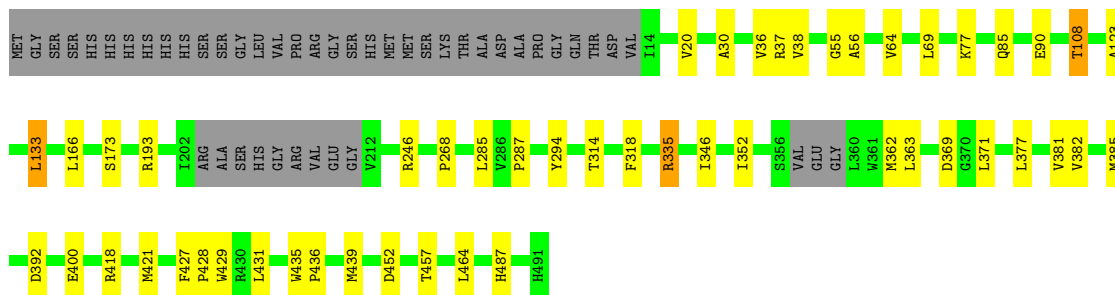


- Molecule 1: N-formimidoyl fortimicin A synthase

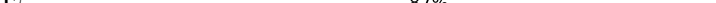


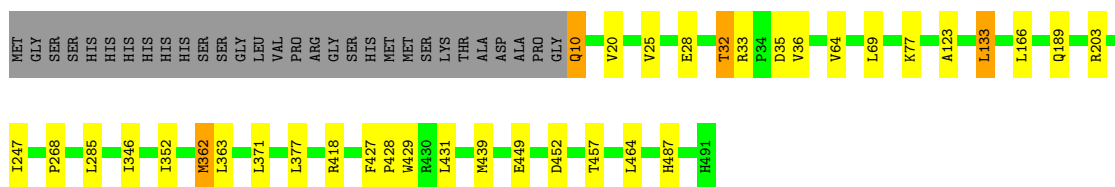
- Molecule 1: N-formimidoyl fortimicin A synthase





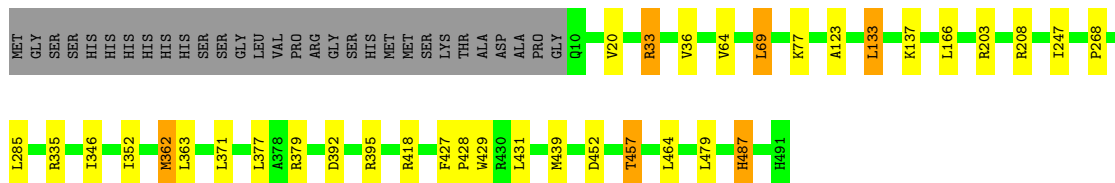
- Molecule 1: N-formimidoyl fortimicin A synthase

Chain E:  87% 6% • 6%



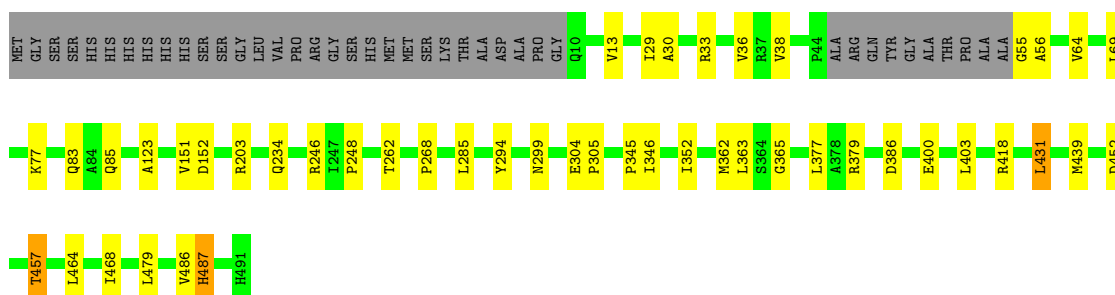
- Molecule 1: N-formimidoyl fortimicin A synthase

Chain F:  87% 6% • 6%



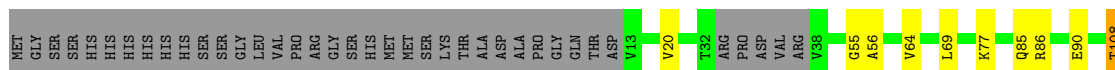
- Molecule 1: N-formimidoyl fortimicin A synthase

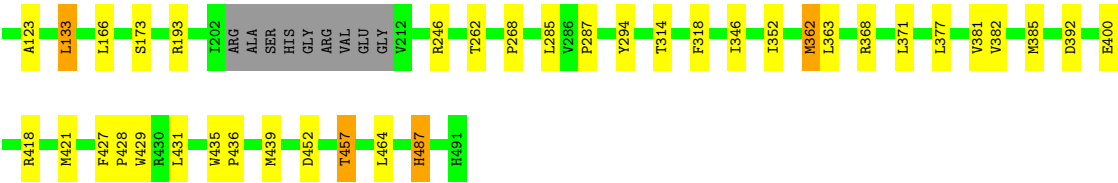
Chain G: 83% 9% • 8%



- Molecule 1: N-formimidoyl fortimicin A synthase

Chain H: 81% 8% • 9%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.64Å 107.88Å 134.78Å 89.96° 90.13° 83.44°	Depositor
Resolution (Å)	29.39 – 2.12 29.39 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.39-2.12) 96.4 (29.39-2.12)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.195 , 0.215 0.202 , 0.203	Depositor DCC
R_{free} test set	16321 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.466 for -h,-k,l 0.011 for -k,-h,-l 0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32019	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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: I60, 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	1.00	1/3737 (0.0%)	1.31	4/5092 (0.1%)
1	B	1.01	1/3743 (0.0%)	1.31	5/5100 (0.1%)
1	C	1.02	0/3670	1.34	8/4998 (0.2%)
1	D	0.97	0/3622	1.32	3/4934 (0.1%)
1	E	1.00	1/3737 (0.0%)	1.31	2/5092 (0.0%)
1	F	1.00	1/3743 (0.0%)	1.31	3/5100 (0.1%)
1	G	1.03	1/3670 (0.0%)	1.34	8/4998 (0.2%)
1	H	0.96	0/3604	1.31	5/4910 (0.1%)
All	All	1.00	5/29526 (0.0%)	1.32	38/40224 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	ILE	N-CA	5.50	1.50	1.46
1	F	247	ILE	N-CA	5.47	1.50	1.46
1	E	247	ILE	N-CA	5.25	1.50	1.46
1	A	247	ILE	N-CA	5.07	1.50	1.46
1	G	431	LEU	N-CA	5.02	1.50	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	VAL	CA-C-N	6.74	130.41	120.90
1	C	151	VAL	C-N-CA	6.74	130.41	120.90
1	G	151	VAL	CA-C-N	6.52	130.09	120.90
1	G	151	VAL	C-N-CA	6.52	130.09	120.90
1	G	152	ASP	CA-C-O	-5.80	114.77	121.15
1	C	152	ASP	CA-C-O	-5.71	114.86	121.15
1	D	392	ASP	CA-C-O	-5.63	114.91	120.82
1	F	392	ASP	CA-C-O	-5.62	114.89	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	392	ASP	CA-C-O	-5.56	114.98	120.82
1	B	392	ASP	CA-C-O	-5.45	115.06	120.90
1	C	152	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	487	HIS	CA-C-N	5.23	127.55	120.38
1	D	487	HIS	C-N-CA	5.23	127.55	120.38
1	F	487	HIS	CA-C-N	5.21	127.51	120.38
1	F	487	HIS	C-N-CA	5.21	127.51	120.38
1	A	262	THR	CA-C-N	5.18	127.48	120.38
1	A	262	THR	C-N-CA	5.18	127.48	120.38
1	E	487	HIS	CA-C-N	5.17	127.46	120.38
1	E	487	HIS	C-N-CA	5.17	127.46	120.38
1	B	487	HIS	CA-C-N	5.16	127.45	120.38
1	B	487	HIS	C-N-CA	5.16	127.45	120.38
1	G	487	HIS	CA-C-N	5.12	127.40	120.38
1	G	487	HIS	C-N-CA	5.12	127.40	120.38
1	C	487	HIS	CA-C-N	5.11	127.38	120.38
1	C	487	HIS	C-N-CA	5.11	127.38	120.38
1	C	262	THR	CA-C-N	5.11	127.38	120.38
1	C	262	THR	C-N-CA	5.11	127.38	120.38
1	G	262	THR	CA-C-N	5.11	127.37	120.38
1	G	262	THR	C-N-CA	5.11	127.37	120.38
1	H	487	HIS	CA-C-N	5.10	127.37	120.38
1	H	487	HIS	C-N-CA	5.10	127.37	120.38
1	A	487	HIS	CA-C-N	5.09	127.36	120.38
1	A	487	HIS	C-N-CA	5.09	127.36	120.38
1	G	152	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	262	THR	CA-C-N	5.04	127.29	120.38
1	B	262	THR	C-N-CA	5.04	127.29	120.38
1	H	262	THR	CA-C-N	5.03	127.28	120.38
1	H	262	THR	C-N-CA	5.03	127.28	120.38

There are no chirality outliers.

There are no planarity outliers.

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	3654	0	3584	19	0
1	B	3660	0	3588	24	0
1	C	3590	0	3520	25	0
1	D	3542	0	3476	36	0
1	E	3654	0	3584	19	0
1	F	3660	0	3588	21	0
1	G	3590	0	3520	26	0
1	H	3525	0	3457	38	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	1	0
2	F	53	0	31	0	0
2	G	53	0	31	0	0
2	H	53	0	31	2	0
3	A	5	0	2	1	0
3	B	5	0	2	1	0
3	C	5	0	2	0	0
3	D	5	0	2	0	0
3	E	5	0	2	0	0
3	F	5	0	2	1	0
3	G	5	0	2	0	0
3	H	5	0	2	2	0
4	A	32	0	0	0	0
4	B	32	0	0	0	0
4	C	32	0	0	0	0
4	D	32	0	0	0	0
4	E	32	0	0	0	0
4	F	32	0	0	0	0
4	G	32	0	0	0	0
4	H	32	0	0	0	0
5	A	368	0	0	4	0
5	B	359	0	0	4	0
5	C	312	0	0	5	0
5	D	200	0	0	1	0
5	E	330	0	0	0	0
5	F	352	0	0	4	0
5	G	310	0	0	3	0
5	H	193	0	0	0	0
All	All	32019	0	28581	206	0

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

All (206) 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:H:382:VAL:HA	1:H:385:MET:HE3	1.48	0.96
1:D:382:VAL:HA	1:D:385:MET:HE3	1.49	0.94
1:H:436:PRO:HA	1:H:439:MET:CE	2.10	0.81
1:D:436:PRO:HA	1:D:439:MET:CE	2.10	0.80
1:H:382:VAL:HA	1:H:385:MET:CE	2.16	0.76
1:D:382:VAL:HA	1:D:385:MET:CE	2.17	0.75
1:G:304:GLU:OE2	1:G:305:PRO:O	2.08	0.72
1:D:436:PRO:HA	1:D:439:MET:HE3	1.72	0.70
1:H:436:PRO:HA	1:H:439:MET:HE3	1.72	0.70
1:C:452:ASP:HB3	5:C:822:HOH:O	1.92	0.70
1:H:108:THR:HG22	1:H:173:SER:OG	1.92	0.69
1:D:108:THR:HG22	1:D:173:SER:OG	1.93	0.69
1:D:123:ALA:HB1	1:D:418:ARG:HD2	1.75	0.68
1:B:439:MET:HE2	1:D:439:MET:HG2	1.77	0.67
1:D:381:VAL:HG12	1:D:385:MET:HE2	1.76	0.67
1:D:108:THR:HG21	1:D:287:PRO:O	1.95	0.67
1:H:381:VAL:HG12	1:H:385:MET:HE2	1.76	0.66
1:H:108:THR:HG21	1:H:287:PRO:O	1.95	0.66
1:A:123:ALA:HB1	1:A:418:ARG:HD2	1.78	0.66
1:B:123:ALA:HB1	1:B:418:ARG:HD2	1.79	0.65
1:C:363:LEU:HD11	1:C:377:LEU:HB3	1.79	0.65
1:E:64:VAL:HG13	1:E:69:LEU:HD22	1.79	0.65
1:H:123:ALA:HB1	1:H:418:ARG:HD2	1.77	0.65
1:A:193:ARG:HD2	5:A:1092:HOH:O	1.97	0.64
1:E:123:ALA:HB1	1:E:418:ARG:HD2	1.78	0.64
1:H:436:PRO:HA	1:H:439:MET:HE2	1.80	0.64
1:G:363:LEU:HD11	1:G:377:LEU:HB3	1.80	0.64
1:D:436:PRO:HA	1:D:439:MET:HE2	1.78	0.63
1:F:439:MET:HE2	1:H:439:MET:HG2	1.80	0.63
1:G:246:ARG:NH1	1:G:400:GLU:OE1	2.32	0.63
1:H:246:ARG:NH1	1:H:400:GLU:OE1	2.31	0.62
1:D:246:ARG:NH1	1:D:400:GLU:OE1	2.32	0.62
1:F:123:ALA:HB1	1:F:418:ARG:HD2	1.80	0.62
1:A:64:VAL:HG13	1:A:69:LEU:HD22	1.81	0.62
1:D:421:MET:HE1	1:D:439:MET:HE3	1.82	0.61
1:H:421:MET:HE1	1:H:439:MET:HE3	1.81	0.61
1:D:64:VAL:HG13	1:D:69:LEU:HD22	1.82	0.61
1:F:64:VAL:HG13	1:F:69:LEU:HD22	1.83	0.60
1:H:64:VAL:HG13	1:H:69:LEU:HD22	1.83	0.60
1:B:64:VAL:HG13	1:B:69:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:VAL:HG13	1:G:69:LEU:HD22	1.83	0.59
1:C:64:VAL:HG13	1:C:69:LEU:HD22	1.85	0.59
1:B:133:LEU:HD13	1:B:166:LEU:HD22	1.84	0.59
1:F:133:LEU:HD13	1:F:166:LEU:HD22	1.83	0.58
1:C:123:ALA:HB1	1:C:418:ARG:HD3	1.85	0.58
1:F:268:PRO:HG3	1:F:285:LEU:HD22	1.86	0.58
1:H:314:THR:HG22	1:H:318:PHE:CE2	2.39	0.58
1:E:133:LEU:HD13	1:E:166:LEU:HD22	1.84	0.57
1:E:268:PRO:HG3	1:E:285:LEU:HD22	1.87	0.57
1:A:268:PRO:HG3	1:A:285:LEU:HD22	1.86	0.57
1:A:133:LEU:HD13	1:A:166:LEU:HD22	1.85	0.57
1:B:268:PRO:HG3	1:B:285:LEU:HD22	1.86	0.57
1:E:346:ILE:HG13	1:E:464:LEU:CD2	2.35	0.57
1:D:314:THR:HG22	1:D:318:PHE:CE2	2.39	0.56
1:A:32:THR:HG22	1:A:33:ARG:HG2	1.87	0.56
1:F:346:ILE:HG13	1:F:464:LEU:CD2	2.36	0.56
1:B:346:ILE:HG13	1:B:464:LEU:CD2	2.36	0.56
1:F:379:ARG:HD3	5:F:1021:HOH:O	2.06	0.56
1:D:133:LEU:HD13	1:D:166:LEU:HD22	1.87	0.55
1:H:133:LEU:HD13	1:H:166:LEU:HD22	1.88	0.55
1:D:108:THR:CG2	1:D:287:PRO:O	2.55	0.55
1:G:123:ALA:HB1	1:G:418:ARG:HD3	1.86	0.55
1:C:268:PRO:HG3	1:C:285:LEU:HD22	1.89	0.55
1:H:268:PRO:HG3	1:H:285:LEU:HD22	1.89	0.55
1:D:268:PRO:HG3	1:D:285:LEU:HD22	1.88	0.55
1:E:32:THR:HG22	1:E:33:ARG:HG2	1.88	0.55
1:H:108:THR:CG2	1:H:287:PRO:O	2.54	0.54
1:D:346:ILE:HG13	1:D:464:LEU:CD2	2.37	0.54
1:G:268:PRO:HG3	1:G:285:LEU:HD22	1.88	0.54
1:G:379:ARG:HD3	5:G:969:HOH:O	2.08	0.54
1:G:457:THR:HG21	1:G:487:HIS:CE1	2.43	0.54
1:H:346:ILE:HG13	1:H:464:LEU:CD2	2.37	0.54
1:H:457:THR:HG21	1:H:487:HIS:CE1	2.43	0.53
1:C:457:THR:HG21	1:C:487:HIS:CE1	2.43	0.53
1:B:352:ILE:HD13	1:B:377:LEU:HD22	1.90	0.53
1:F:352:ILE:HD13	1:F:377:LEU:HD22	1.91	0.53
1:D:436:PRO:CA	1:D:439:MET:HE2	2.38	0.53
1:B:379:ARG:HD3	5:B:1072:HOH:O	2.09	0.53
1:C:379:ARG:HD3	5:C:993:HOH:O	2.08	0.53
1:C:346:ILE:HG13	1:C:464:LEU:CD2	2.39	0.52
1:G:13:VAL:HG11	1:G:29:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:VAL:HG11	1:C:29:ILE:HD13	1.89	0.52
1:G:346:ILE:HG13	1:G:464:LEU:CD2	2.39	0.52
1:D:363:LEU:HD11	1:D:377:LEU:HB3	1.91	0.51
1:H:363:LEU:HD11	1:H:377:LEU:HB3	1.92	0.51
1:B:206:HIS:O	1:H:86:ARG:HD2	2.10	0.51
1:E:352:ILE:HD13	1:E:377:LEU:HD22	1.93	0.51
1:F:457:THR:HG21	1:F:487:HIS:CE1	2.46	0.51
1:A:429:TRP:CG	1:A:431:LEU:HD13	2.46	0.50
1:B:208:ARG:HH11	1:B:208:ARG:CG	2.24	0.50
1:B:457:THR:HG21	1:B:487:HIS:CE1	2.45	0.50
1:H:436:PRO:CA	1:H:439:MET:HE2	2.39	0.50
1:F:479:LEU:CD2	5:F:849:HOH:O	2.60	0.50
1:H:429:TRP:CG	1:H:431:LEU:HD13	2.46	0.50
1:B:479:LEU:CD2	5:B:862:HOH:O	2.60	0.49
1:B:208:ARG:HH11	1:B:208:ARG:HG2	1.78	0.49
1:B:429:TRP:CG	1:B:431:LEU:HD13	2.48	0.49
1:C:30:ALA:HB2	1:C:38:VAL:HG11	1.94	0.49
1:D:429:TRP:CG	1:D:431:LEU:HD13	2.47	0.49
1:G:304:GLU:OE2	1:G:304:GLU:C	2.55	0.49
1:F:208:ARG:HH11	1:F:208:ARG:CG	2.26	0.49
1:G:30:ALA:HB2	1:G:38:VAL:HG11	1.95	0.49
1:G:345:PRO:HG3	1:G:365:GLY:HA3	1.94	0.49
1:E:10:GLN:CB	1:E:35:ASP:O	2.60	0.49
1:E:429:TRP:CG	1:E:431:LEU:HD13	2.47	0.48
1:F:429:TRP:CG	1:F:431:LEU:HD13	2.47	0.48
1:A:457:THR:CG2	5:A:1134:HOH:O	2.61	0.48
1:F:208:ARG:HH11	1:F:208:ARG:HG2	1.79	0.48
1:C:83:GLN:NE2	5:C:802:HOH:O	2.39	0.48
1:A:352:ILE:HD13	1:A:377:LEU:HD22	1.94	0.48
1:G:345:PRO:HG3	1:G:365:GLY:CA	2.44	0.47
1:G:362:MET:HE2	1:G:362:MET:HB3	1.75	0.47
1:H:314:THR:CG2	1:H:318:PHE:CE2	2.98	0.47
1:H:429:TRP:CH2	1:H:439:MET:HE1	2.49	0.47
3:F:702:GLY:N	5:F:818:HOH:O	2.48	0.47
3:A:702:GLY:N	5:A:814:HOH:O	2.47	0.47
1:E:10:GLN:HB2	1:E:35:ASP:O	2.14	0.47
1:E:439:MET:HG2	1:G:439:MET:HE2	1.96	0.47
1:B:363:LEU:HD11	1:B:377:LEU:HB3	1.97	0.47
1:A:363:LEU:HD11	1:A:377:LEU:HB3	1.97	0.47
1:A:439:MET:HG2	1:C:439:MET:HE2	1.96	0.47
1:F:363:LEU:HD11	1:F:377:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:THR:CG2	1:D:318:PHE:CE2	2.98	0.46
1:E:363:LEU:HD11	1:E:377:LEU:HB3	1.96	0.46
1:G:468:ILE:HD13	1:G:479:LEU:CD2	2.46	0.46
1:D:429:TRP:CH2	1:D:439:MET:HE1	2.50	0.46
1:C:76:LYS:NZ	5:C:819:HOH:O	2.48	0.46
1:E:431:LEU:HD21	1:E:439:MET:HE1	1.98	0.45
1:G:83:GLN:NE2	5:G:804:HOH:O	2.42	0.45
1:C:468:ILE:HD13	1:C:479:LEU:CD2	2.46	0.45
1:H:381:VAL:C	1:H:385:MET:HE2	2.42	0.45
2:B:701:FAD:H9	2:B:701:FAD:H1'2	1.75	0.45
1:D:381:VAL:C	1:D:385:MET:HE2	2.42	0.45
1:D:335:ARG:HD3	1:D:335:ARG:HA	1.52	0.45
1:A:431:LEU:HD21	1:A:439:MET:HE1	1.98	0.44
1:D:20:VAL:HG11	1:D:371:LEU:HA	1.98	0.44
1:F:362:MET:HE2	1:F:362:MET:HB2	1.88	0.44
1:C:362:MET:HE2	1:C:362:MET:HB3	1.75	0.44
1:C:281[B]:CYS:SG	1:C:299:ASN:N	2.83	0.44
2:E:701:FAD:H9	2:E:701:FAD:H1'2	1.76	0.43
1:H:20:VAL:HG11	1:H:371:LEU:HA	1.99	0.43
1:C:55:GLY:HA2	1:C:294:TYR:CD2	2.53	0.43
1:G:363:LEU:HD12	1:G:363:LEU:HA	1.88	0.43
1:H:435:TRP:C	1:H:439:MET:HE2	2.43	0.43
1:H:436:PRO:N	1:H:439:MET:HE2	2.33	0.43
1:B:439:MET:CE	1:D:439:MET:HG2	2.48	0.43
1:A:311:ILE:HG23	1:B:318:PHE:HB3	2.01	0.43
1:G:55:GLY:HA2	1:G:294:TYR:CD2	2.53	0.43
1:H:362:MET:HE2	1:H:362:MET:HB2	1.91	0.43
1:D:436:PRO:N	1:D:439:MET:HE2	2.33	0.43
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.85	0.43
1:E:20:VAL:HG11	1:E:371:LEU:HA	2.00	0.43
1:D:435:TRP:C	1:D:439:MET:HE2	2.44	0.43
1:B:352:ILE:HG23	1:B:363:LEU:CD1	2.49	0.43
3:B:702:GLY:N	5:B:828:HOH:O	2.51	0.43
1:E:439:MET:CG	1:G:439:MET:HE2	2.49	0.43
1:A:20:VAL:HG11	1:A:371:LEU:HA	2.00	0.42
2:A:701:FAD:H9	2:A:701:FAD:H1'2	1.74	0.42
1:B:427:PHE:N	1:B:428:PRO:HA	2.34	0.42
1:E:427:PHE:N	1:E:428:PRO:HA	2.35	0.42
1:G:403:LEU:HG	1:G:486:VAL:HG11	2.02	0.42
1:H:363:LEU:HD12	1:H:363:LEU:HA	1.87	0.42
1:C:352:ILE:HG23	1:C:363:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:ILE:HG23	1:F:363:LEU:CD1	2.49	0.42
1:G:352:ILE:HG23	1:G:363:LEU:CD1	2.50	0.42
1:D:369:ASP:HB2	5:D:804:HOH:O	2.20	0.42
1:H:368:ARG:NH2	3:H:702:GLY:HA2	2.35	0.42
2:H:701:FAD:O4	3:H:702:GLY:HA3	2.19	0.42
1:A:352:ILE:HG23	1:A:363:LEU:CD1	2.50	0.42
1:A:427:PHE:N	1:A:428:PRO:HA	2.35	0.42
1:E:362:MET:HE2	1:E:362:MET:HB2	1.90	0.42
1:E:28:GLU:O	1:E:32:THR:HB	2.19	0.42
1:H:133:LEU:HD12	1:H:133:LEU:HA	1.96	0.42
1:D:55:GLY:N	1:D:56:ALA:HA	2.35	0.41
1:F:427:PHE:N	1:F:428:PRO:HA	2.35	0.41
1:C:249:ARG:CG	5:C:877:HOH:O	2.68	0.41
1:G:299:ASN:ND2	5:G:820:HOH:O	2.53	0.41
1:H:55:GLY:N	1:H:56:ALA:HA	2.35	0.41
1:H:55:GLY:HA2	1:H:294:TYR:CD2	2.55	0.41
1:D:352:ILE:HG23	1:D:363:LEU:CD1	2.51	0.41
1:D:427:PHE:N	1:D:428:PRO:HA	2.35	0.41
1:B:362:MET:HE2	1:B:362:MET:HB2	1.87	0.41
1:G:234:GLN:HG3	1:G:248:PRO:O	2.21	0.41
1:B:20:VAL:HG11	1:B:371:LEU:HA	2.02	0.41
1:C:403:LEU:HG	1:C:486:VAL:HG11	2.01	0.41
1:C:427:PHE:N	1:C:428:PRO:HA	2.35	0.41
1:A:28:GLU:O	1:A:32:THR:HB	2.20	0.41
1:A:457:THR:HG23	5:A:1134:HOH:O	2.20	0.41
1:F:33:ARG:HD2	5:F:927:HOH:O	2.21	0.41
1:A:439:MET:CG	1:C:439:MET:HE2	2.50	0.41
1:D:30:ALA:HB2	1:D:38:VAL:HG11	2.02	0.41
1:D:55:GLY:HA2	1:D:294:TYR:CD2	2.55	0.41
1:F:363:LEU:HD12	1:F:363:LEU:HA	1.88	0.41
1:H:352:ILE:HG23	1:H:363:LEU:CD1	2.50	0.41
1:E:352:ILE:HG23	1:E:363:LEU:CD1	2.50	0.40
1:F:20:VAL:HG11	1:F:371:LEU:HA	2.02	0.40
2:H:701:FAD:H9	2:H:701:FAD:H1'2	1.83	0.40
1:B:208:ARG:CG	1:B:208:ARG:NH1	2.84	0.40
1:C:240:LEU:HB2	1:C:243:LEU:HD22	2.04	0.40
1:D:123:ALA:CB	1:D:418:ARG:HD2	2.48	0.40
1:B:69:LEU:HD23	5:B:1003:HOH:O	2.21	0.40
1:B:137:LYS:HD3	1:B:143:HIS:CE1	2.56	0.40
1:H:427:PHE:N	1:H:428:PRO:HA	2.36	0.40
1:C:137:LYS:HA	1:C:137:LYS:HD3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:439:MET:CE	1:H:439:MET:HG2	2.49	0.40
1:G:55:GLY:N	1:G:56:ALA:HA	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/512 (94%)	468 (98%)	12 (2%)	0	100	100
1	B	481/512 (94%)	469 (98%)	12 (2%)	0	100	100
1	C	469/512 (92%)	458 (98%)	11 (2%)	0	100	100
1	D	461/512 (90%)	450 (98%)	11 (2%)	0	100	100
1	E	480/512 (94%)	468 (98%)	12 (2%)	0	100	100
1	F	481/512 (94%)	469 (98%)	12 (2%)	0	100	100
1	G	469/512 (92%)	458 (98%)	11 (2%)	0	100	100
1	H	460/512 (90%)	448 (97%)	12 (3%)	0	100	100
All	All	3781/4096 (92%)	3688 (98%)	93 (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	376/400 (94%)	362 (96%)	14 (4%)	30	31
1	B	377/400 (94%)	367 (97%)	10 (3%)	39	44
1	C	372/400 (93%)	362 (97%)	10 (3%)	39	44
1	D	365/400 (91%)	353 (97%)	12 (3%)	33	36
1	E	376/400 (94%)	364 (97%)	12 (3%)	34	37
1	F	377/400 (94%)	365 (97%)	12 (3%)	34	37
1	G	372/400 (93%)	363 (98%)	9 (2%)	43	48
1	H	363/400 (91%)	354 (98%)	9 (2%)	42	47
All	All	2978/3200 (93%)	2890 (97%)	88 (3%)	36	40

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	25	VAL
1	A	32	THR
1	A	36	VAL
1	A	77	LYS
1	A	133	LEU
1	A	189	GLN
1	A	193	ARG
1	A	203	ARG
1	A	362	MET
1	A	449	GLU
1	A	452	ASP
1	A	457	THR
1	A	464	LEU
1	B	33	ARG
1	B	36	VAL
1	B	77	LYS
1	B	133	LEU
1	B	137	LYS
1	B	203	ARG
1	B	362	MET
1	B	395	ARG
1	B	452	ASP
1	B	457	THR
1	C	33	ARG
1	C	36	VAL
1	C	77	LYS

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	203	ARG
1	C	335	ARG
1	C	386	ASP
1	C	431	LEU
1	C	452	ASP
1	C	457	THR
1	D	36	VAL
1	D	37	ARG
1	D	77	LYS
1	D	85	GLN
1	D	90	GLU
1	D	108	THR
1	D	133	LEU
1	D	193	ARG
1	D	335	ARG
1	D	362	MET
1	D	452	ASP
1	D	457	THR
1	E	10	GLN
1	E	25	VAL
1	E	32	THR
1	E	36	VAL
1	E	77	LYS
1	E	133	LEU
1	E	189	GLN
1	E	203	ARG
1	E	362	MET
1	E	449	GLU
1	E	452	ASP
1	E	457	THR
1	F	33	ARG
1	F	36	VAL
1	F	69	LEU
1	F	77	LYS
1	F	133	LEU
1	F	137	LYS
1	F	203	ARG
1	F	335	ARG
1	F	362	MET
1	F	395	ARG
1	F	452	ASP

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Mol	Chain	Res	Type
1	F	457	THR
1	G	33	ARG
1	G	36	VAL
1	G	77	LYS
1	G	85	GLN
1	G	203	ARG
1	G	386	ASP
1	G	431	LEU
1	G	452	ASP
1	G	457	THR
1	H	77	LYS
1	H	85	GLN
1	H	90	GLU
1	H	108	THR
1	H	133	LEU
1	H	193	ARG
1	H	362	MET
1	H	452	ASP
1	H	457	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	437	HIS
1	A	487	HIS
1	B	444	GLN
1	C	159	ASN
1	C	437	HIS
1	D	85	GLN
1	D	159	ASN
1	D	437	HIS
1	D	487	HIS
1	E	437	HIS
1	E	487	HIS
1	F	444	GLN
1	G	159	ASN
1	H	85	GLN
1	H	245	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GLY	G	702	-	4,4,4	1.18	1 (25%)	3,4,4	1.86	1 (33%)
2	FAD	F	701	-	58,58,58	0.78	1 (1%)	85,89,89	0.78	3 (3%)
2	FAD	H	701	-	58,58,58	0.63	1 (1%)	85,89,89	0.66	0
3	GLY	F	702	-	4,4,4	1.04	0	3,4,4	1.25	0
3	GLY	H	702	-	4,4,4	0.98	0	3,4,4	2.19	2 (66%)
3	GLY	B	702	-	4,4,4	1.16	0	3,4,4	0.95	0
4	I60	G	703	-	31,34,34	0.81	1 (3%)	36,48,48	0.92	1 (2%)
4	I60	A	703	-	31,34,34	1.05	2 (6%)	36,48,48	0.94	3 (8%)
2	FAD	D	701	-	58,58,58	0.62	0	85,89,89	0.67	2 (2%)
3	GLY	D	702	-	4,4,4	1.02	0	3,4,4	2.34	2 (66%)
2	FAD	B	701	-	58,58,58	0.86	2 (3%)	85,89,89	0.83	3 (3%)
3	GLY	A	702	-	4,4,4	0.97	0	3,4,4	0.75	0
2	FAD	C	701	-	58,58,58	0.65	1 (1%)	85,89,89	0.67	1 (1%)
2	FAD	E	701	-	58,58,58	0.91	2 (3%)	85,89,89	0.84	4 (4%)
3	GLY	C	702	-	4,4,4	1.23	1 (25%)	3,4,4	1.85	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLY	E	702	-	4,4,4	1.01	0	3,4,4	1.22	0
2	FAD	G	701	-	58,58,58	0.69	2 (3%)	85,89,89	0.73	1 (1%)
2	FAD	A	701	-	58,58,58	0.82	2 (3%)	85,89,89	0.81	2 (2%)
4	I60	E	703	-	31,34,34	1.17	2 (6%)	36,48,48	0.98	3 (8%)
4	I60	B	703	-	31,34,34	0.86	1 (3%)	36,48,48	0.95	3 (8%)
4	I60	D	703	-	31,34,34	0.93	1 (3%)	36,48,48	0.88	1 (2%)
4	I60	C	703	-	31,34,34	0.78	1 (3%)	36,48,48	1.12	2 (5%)
4	I60	H	703	-	31,34,34	0.73	1 (3%)	36,48,48	0.85	2 (5%)
4	I60	F	703	-	31,34,34	0.90	1 (3%)	36,48,48	0.93	1 (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
3	GLY	G	702	-	-	2/2/2/2	-
2	FAD	F	701	-	-	3/34/50/50	0/6/6/6
2	FAD	H	701	-	-	6/34/50/50	0/6/6/6
3	GLY	F	702	-	-	0/2/2/2	-
3	GLY	H	702	-	-	0/2/2/2	-
3	GLY	B	702	-	-	0/2/2/2	-
4	I60	G	703	-	-	4/16/63/63	0/3/3/3
4	I60	A	703	-	-	1/16/63/63	0/3/3/3
2	FAD	D	701	-	-	7/34/50/50	0/6/6/6
3	GLY	D	702	-	-	0/2/2/2	-
2	FAD	B	701	-	-	3/34/50/50	0/6/6/6
3	GLY	A	702	-	-	0/2/2/2	-
2	FAD	C	701	-	-	11/34/50/50	0/6/6/6
2	FAD	E	701	-	-	3/34/50/50	0/6/6/6
3	GLY	C	702	-	-	0/2/2/2	-
3	GLY	E	702	-	-	0/2/2/2	-
2	FAD	G	701	-	-	13/34/50/50	0/6/6/6
2	FAD	A	701	-	-	3/34/50/50	0/6/6/6
4	I60	E	703	-	-	1/16/63/63	0/3/3/3
4	I60	B	703	-	-	1/16/63/63	0/3/3/3
4	I60	D	703	-	-	4/16/63/63	0/3/3/3
4	I60	C	703	-	-	4/16/63/63	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	I60	H	703	-	-	2/16/63/63	0/3/3/3
4	I60	F	703	-	-	1/16/63/63	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	703	I60	C11-C5	-5.41	1.49	1.53
4	A	703	I60	C11-C5	-4.77	1.50	1.53
4	D	703	I60	C11-C5	-4.48	1.50	1.53
2	B	701	FAD	PA-O3P	3.92	1.63	1.59
2	E	701	FAD	PA-O3P	3.76	1.63	1.59
4	F	703	I60	C11-C5	-3.67	1.50	1.53
4	B	703	I60	C11-C5	-3.41	1.51	1.53
2	A	701	FAD	PA-O3P	3.28	1.63	1.59
2	F	701	FAD	PA-O3P	3.07	1.62	1.59
4	G	703	I60	C11-C5	-3.00	1.51	1.53
4	H	703	I60	C11-C5	-2.98	1.51	1.53
2	E	701	FAD	C1'-C2'	-2.85	1.48	1.52
2	A	701	FAD	C1'-C2'	-2.50	1.49	1.52
4	C	703	I60	C11-C5	-2.48	1.51	1.53
4	E	703	I60	C15-C16	2.44	1.54	1.52
4	A	703	I60	C15-C16	2.38	1.54	1.52
3	C	702	GLY	OXT-C	-2.37	1.23	1.30
2	G	701	FAD	PA-O3P	2.36	1.62	1.59
2	B	701	FAD	C1'-C2'	-2.31	1.49	1.52
3	G	702	GLY	OXT-C	-2.25	1.23	1.30
2	G	701	FAD	P-O3P	2.11	1.61	1.59
2	H	701	FAD	PA-O3P	2.04	1.61	1.59
2	C	701	FAD	PA-O3P	2.04	1.61	1.59

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	703	I60	C13-C14-N6	-3.42	114.11	118.14
4	C	703	I60	C11-C5-N2	3.35	115.94	111.08
4	D	703	I60	C13-C14-N6	-3.06	114.54	118.14
4	B	703	I60	C16-C15-N6	2.98	112.87	109.83
4	E	703	I60	C17-N7-C12	-2.97	107.20	112.17
3	D	702	GLY	OXT-C-O	-2.92	115.81	123.33
2	A	701	FAD	C4'-C3'-C2'	2.90	118.39	113.57
2	F	701	FAD	C4'-C3'-C2'	2.88	118.37	113.57
2	E	701	FAD	C4'-C3'-C2'	2.80	118.23	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	O2A-PA-O1A	2.78	125.36	112.44
2	B	701	FAD	C4'-C3'-C2'	2.77	118.18	113.57
3	D	702	GLY	OXT-C-CA	2.74	124.30	113.38
3	H	702	GLY	OXT-C-CA	2.71	124.16	113.38
4	E	703	I60	C16-C15-N6	2.61	112.49	109.83
3	C	702	GLY	OXT-C-O	-2.58	116.70	123.33
3	G	702	GLY	OXT-C-O	-2.58	116.71	123.33
4	A	703	I60	C17-N7-C12	-2.55	107.92	112.17
3	H	702	GLY	OXT-C-O	-2.54	116.81	123.33
4	F	703	I60	C16-C15-N6	2.48	112.36	109.83
2	A	701	FAD	O2A-PA-O1A	2.42	123.72	112.44
4	A	703	I60	N7-C12-N5	-2.38	106.79	109.21
2	F	701	FAD	O2A-PA-O1A	2.31	123.18	112.44
2	E	701	FAD	O2A-PA-O1A	2.29	123.09	112.44
4	E	703	I60	N7-C12-N5	-2.28	106.89	109.21
2	E	701	FAD	O3P-PA-O1A	-2.23	103.99	110.70
4	G	703	I60	C11-C5-N2	2.18	114.25	111.08
4	B	703	I60	N7-C12-N5	-2.17	107.00	109.21
4	A	703	I60	C16-C15-N6	2.14	112.02	109.83
4	H	703	I60	N7-C12-N5	-2.12	107.05	109.21
2	B	701	FAD	C4-N3-C2	-2.12	121.88	125.64
4	H	703	I60	C11-C5-N2	2.11	114.14	111.08
4	B	703	I60	C11-C5-N2	2.10	114.13	111.08
2	E	701	FAD	C4-N3-C2	-2.08	121.94	125.64
2	G	701	FAD	C4-N3-C2	-2.08	121.95	125.64
2	D	701	FAD	O2P-P-O1P	2.07	122.09	112.44
2	F	701	FAD	C4-N3-C2	-2.06	121.98	125.64
2	D	701	FAD	C4-N3-C2	-2.03	122.04	125.64
2	C	701	FAD	C4-N3-C2	-2.01	122.08	125.64

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	FAD	C2'-C3'-C4'-O4'
2	C	701	FAD	C2'-C3'-C4'-C5'
2	C	701	FAD	O3'-C3'-C4'-O4'
2	C	701	FAD	O3'-C3'-C4'-C5'
2	C	701	FAD	O4'-C4'-C5'-O5'
2	C	701	FAD	C5'-O5'-P-O2P
2	D	701	FAD	C5B-O5B-PA-O2A
2	G	701	FAD	P-O3P-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	G	701	FAD	C2'-C3'-C4'-O4'
2	G	701	FAD	C2'-C3'-C4'-C5'
2	G	701	FAD	O3'-C3'-C4'-O4'
2	G	701	FAD	O3'-C3'-C4'-C5'
2	G	701	FAD	C3'-C4'-C5'-O5'
2	G	701	FAD	O4'-C4'-C5'-O5'
2	G	701	FAD	C5'-O5'-P-O2P
2	G	701	FAD	C5'-O5'-P-O3P
2	H	701	FAD	C5B-O5B-PA-O2A
4	C	703	I60	N5-C12-N4-C11
4	C	703	I60	N7-C12-N4-C11
4	D	703	I60	C6-C7-O3-C8
4	D	703	I60	C9-C7-O3-C8
4	D	703	I60	N5-C12-N4-C11
4	D	703	I60	N7-C12-N4-C11
4	G	703	I60	N5-C12-N4-C11
4	G	703	I60	N7-C12-N4-C11
2	H	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C3'-C4'-C5'-O5'
2	D	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	O4B-C4B-C5B-O5B
2	H	701	FAD	C3B-C4B-C5B-O5B
2	C	701	FAD	P-O3P-PA-O5B
2	D	701	FAD	P-O3P-PA-O5B
2	H	701	FAD	P-O3P-PA-O5B
3	G	702	GLY	OXT-C-CA-N
2	D	701	FAD	C3B-C4B-C5B-O5B
2	A	701	FAD	C2B-C1B-N9A-C8A
2	B	701	FAD	C2B-C1B-N9A-C8A
2	E	701	FAD	C2B-C1B-N9A-C8A
2	F	701	FAD	C2B-C1B-N9A-C8A
2	H	701	FAD	C2B-C1B-N9A-C8A
4	A	703	I60	C6-C7-O3-C8
4	B	703	I60	C6-C7-O3-C8
4	C	703	I60	C6-C7-O3-C8
4	C	703	I60	C9-C7-O3-C8
4	E	703	I60	C6-C7-O3-C8
4	F	703	I60	C6-C7-O3-C8
4	G	703	I60	C6-C7-O3-C8
4	G	703	I60	C9-C7-O3-C8
4	H	703	I60	C6-C7-O3-C8
4	H	703	I60	C9-C7-O3-C8

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Mol	Chain	Res	Type	Atoms
2	D	701	FAD	C2B-C1B-N9A-C8A
2	C	701	FAD	C5'-O5'-P-O3P
2	G	701	FAD	C5'-O5'-P-O1P
2	G	701	FAD	C3B-C4B-C5B-O5B
2	B	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	C2B-C1B-N9A-C8A
2	A	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	O4B-C1B-N9A-C8A
3	G	702	GLY	O-C-CA-N
2	D	701	FAD	O4B-C1B-N9A-C8A
2	H	701	FAD	O4B-C1B-N9A-C8A
2	C	701	FAD	C2B-C1B-N9A-C8A
2	A	701	FAD	O4B-C1B-N9A-C8A
2	F	701	FAD	O4B-C1B-N9A-C8A
2	E	701	FAD	O4B-C4B-C5B-O5B
2	E	701	FAD	O4B-C1B-N9A-C8A
2	D	701	FAD	PA-O3P-P-O2P

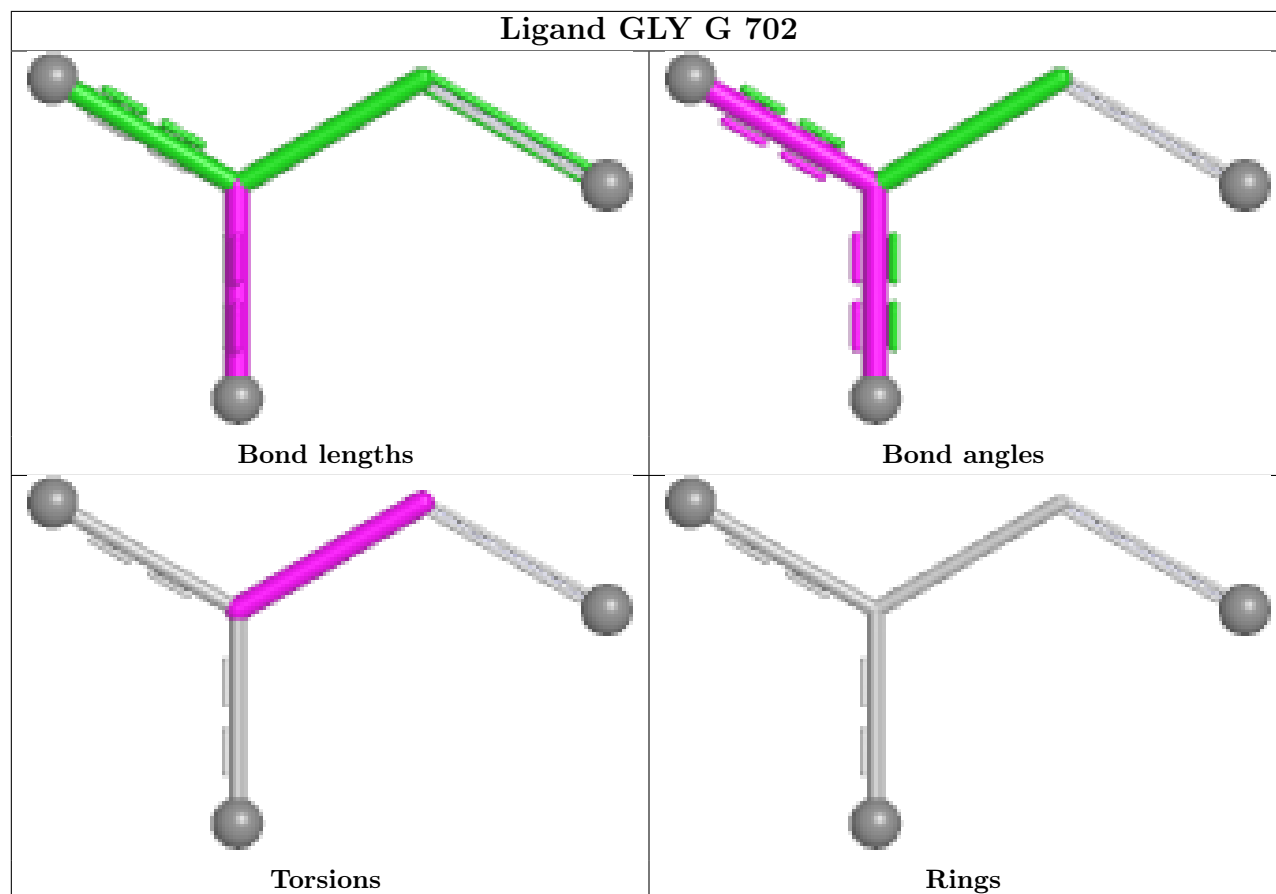
There are no ring outliers.

8 monomers are involved in 9 short contacts:

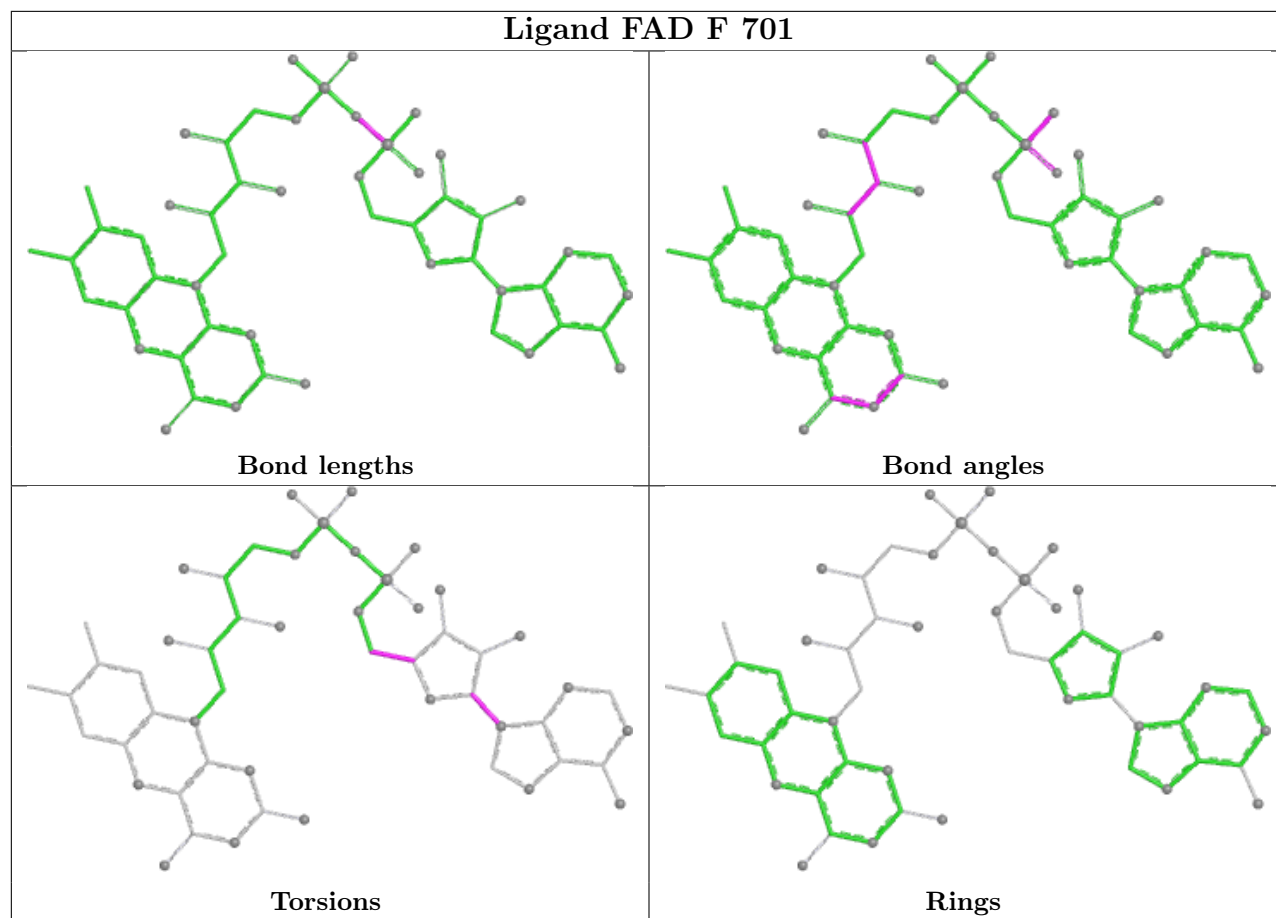
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	701	FAD	2	0
3	F	702	GLY	1	0
3	H	702	GLY	2	0
3	B	702	GLY	1	0
2	B	701	FAD	1	0
3	A	702	GLY	1	0
2	E	701	FAD	1	0
2	A	701	FAD	1	0

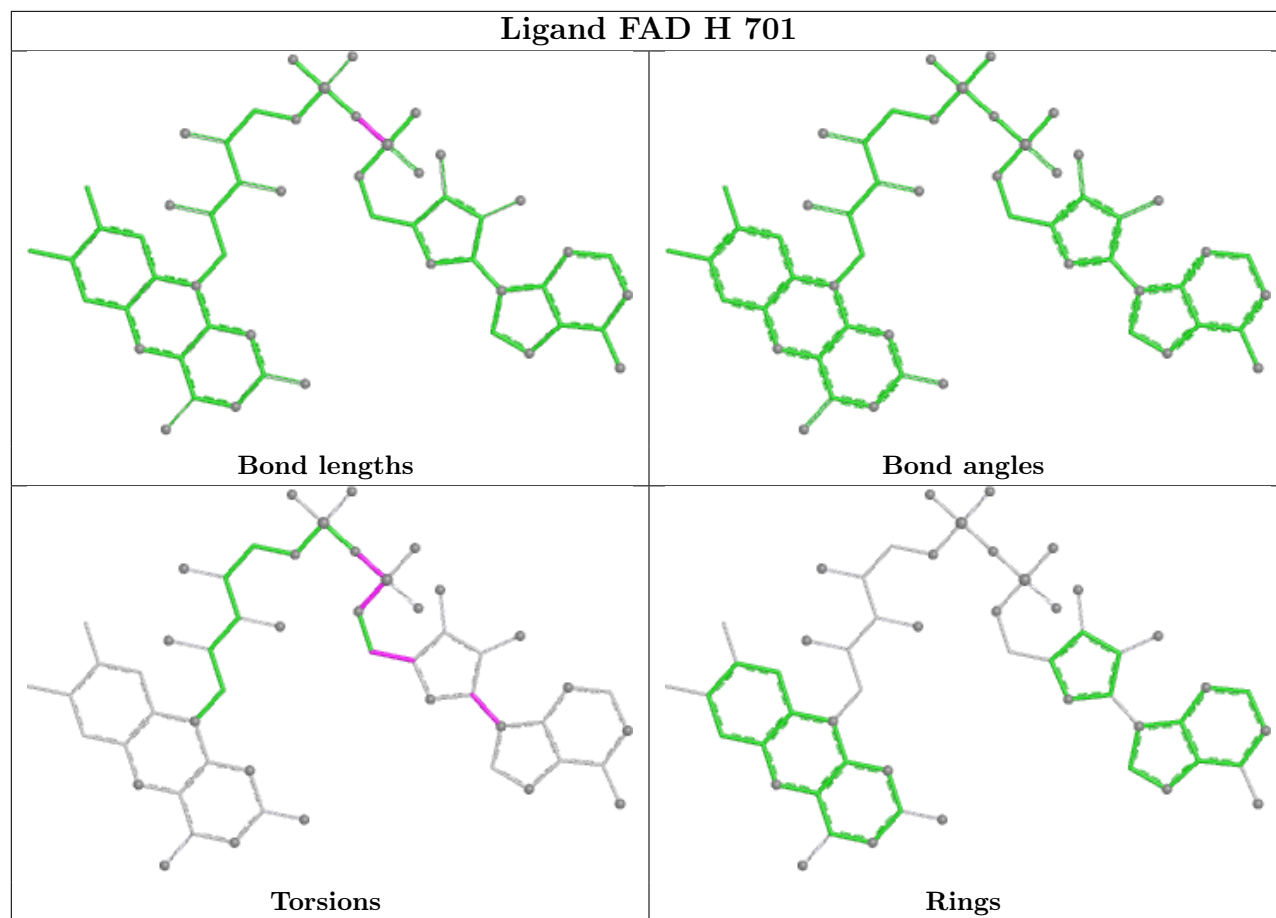
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

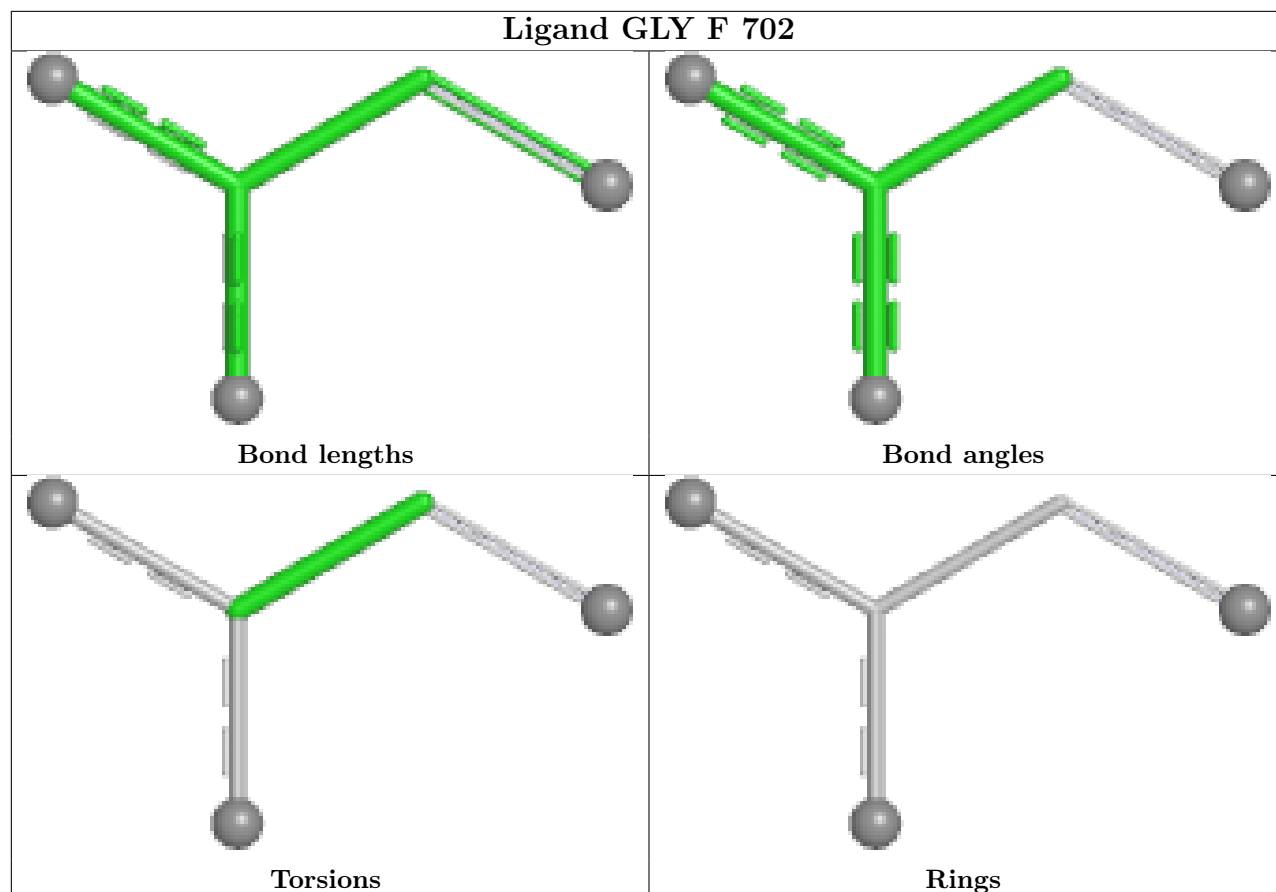


Ligand FAD F 701

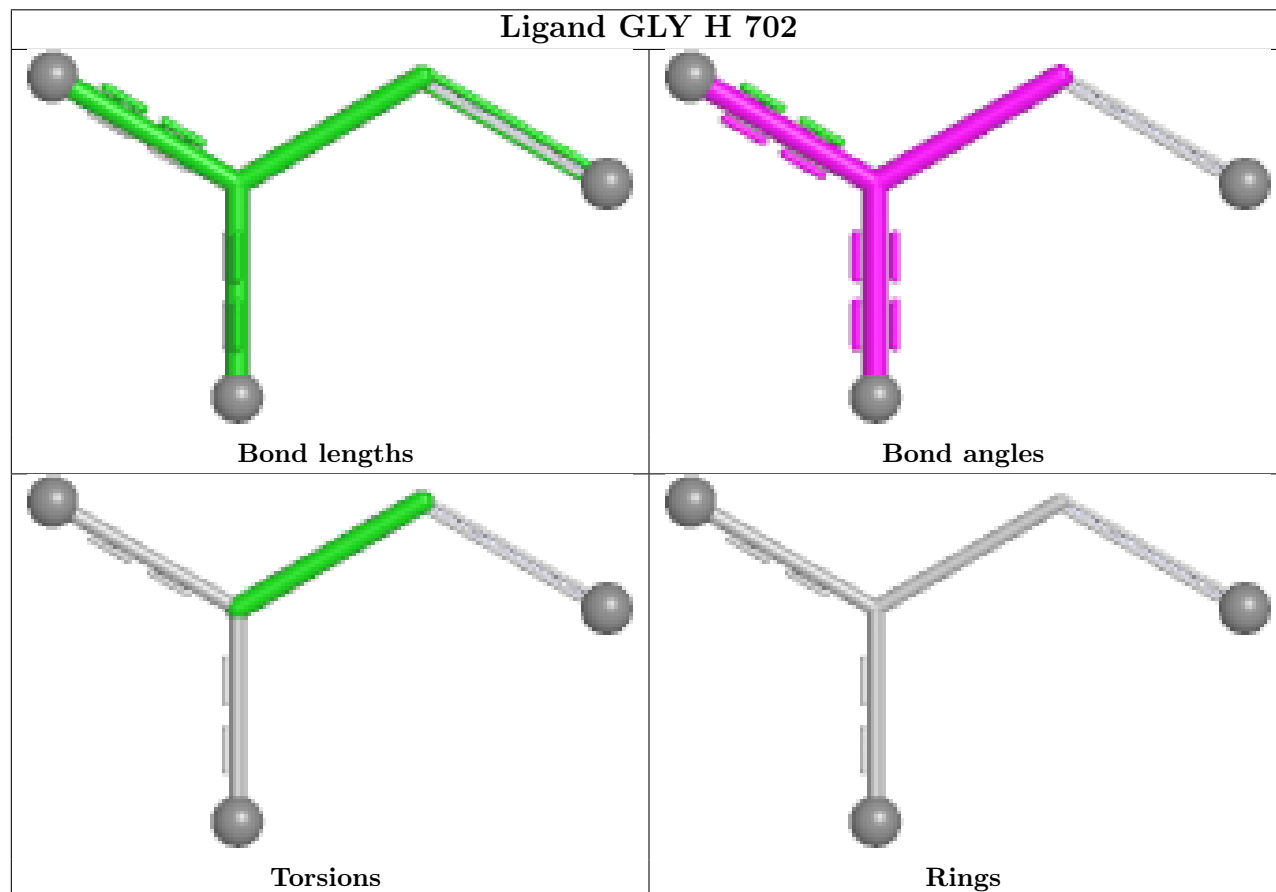


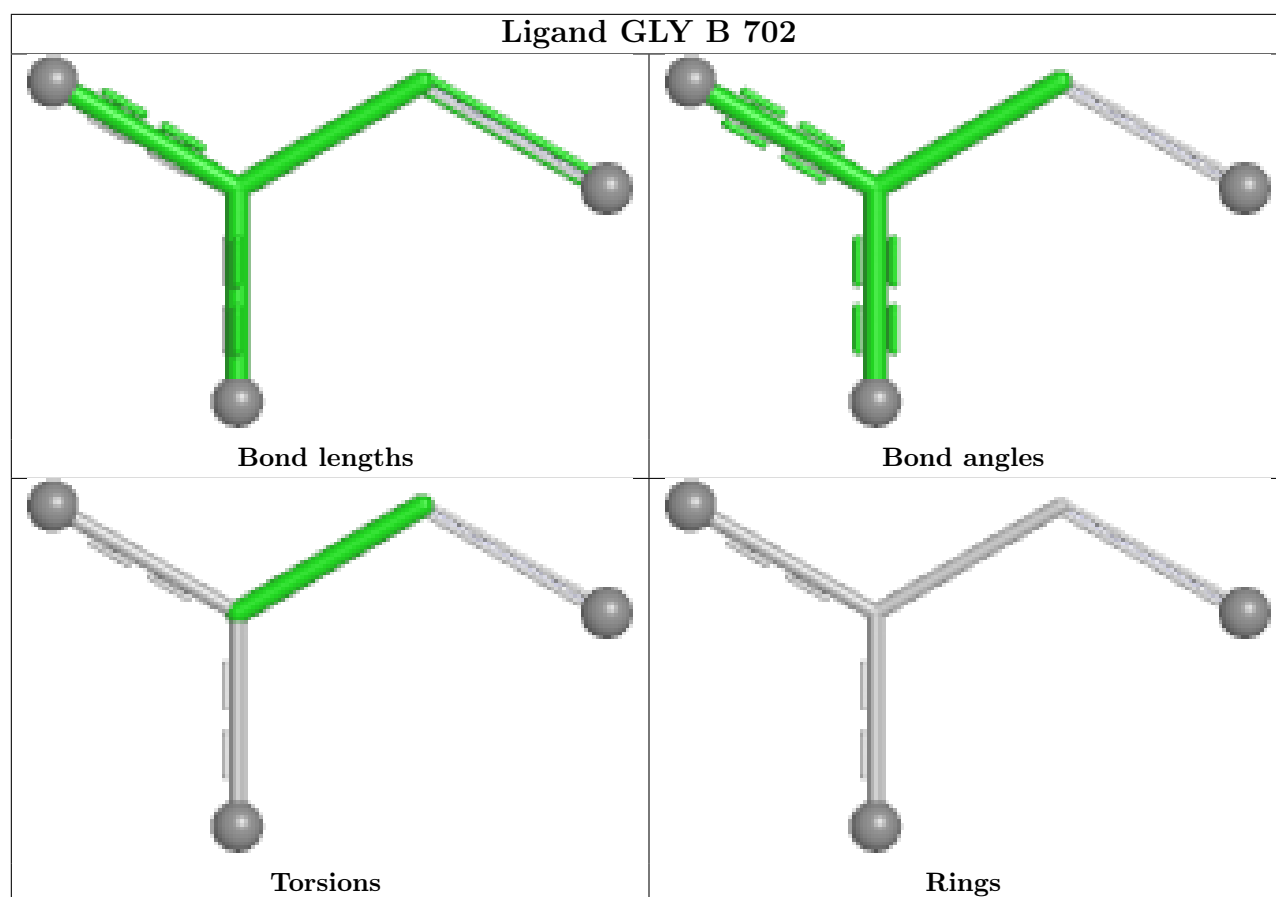


Ligand GLY F 702

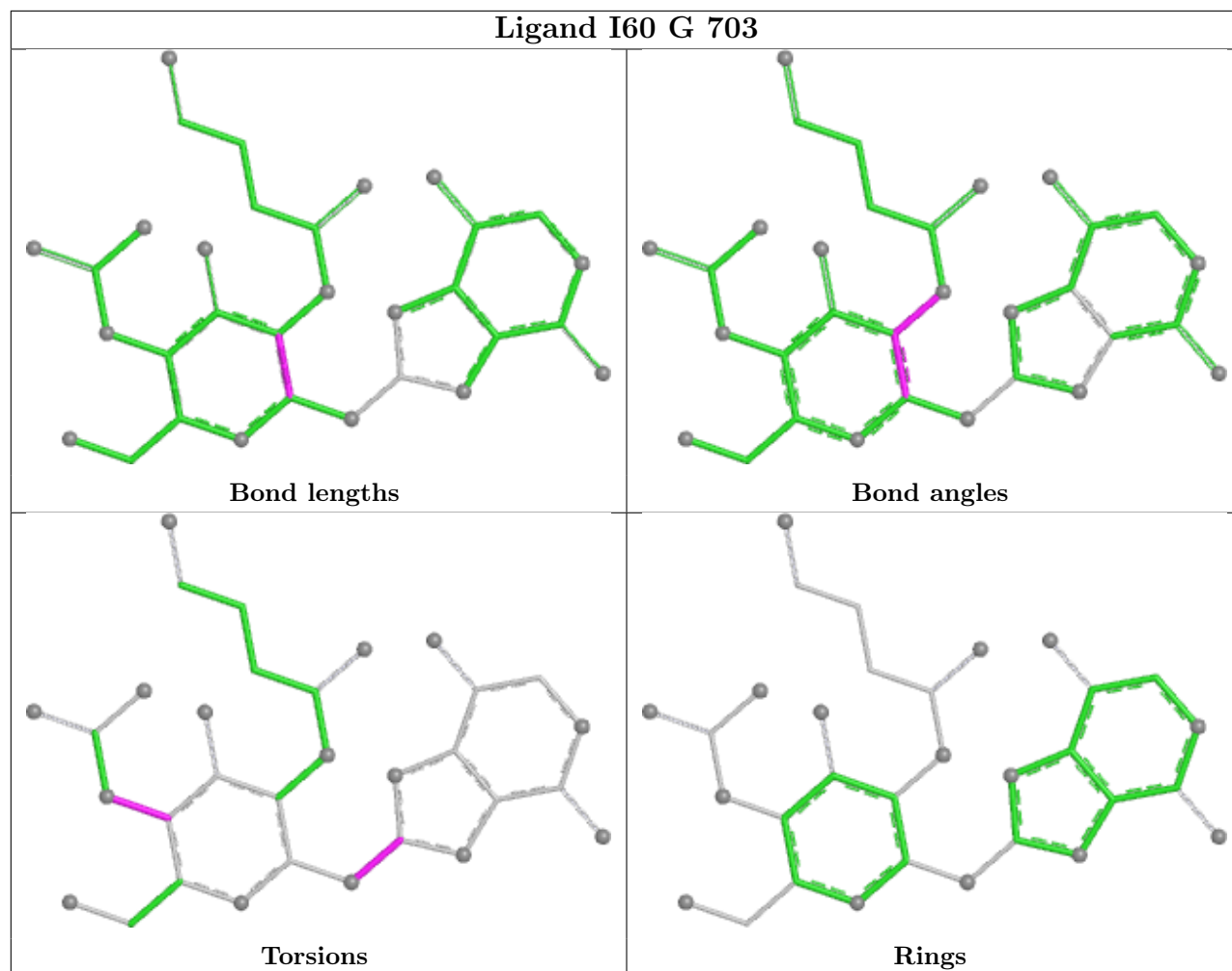


Ligand GLY H 702

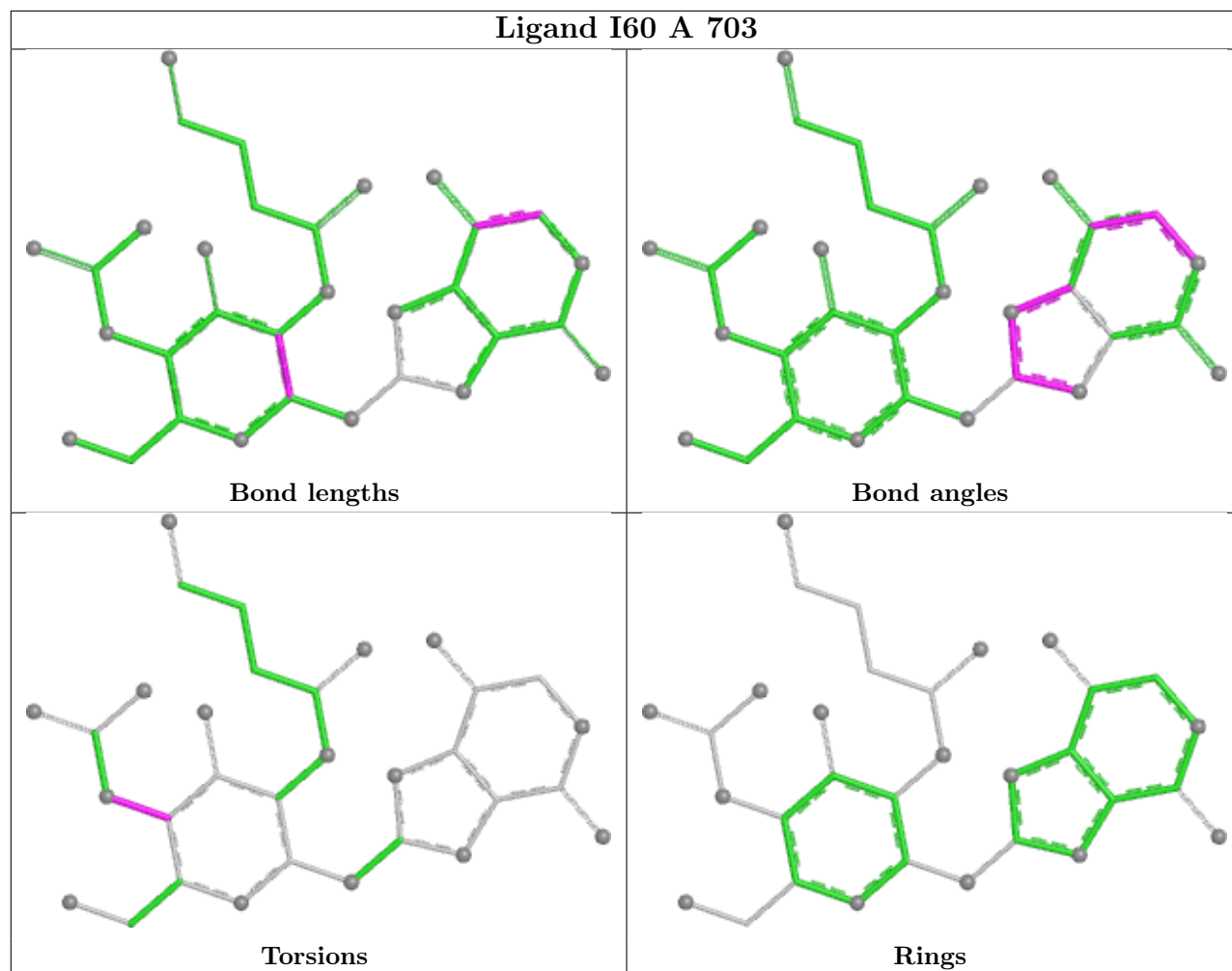


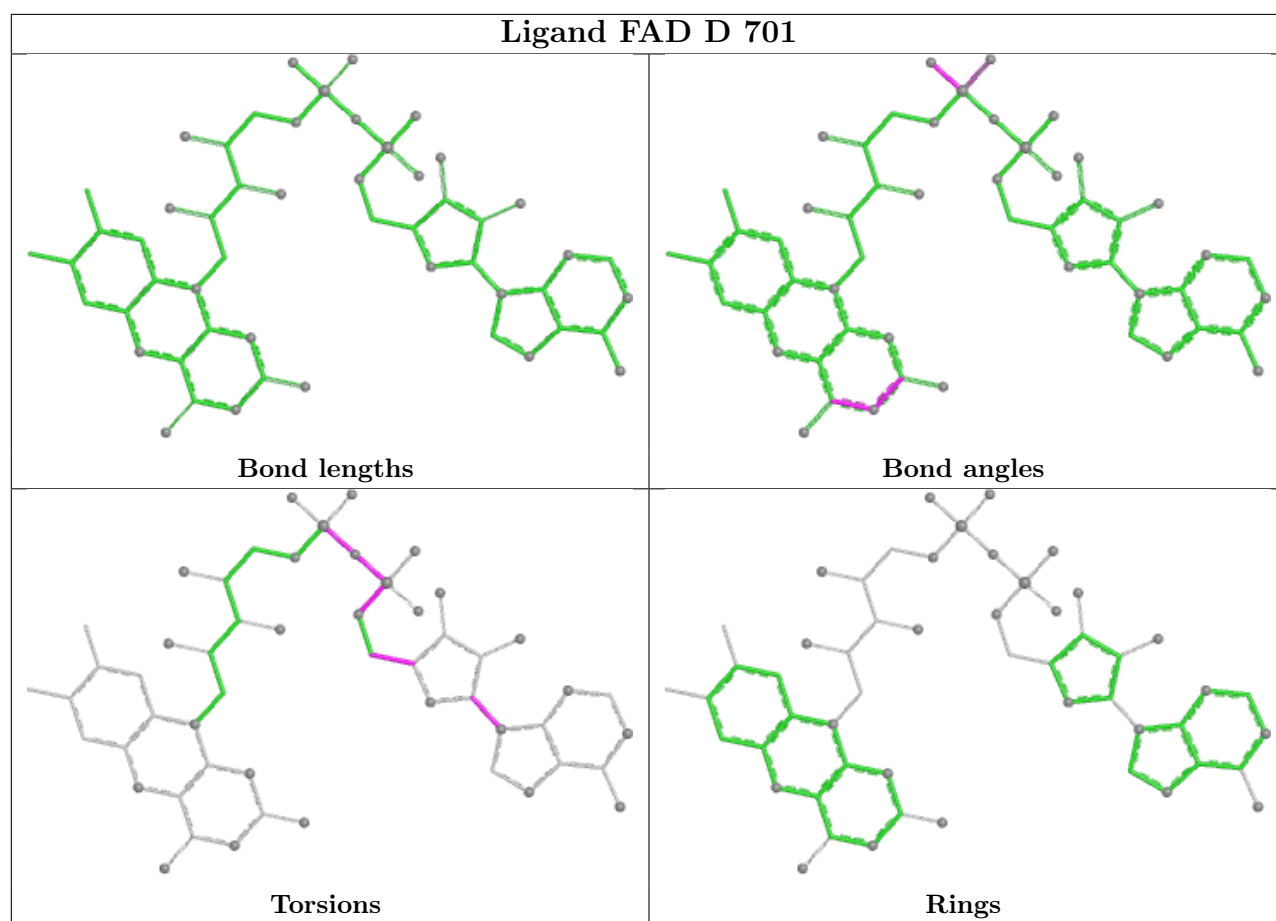


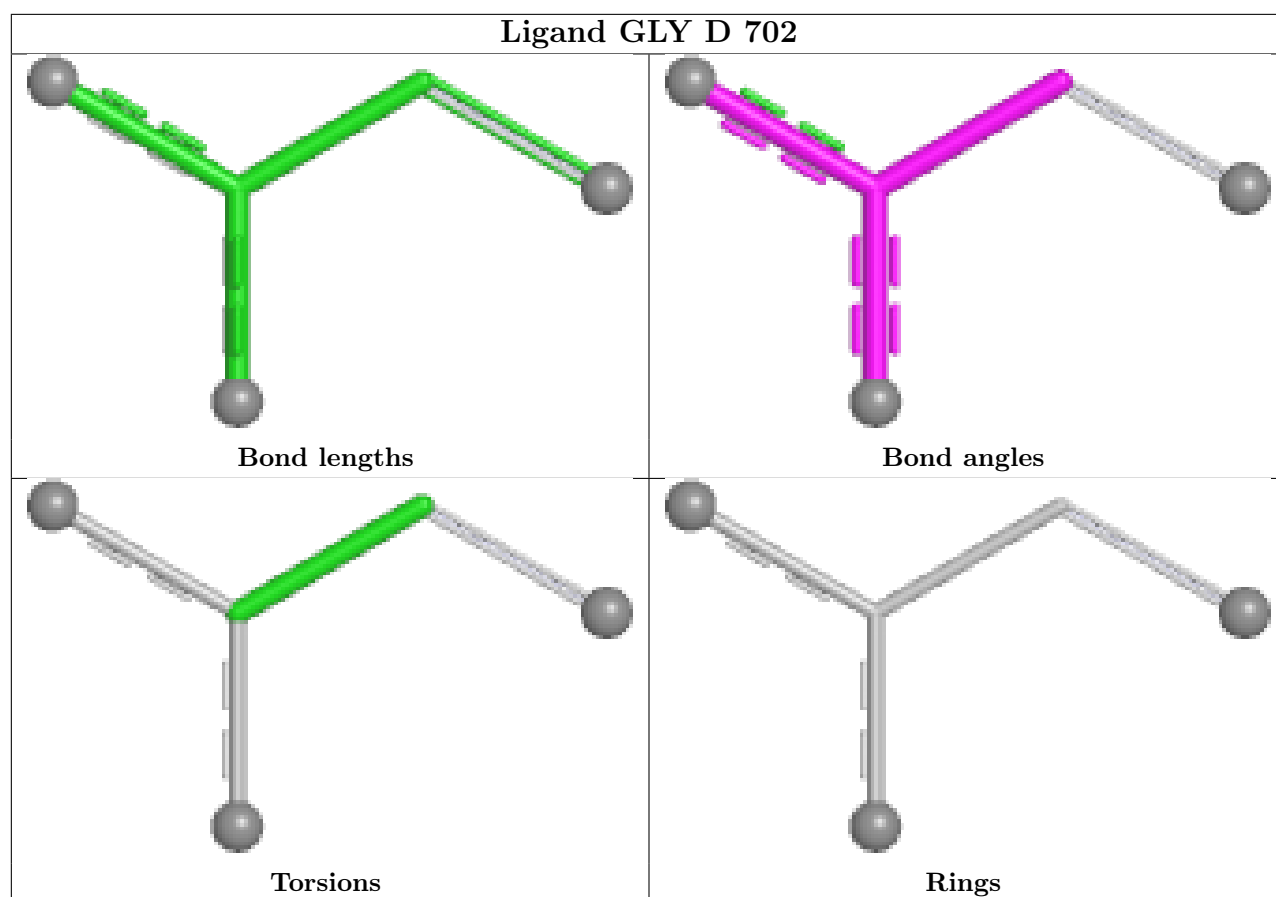
Ligand I60 G 703

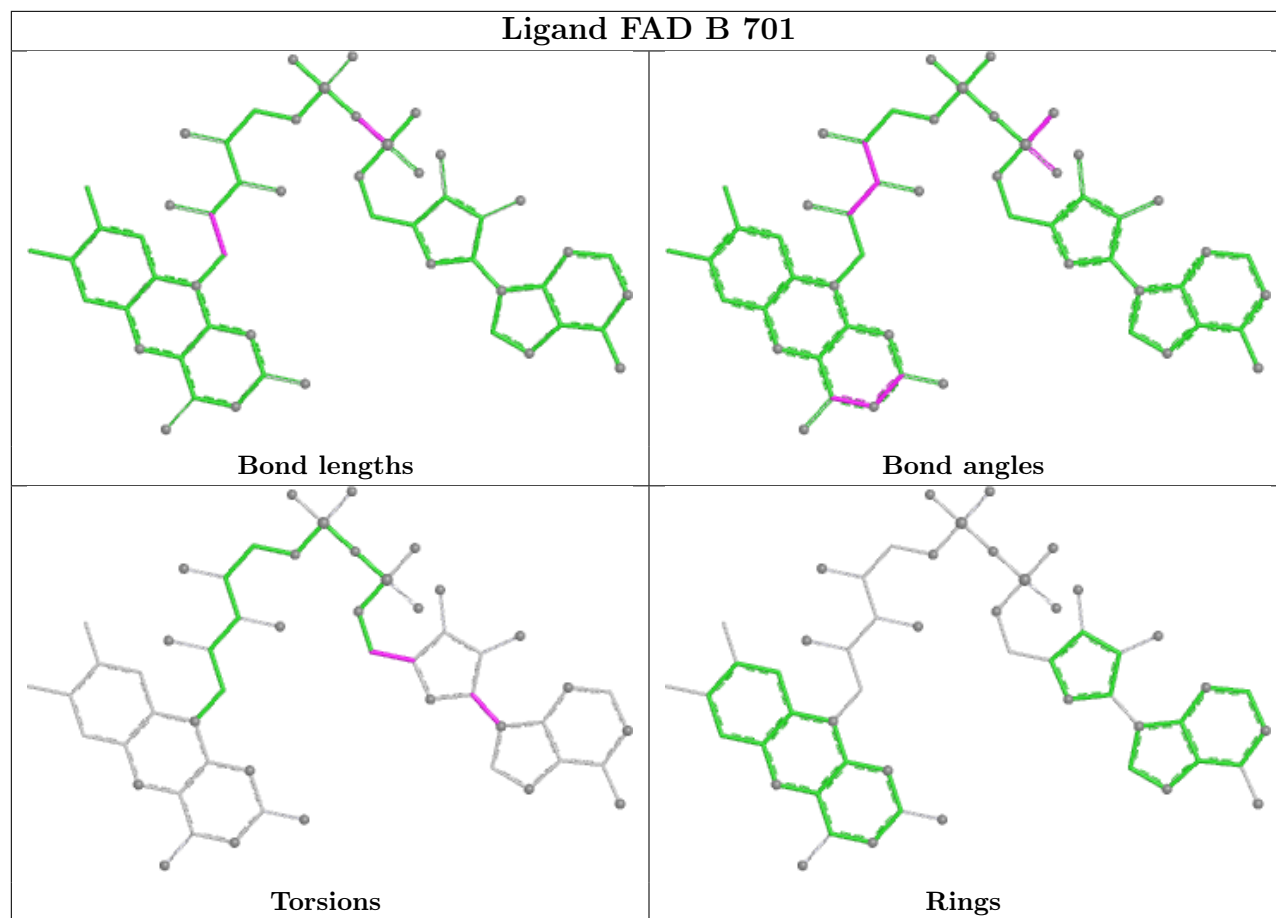


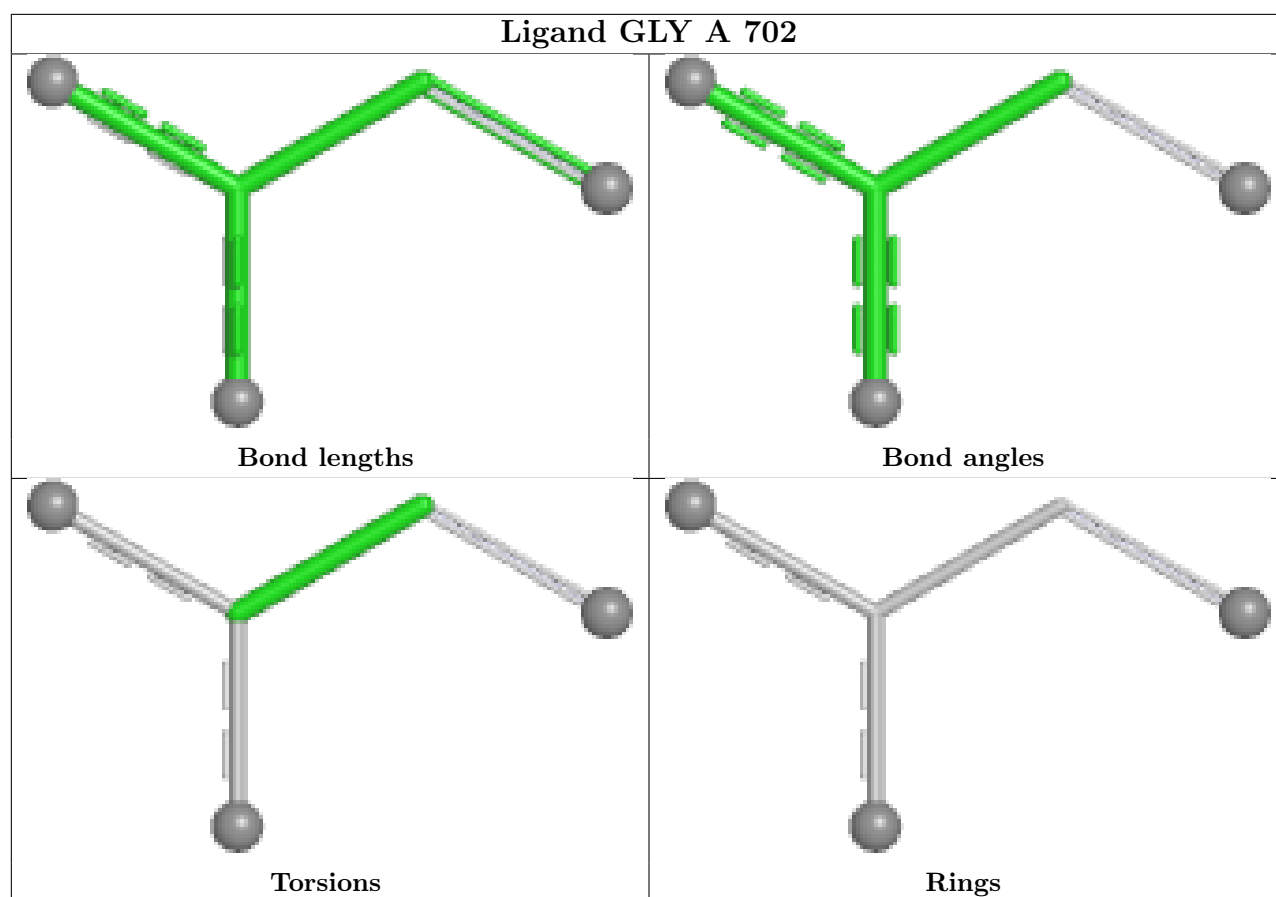
Ligand I60 A 703

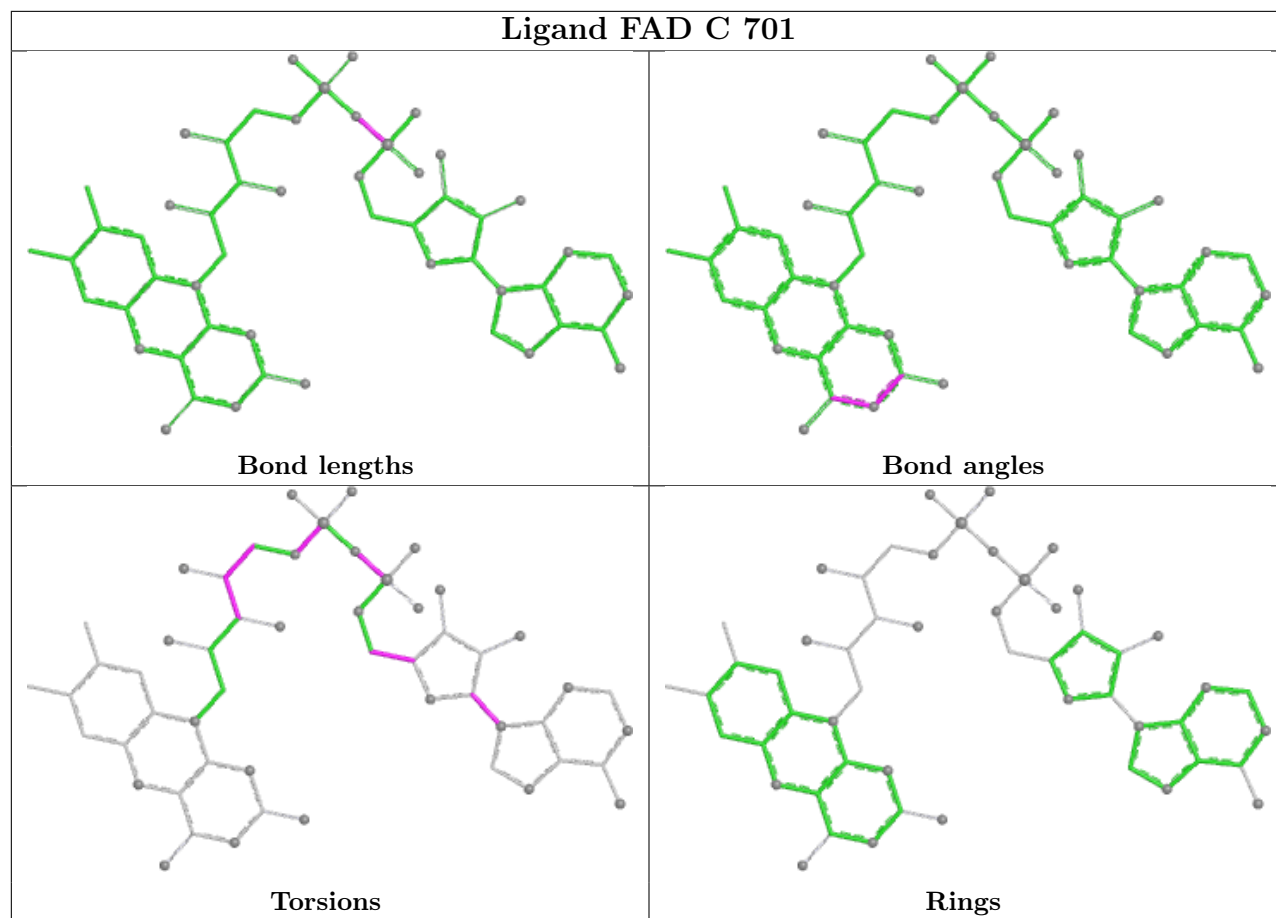


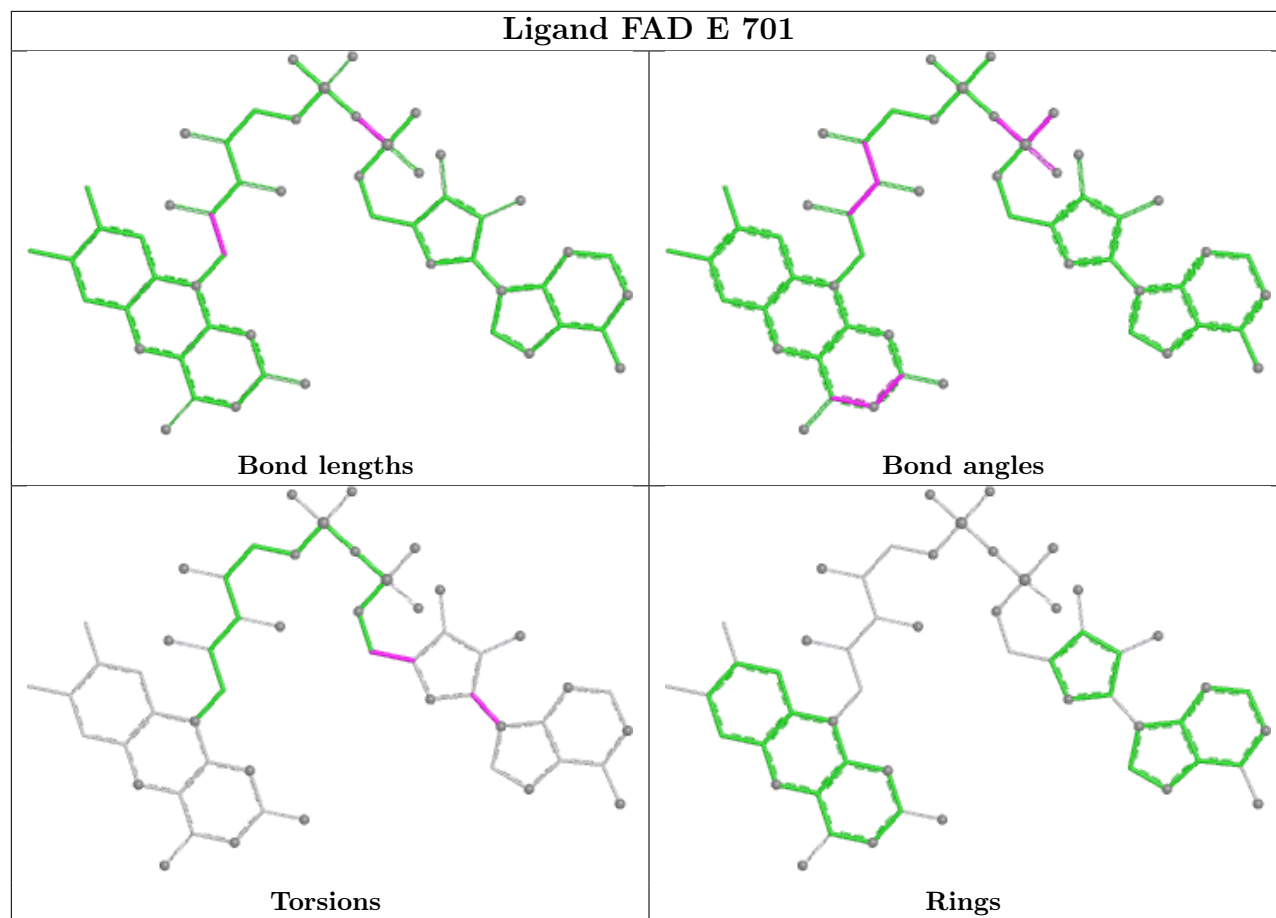


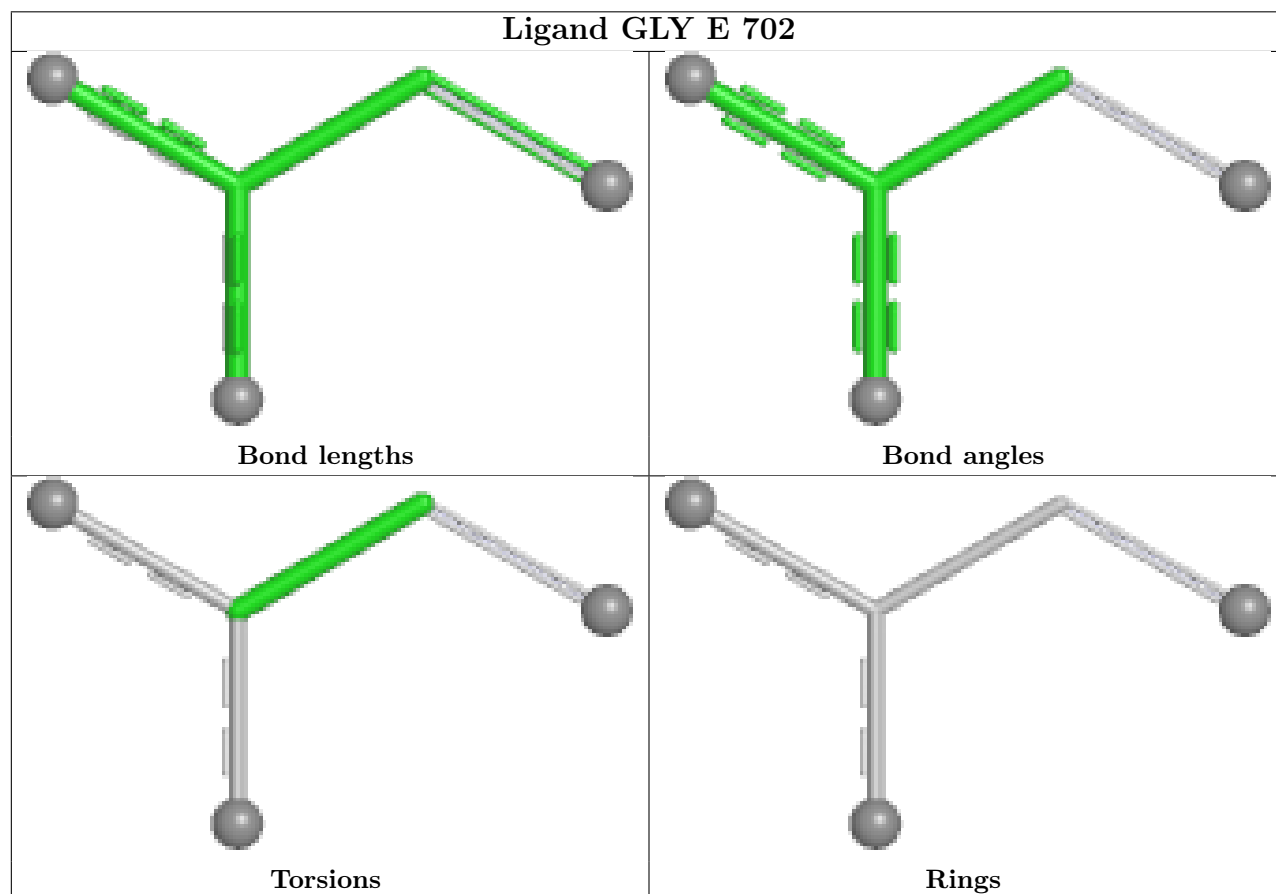
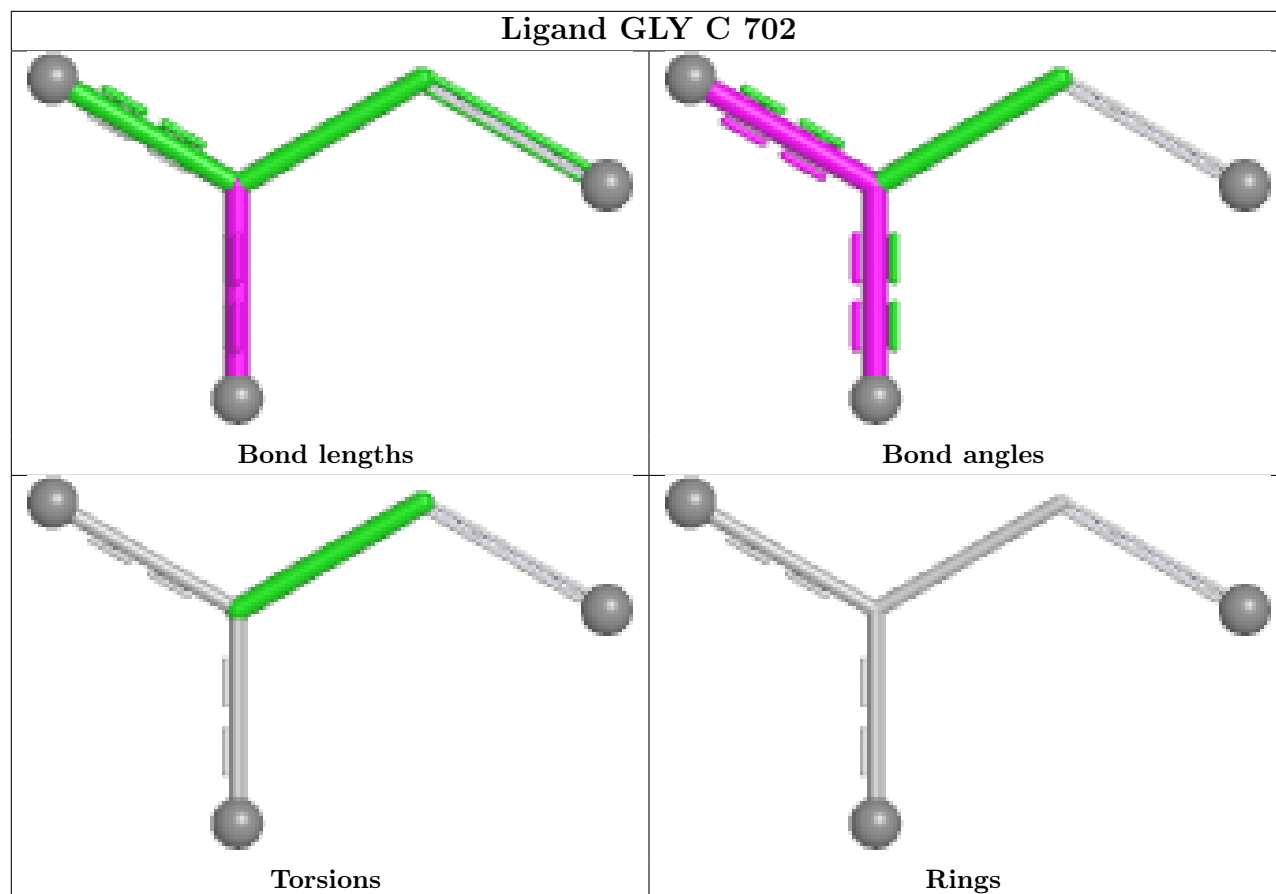


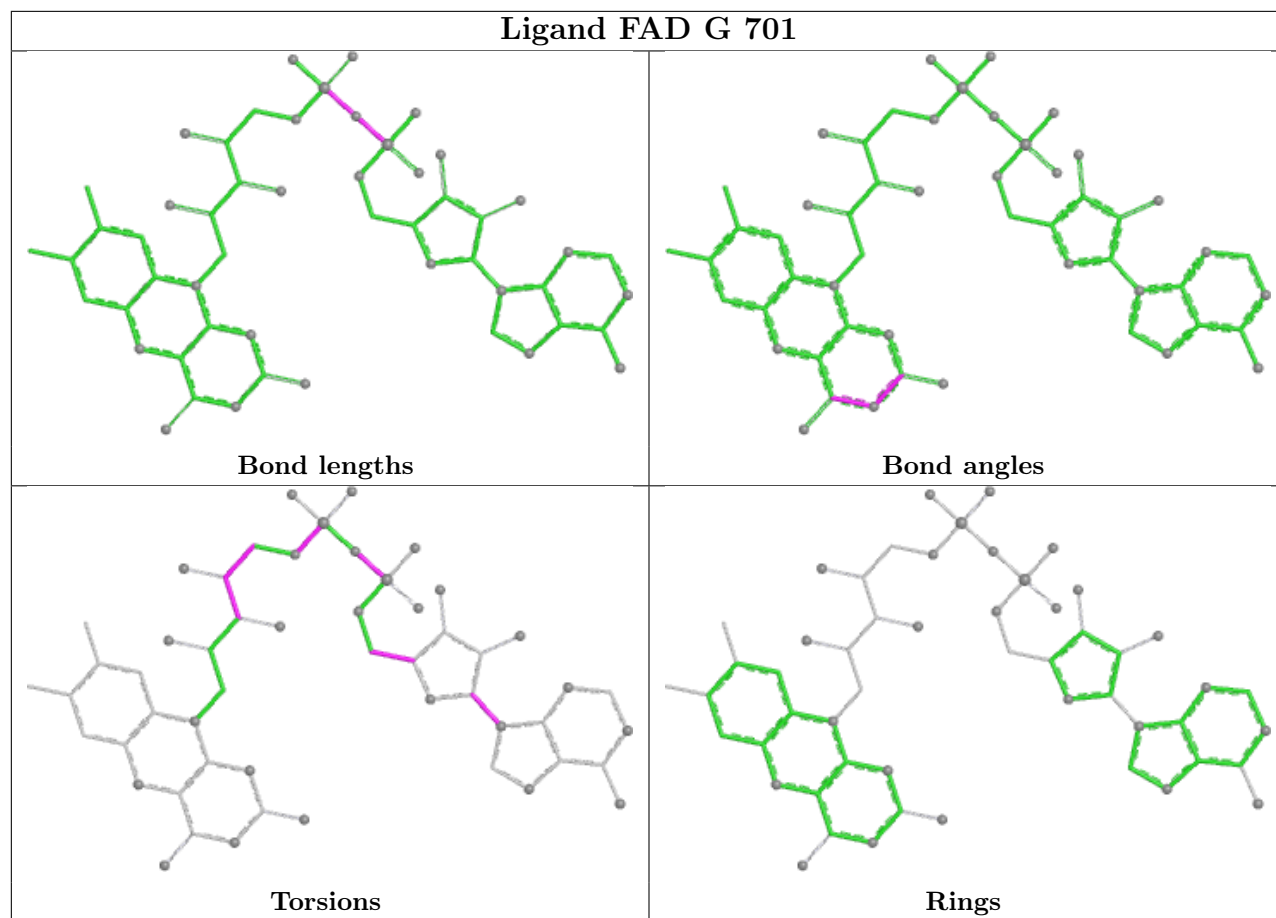


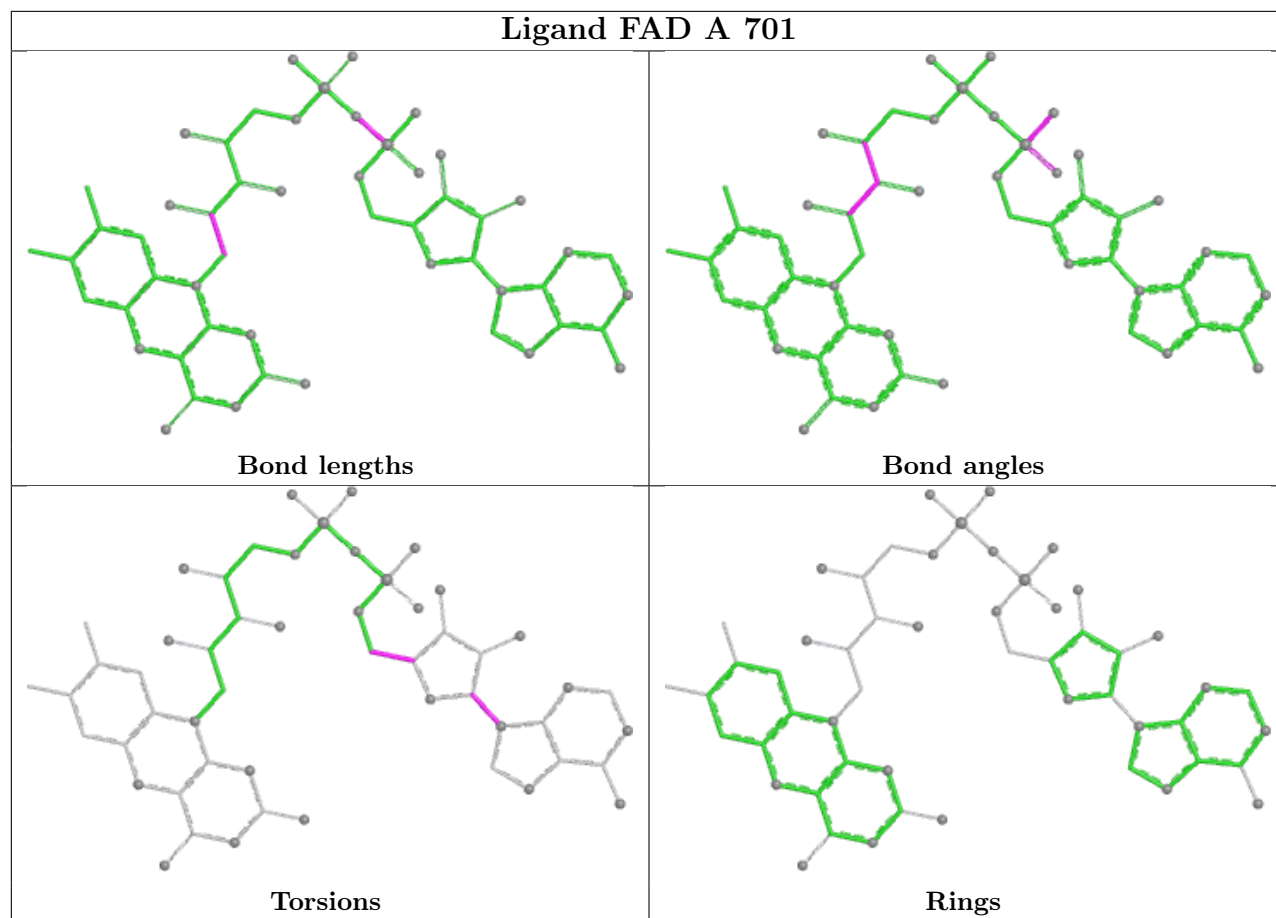




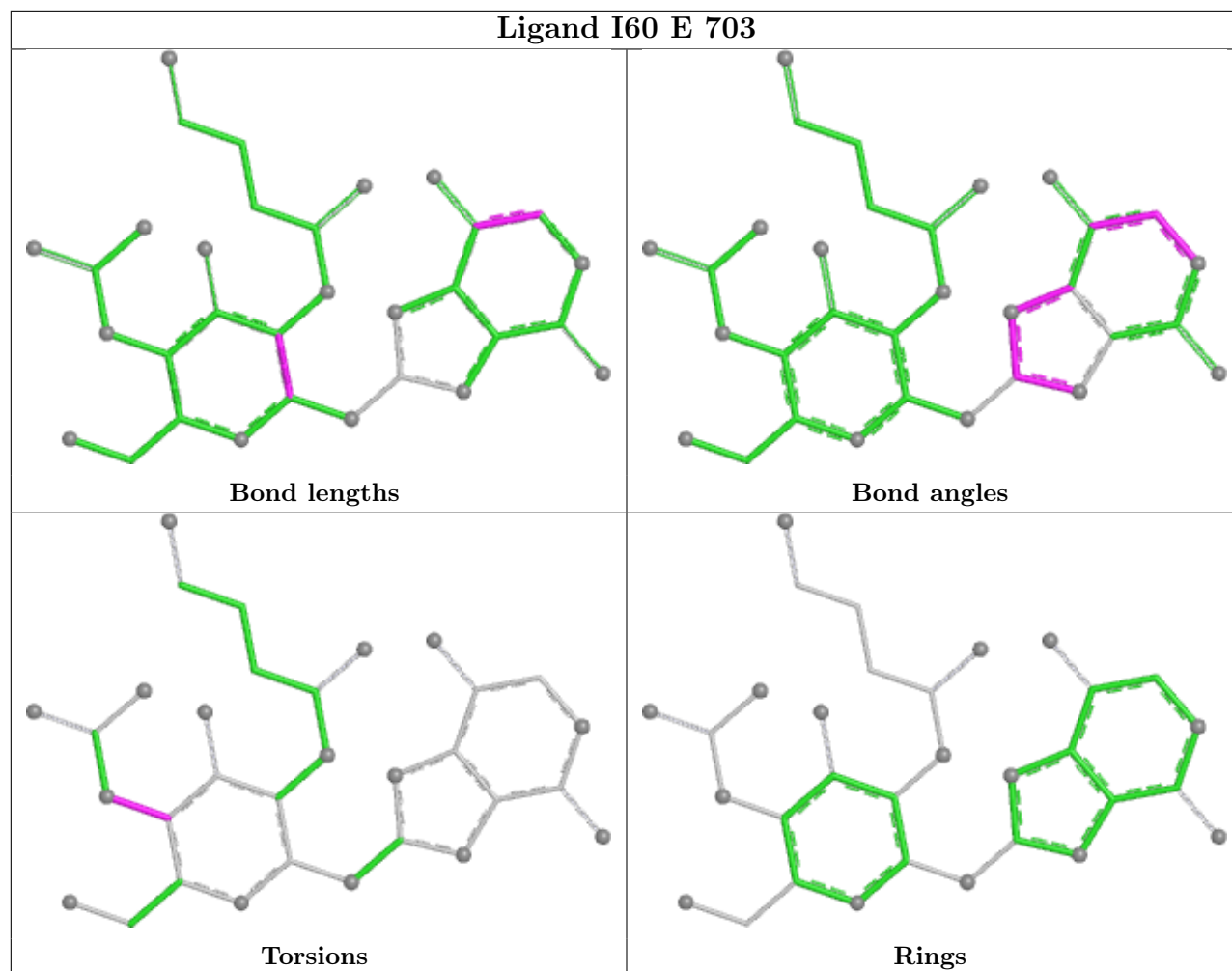




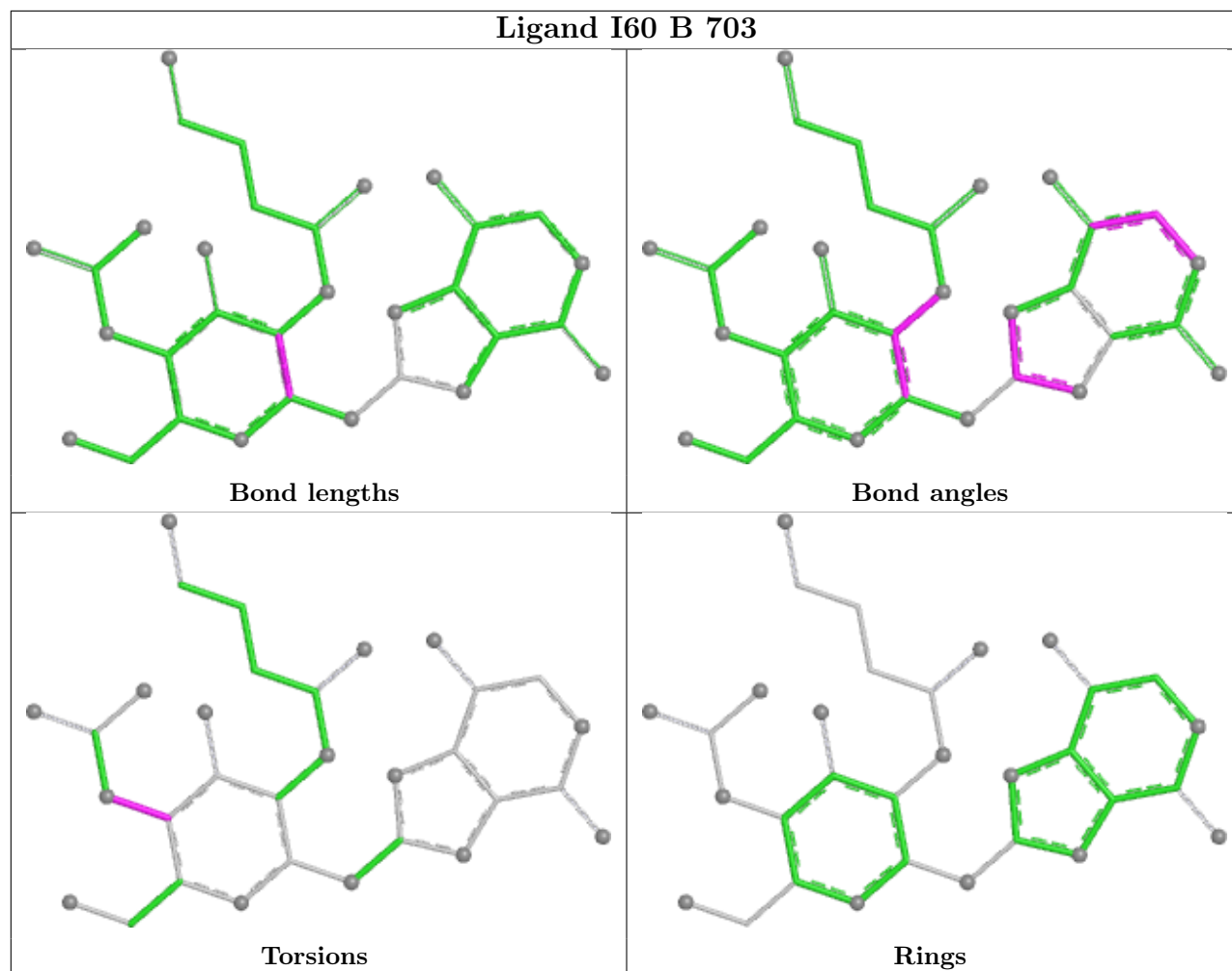




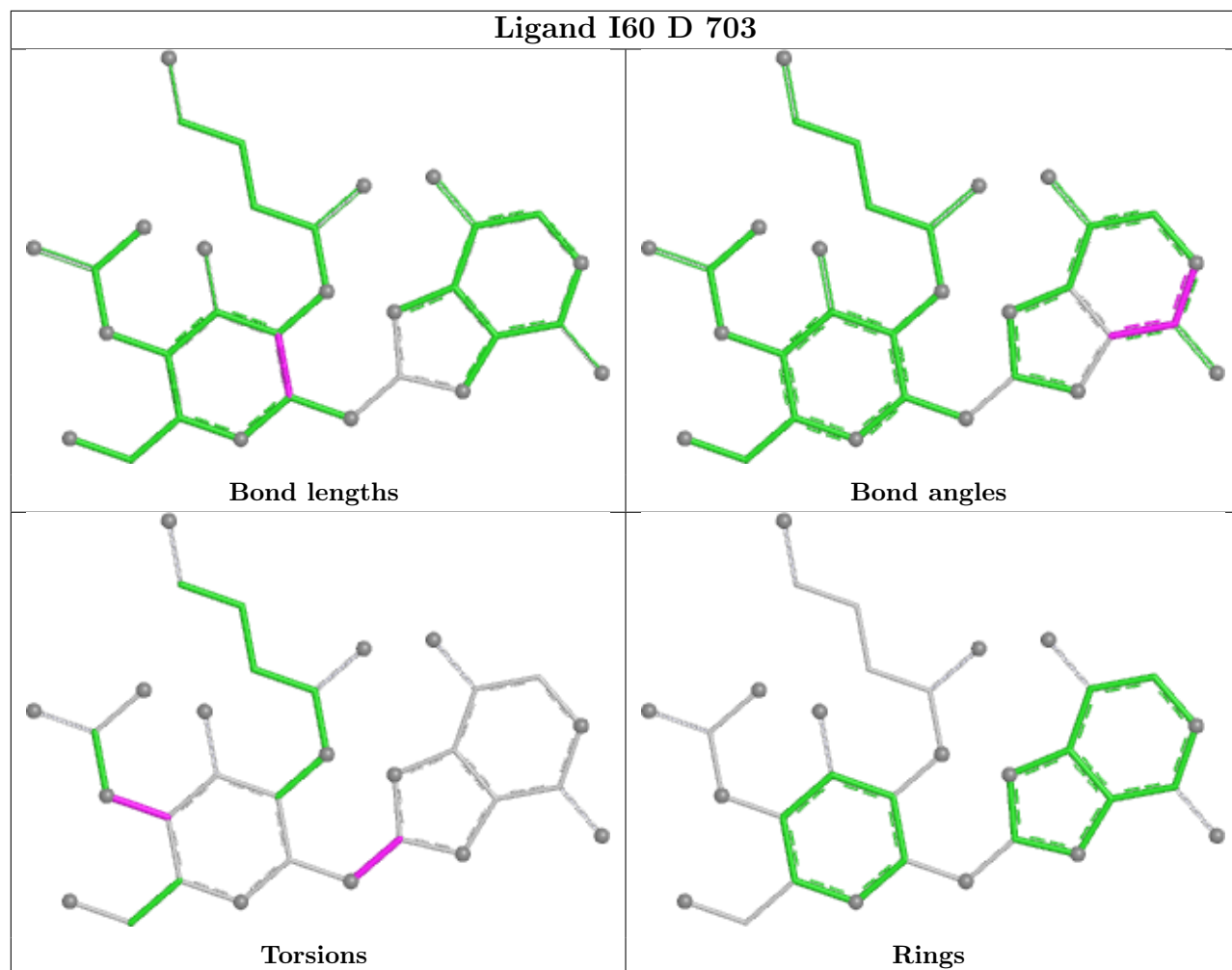
Ligand I60 E 703



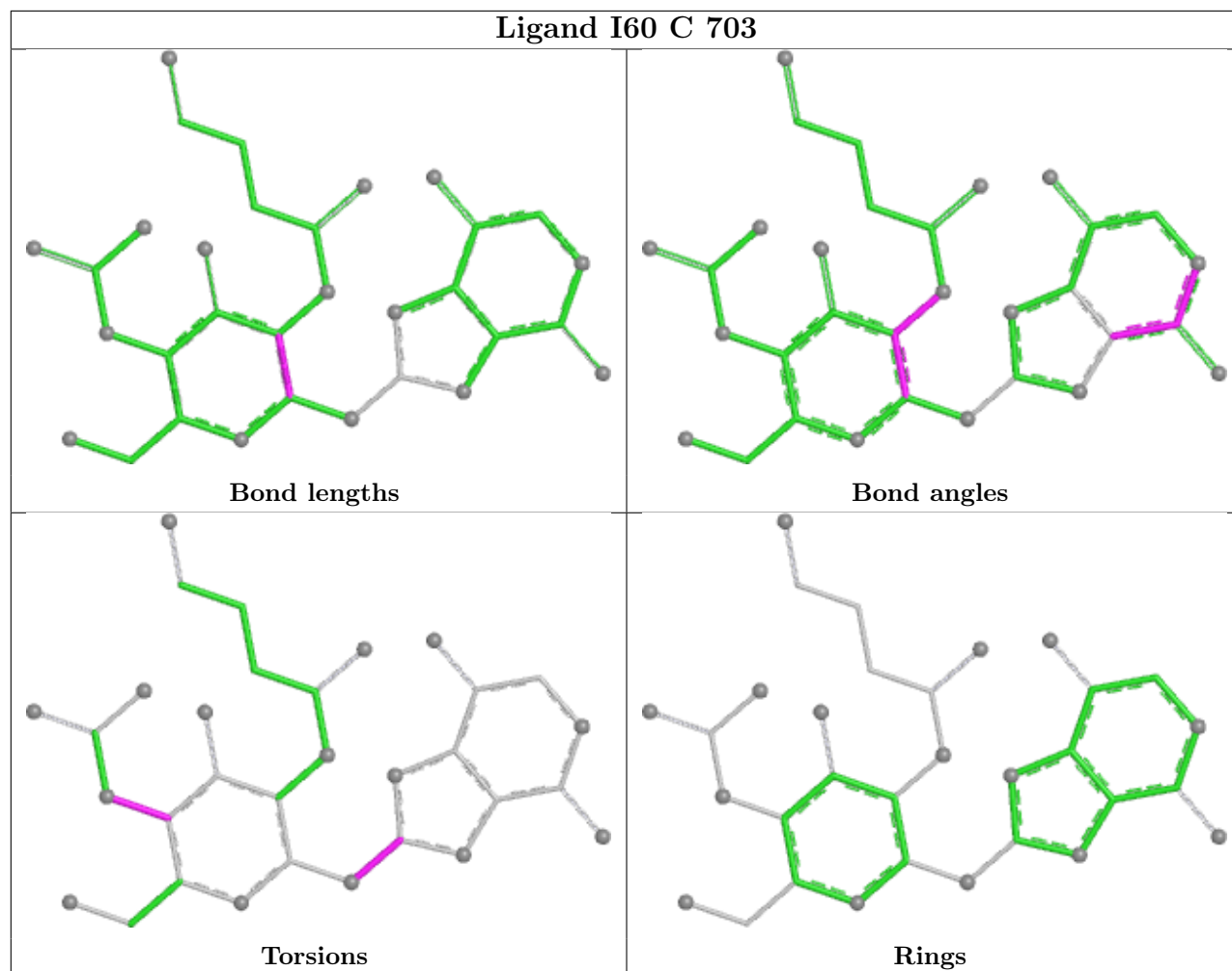
Ligand I60 B 703



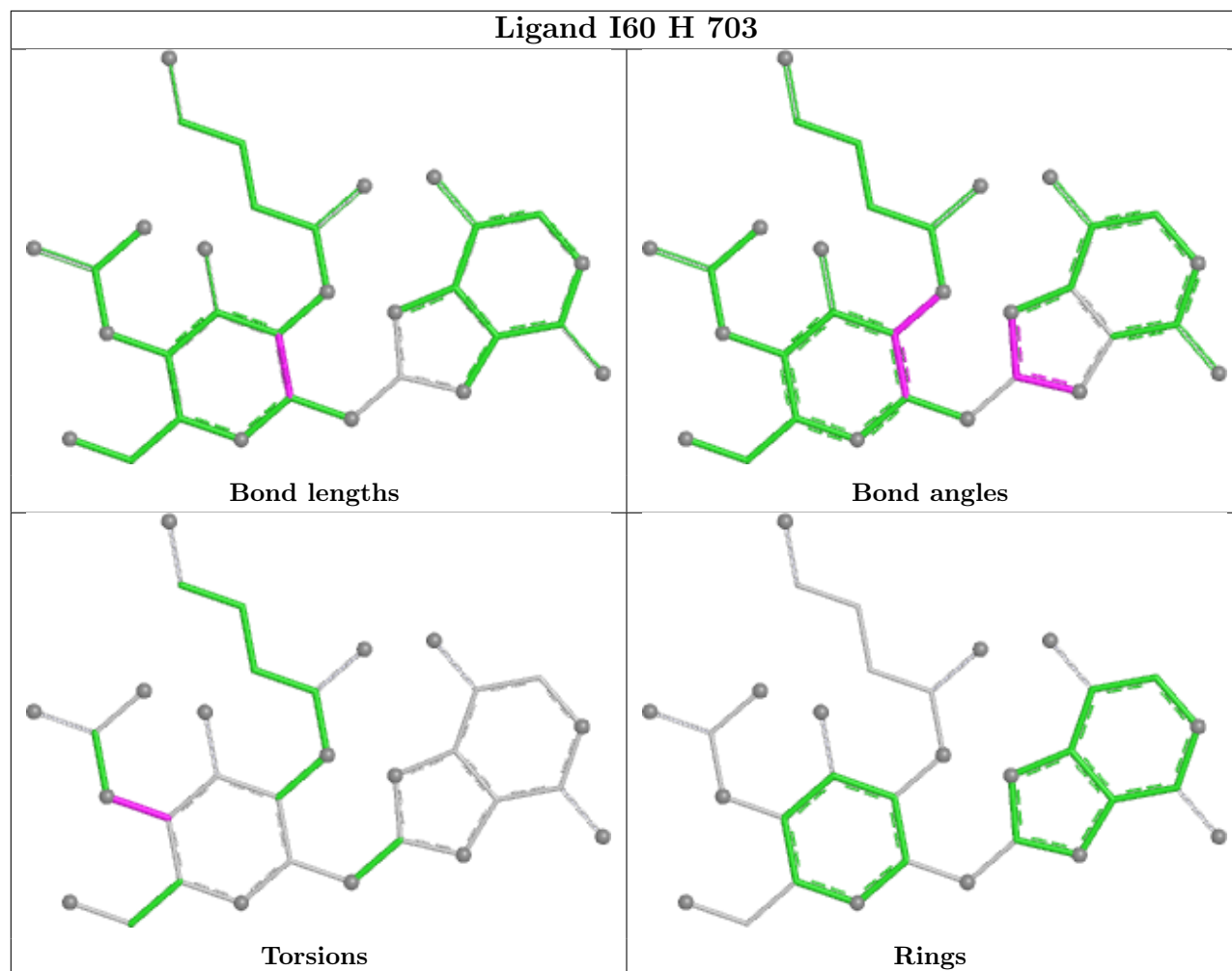
Ligand I60 D 703

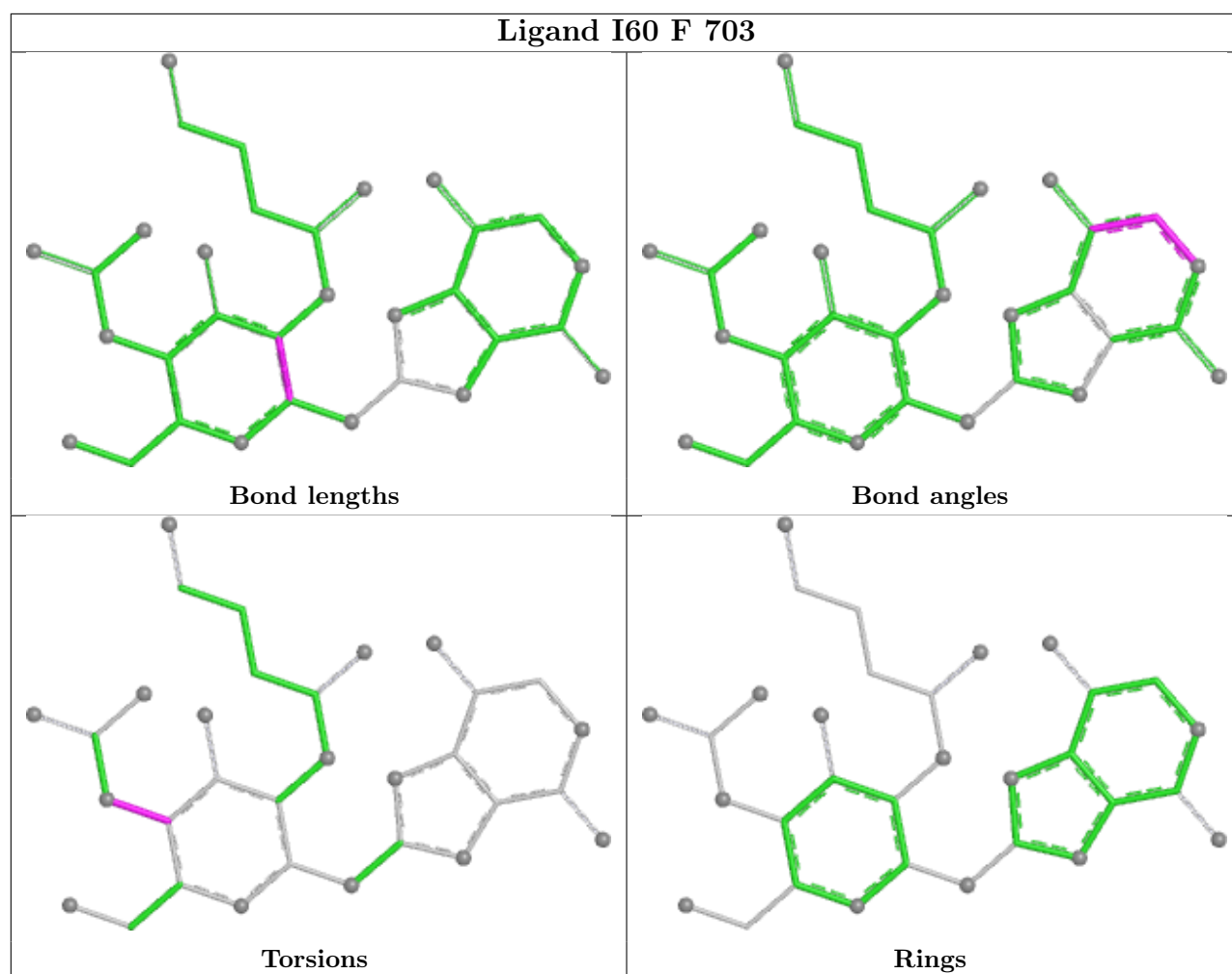


Ligand I60 C 703



Ligand I60 H 703





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	482/512 (94%)	-1.39	0 100 100	12, 25, 47, 77	0
1	B	482/512 (94%)	-1.39	0 100 100	12, 24, 45, 73	1 (0%)
1	C	472/512 (92%)	-1.34	0 100 100	12, 27, 58, 82	1 (0%)
1	D	466/512 (91%)	-1.08	0 100 100	15, 41, 84, 104	1 (0%)
1	E	482/512 (94%)	-1.39	0 100 100	11, 25, 46, 76	0
1	F	482/512 (94%)	-1.41	0 100 100	12, 25, 46, 72	1 (0%)
1	G	472/512 (92%)	-1.33	0 100 100	12, 27, 58, 85	1 (0%)
1	H	465/512 (90%)	-1.07	0 100 100	15, 41, 83, 96	1 (0%)
All	All	3803/4096 (92%)	-1.30	0 100 100	11, 28, 68, 104	6 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

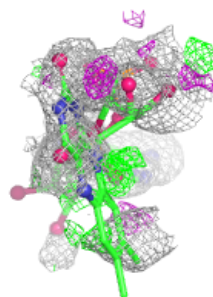
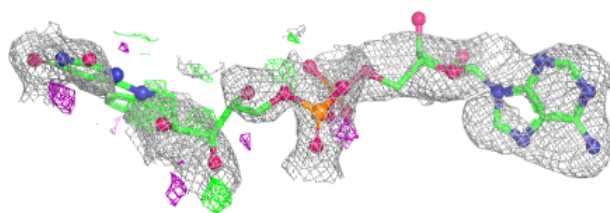
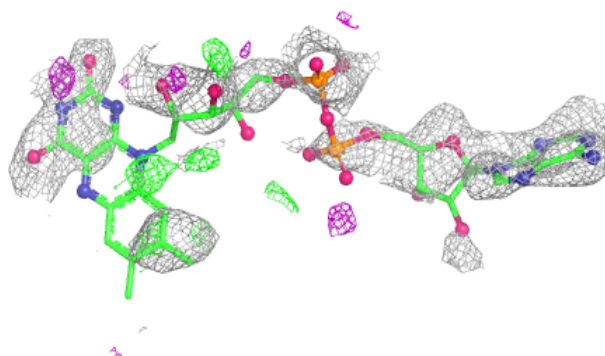
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	701	53/53	0.98	0.10	66,93,119,124	0
2	FAD	D	701	53/53	0.98	0.05	52,62,82,84	0
2	FAD	G	701	53/53	0.98	0.09	67,91,115,120	0
2	FAD	H	701	53/53	0.98	0.06	52,62,83,85	0
3	GLY	C	702	5/5	0.98	0.08	58,70,75,76	0
3	GLY	D	702	5/5	0.98	0.06	47,52,53,54	0
3	GLY	G	702	5/5	0.98	0.08	53,65,70,71	0
3	GLY	H	702	5/5	0.98	0.04	43,49,52,53	0
2	FAD	F	701	53/53	0.99	0.03	16,18,20,22	0
3	GLY	E	702	5/5	0.99	0.03	23,25,33,33	0
4	I60	A	703	32/32	0.99	0.04	20,34,45,49	0
4	I60	B	703	32/32	0.99	0.04	23,42,51,56	0
4	I60	C	703	32/32	0.99	0.06	23,40,80,90	0
4	I60	D	703	32/32	0.99	0.05	25,49,81,82	0
4	I60	E	703	32/32	0.99	0.04	19,33,41,44	0
4	I60	F	703	32/32	0.99	0.05	21,41,51,54	0
4	I60	G	703	32/32	0.99	0.05	25,40,74,75	0
4	I60	H	703	32/32	0.99	0.05	28,46,70,70	0
2	FAD	E	701	53/53	1.00	0.03	18,22,24,26	0
3	GLY	F	702	5/5	1.00	0.05	21,25,27,27	0
3	GLY	A	702	5/5	1.00	0.02	22,24,31,31	0
3	GLY	B	702	5/5	1.00	0.04	21,24,26,27	0
2	FAD	A	701	53/53	1.00	0.02	18,20,23,25	0
2	FAD	B	701	53/53	1.00	0.02	17,18,20,21	0

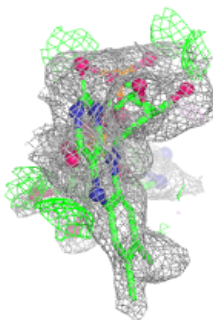
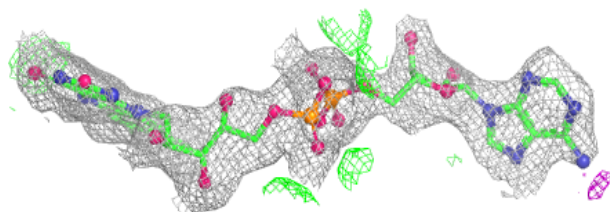
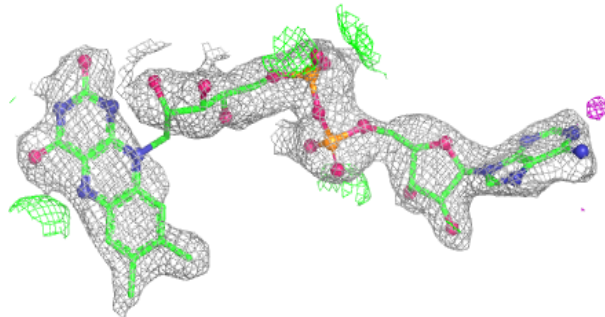
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

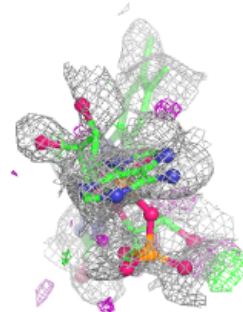
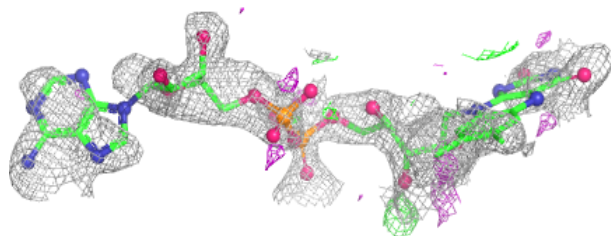
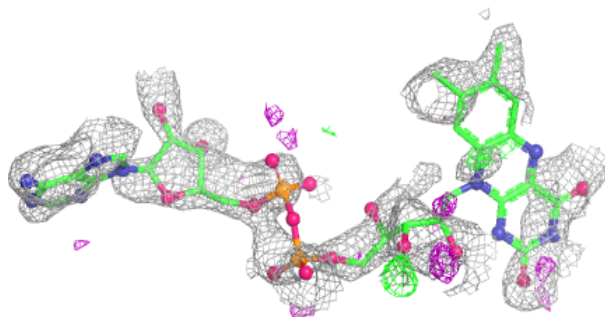
**Electron density around FAD D 701:**

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

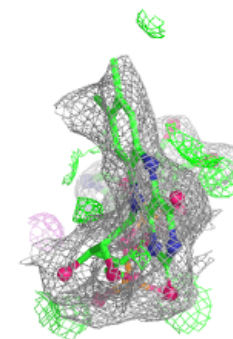
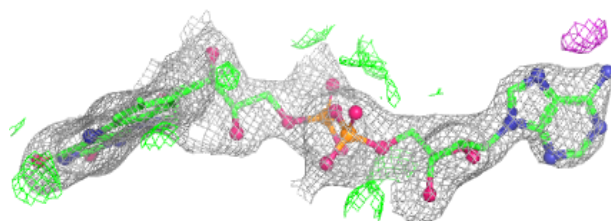
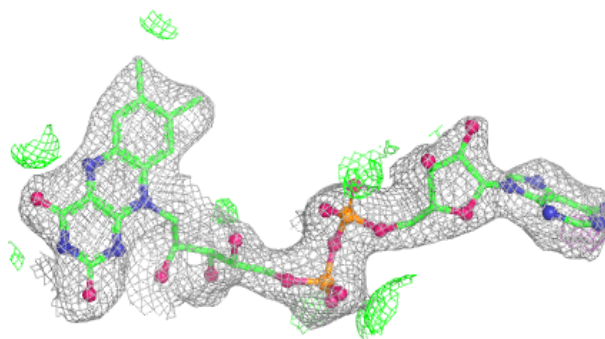


Electron density around FAD G 701:

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and green (positive)

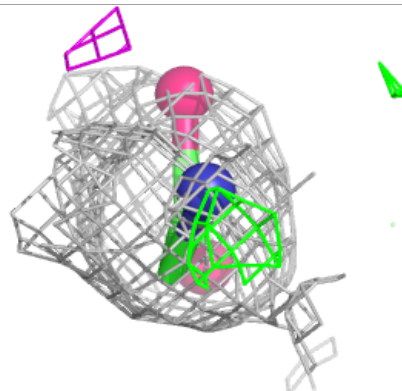
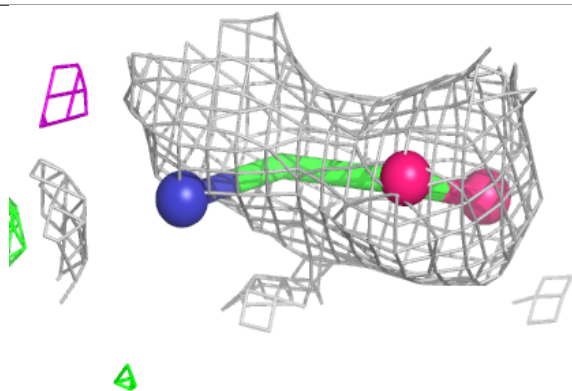
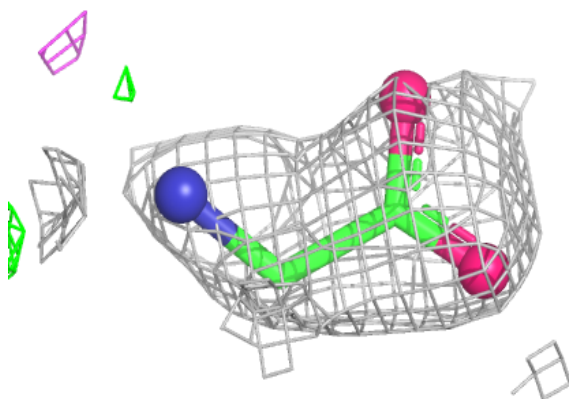
**Electron density around FAD H 701:**

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and green (positive)

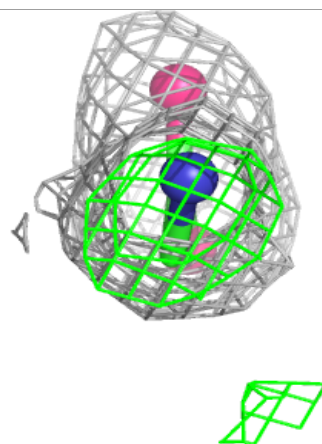
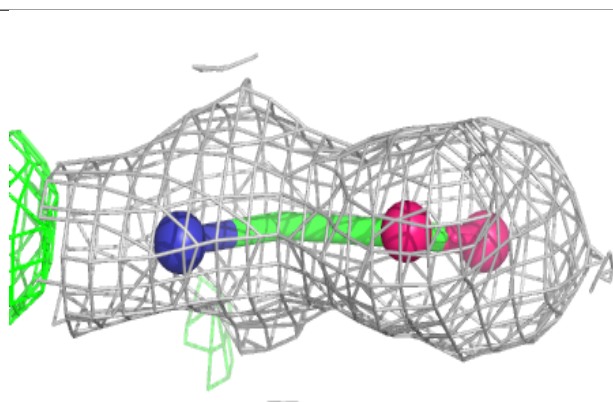
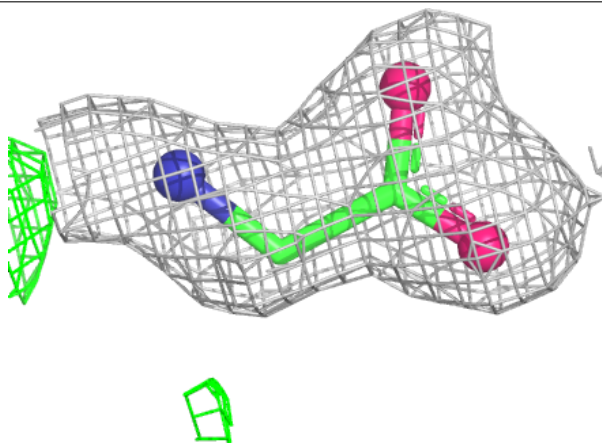


Electron density around GLY C 702:

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and green (positive)

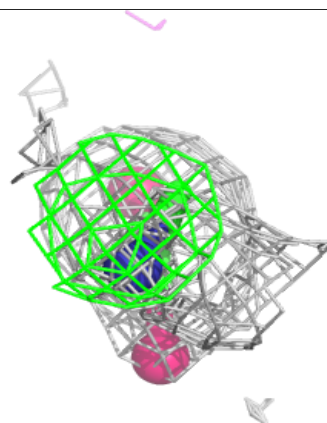
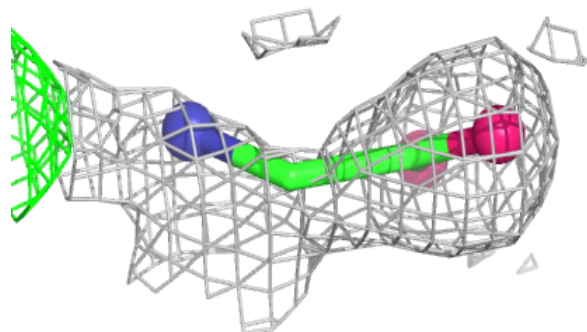
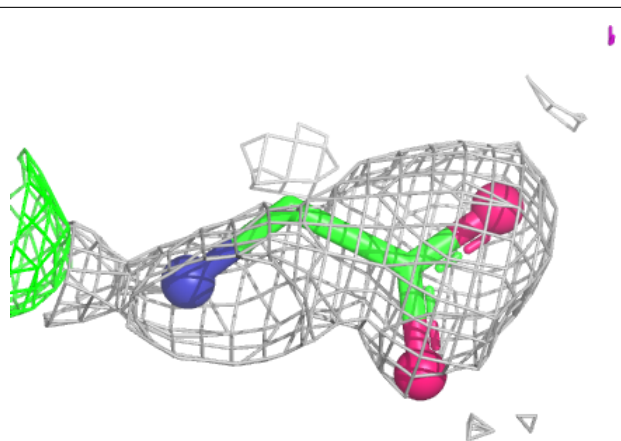
**Electron density around GLY D 702:**

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and green (positive)

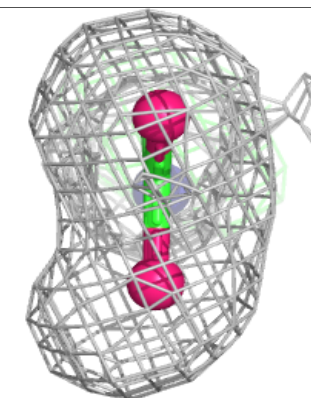
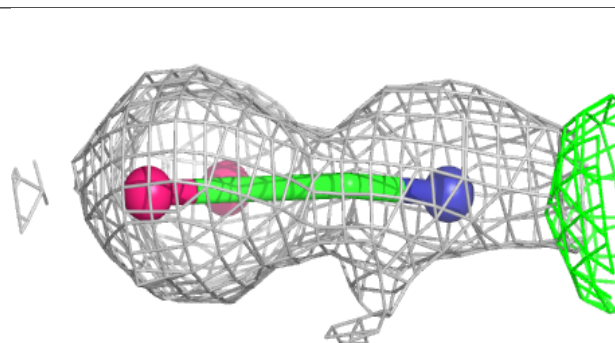
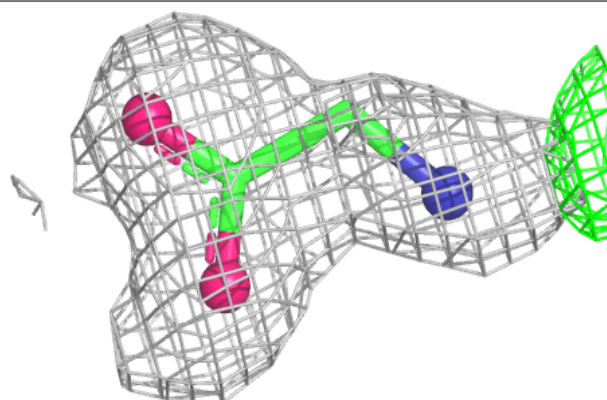


Electron density around GLY G 702:

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

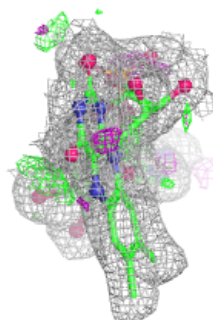
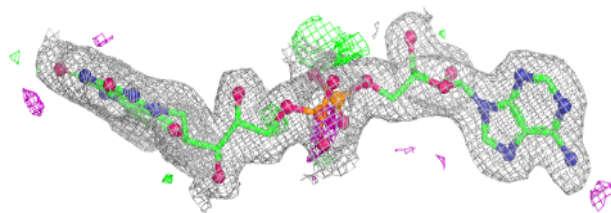
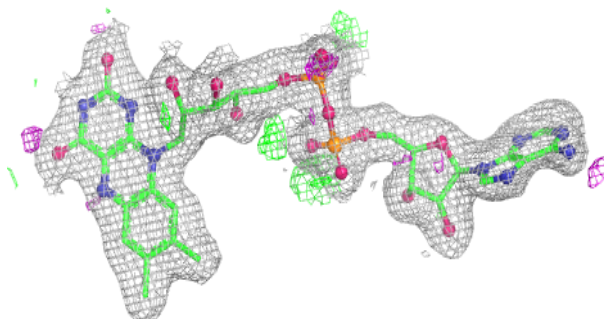
**Electron density around GLY H 702:**

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

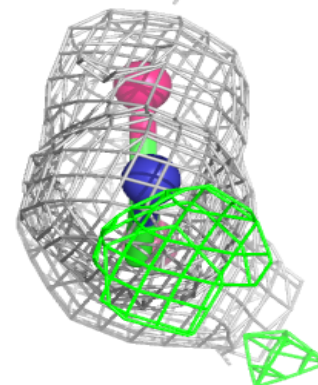
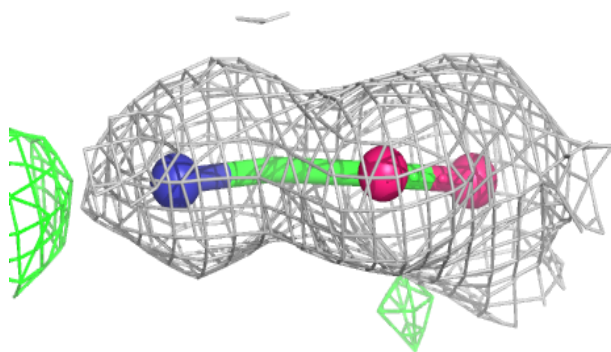
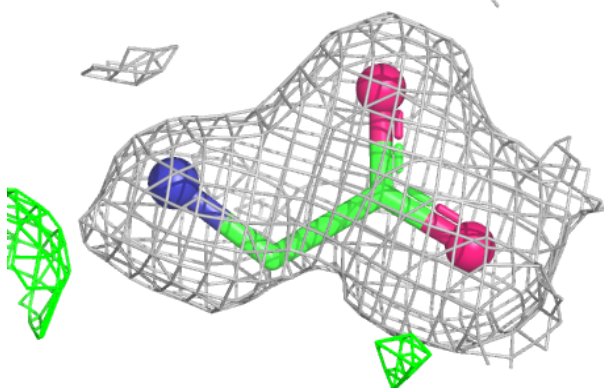


Electron density around FAD F 701:

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

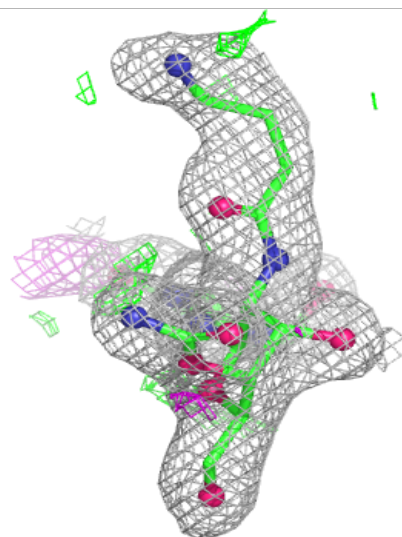
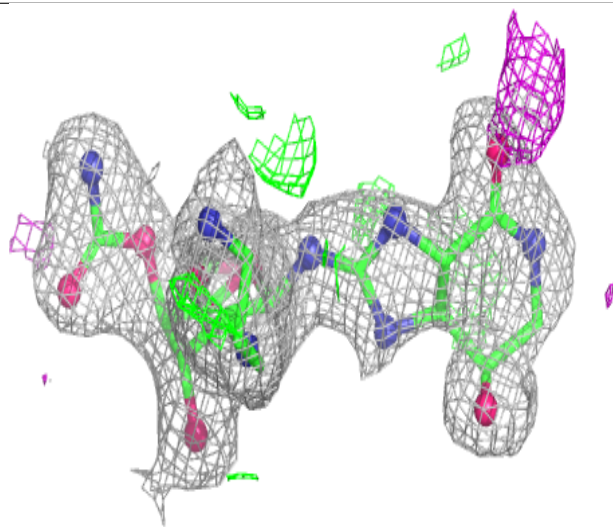
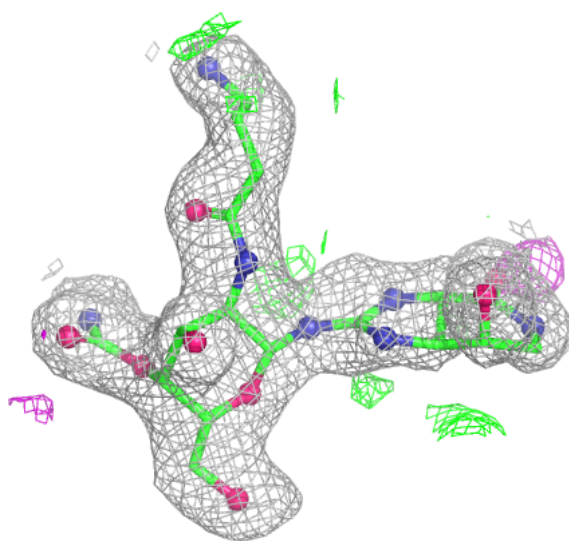
**Electron density around GLY E 702:**

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



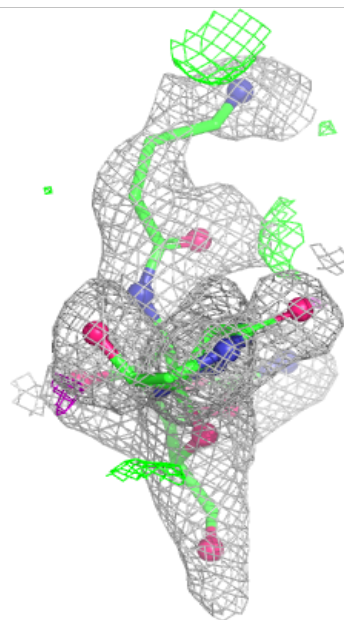
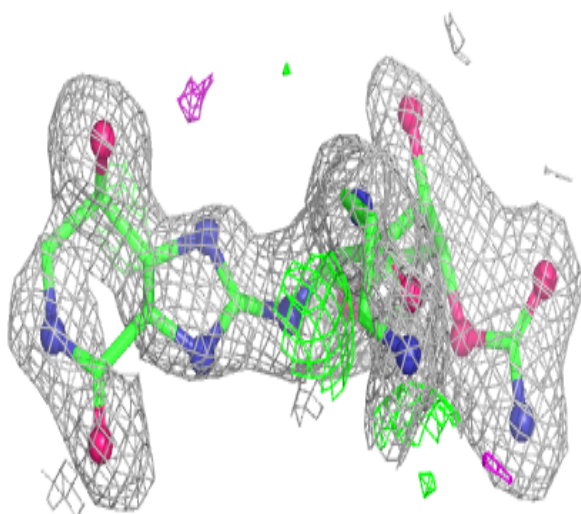
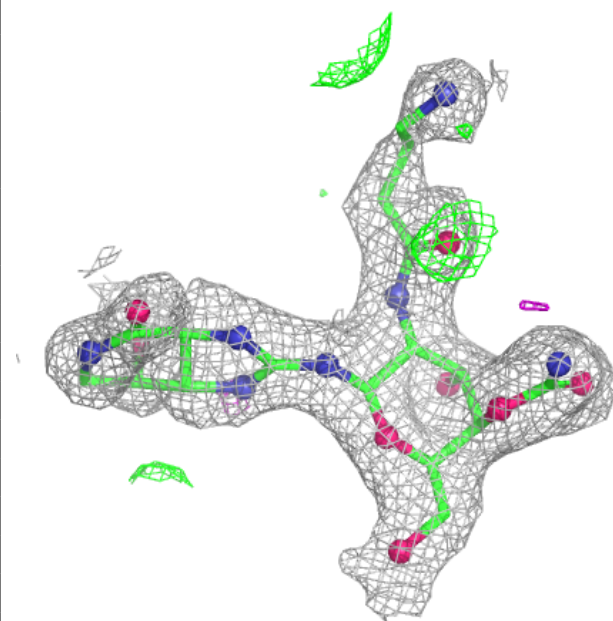
Electron density around I60 A 703:

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



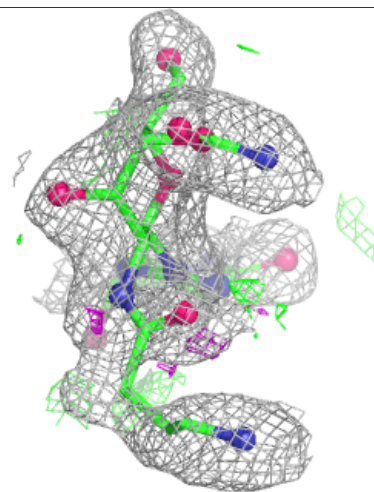
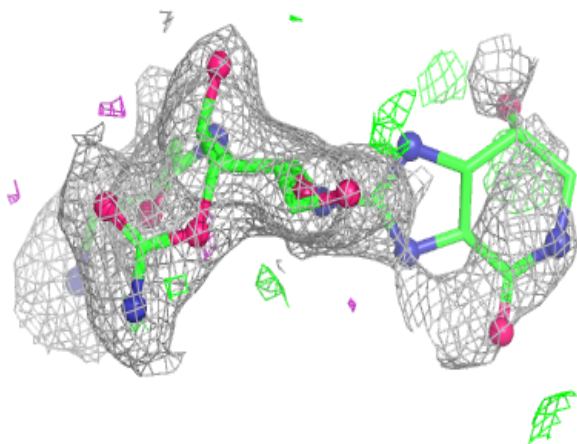
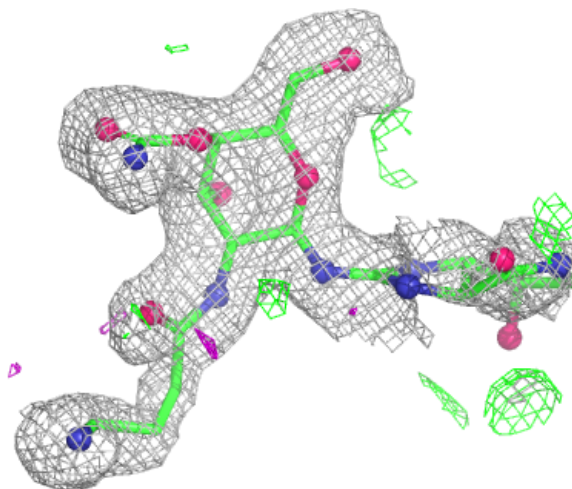
Electron density around I60 B 703:

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



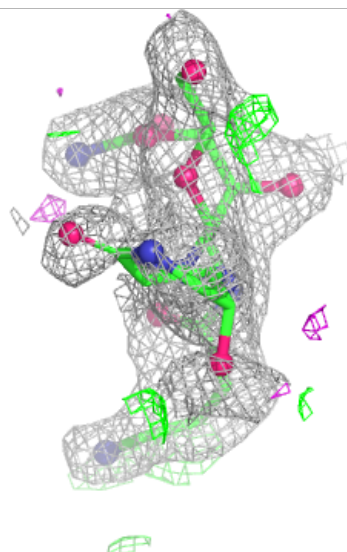
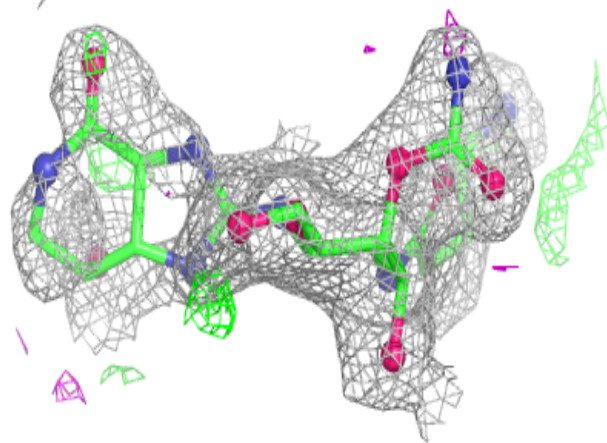
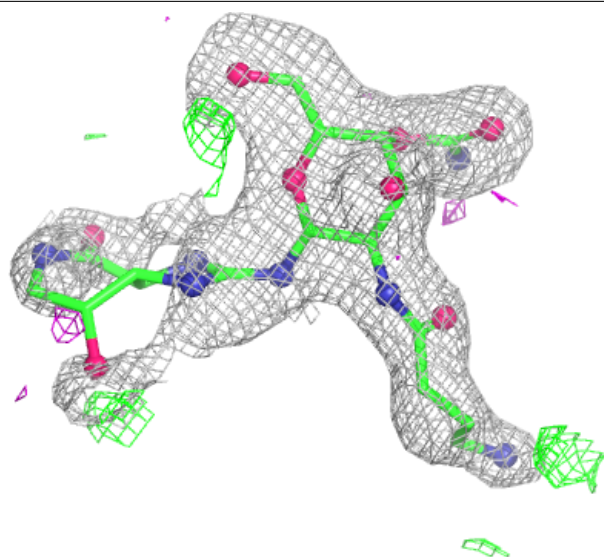
Electron density around I60 C 703:

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



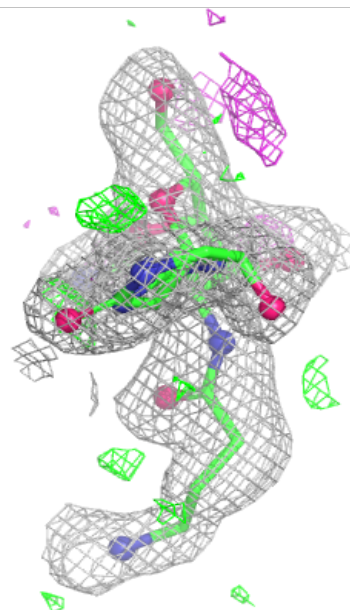
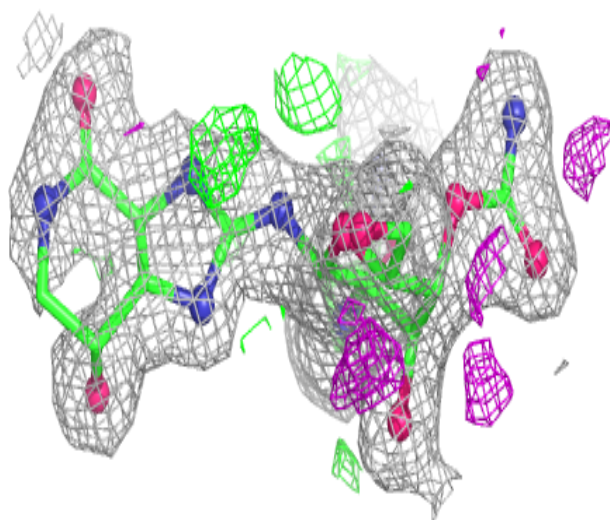
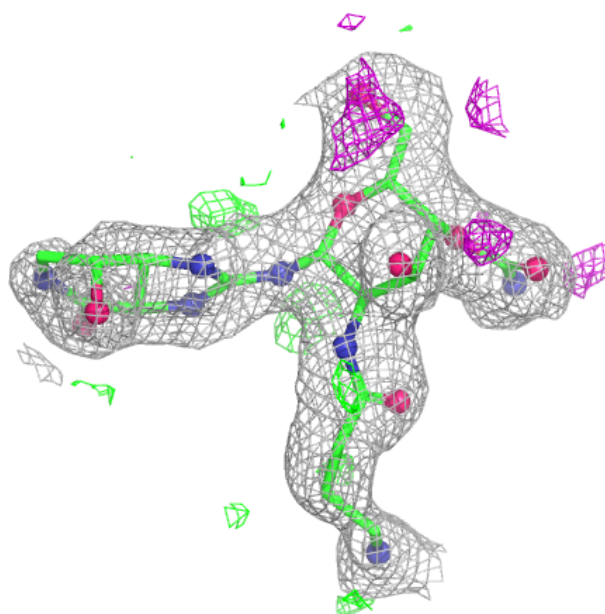
Electron density around I60 D 703:

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



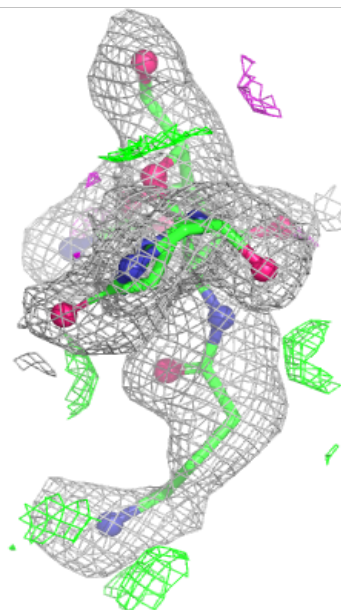
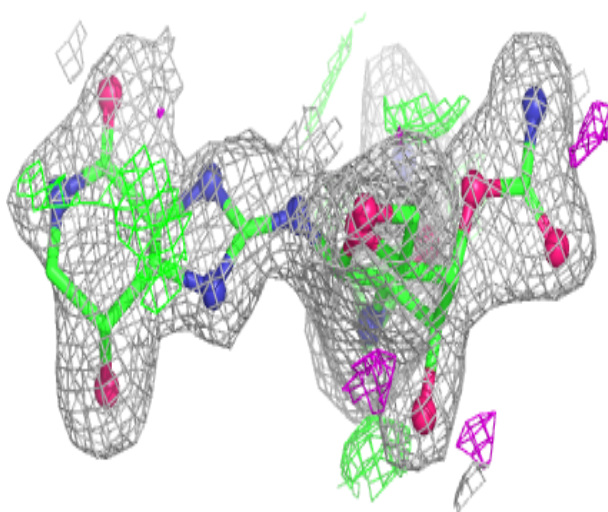
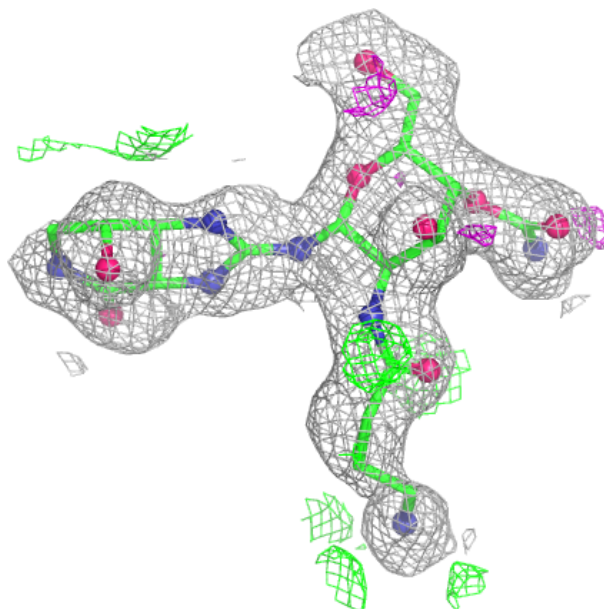
Electron density around I60 E 703:

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



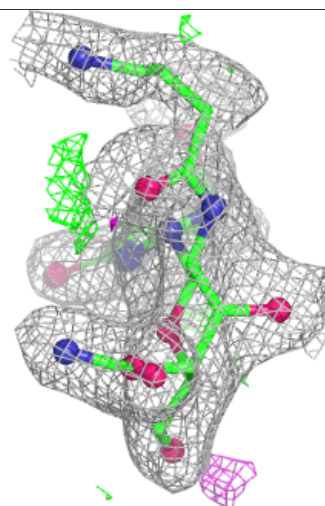
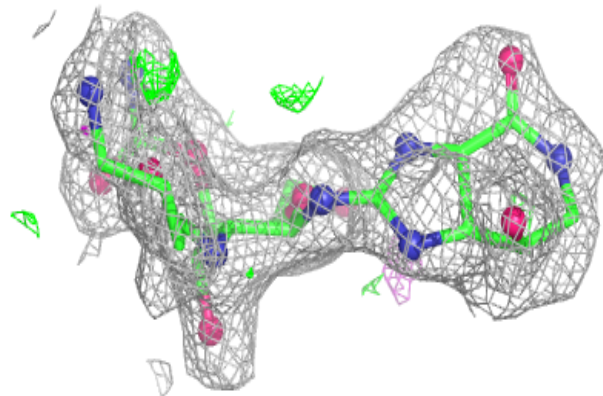
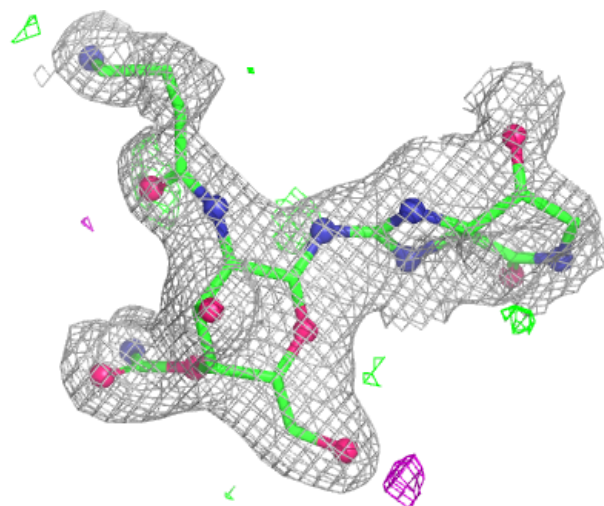
Electron density around I60 F 703:

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



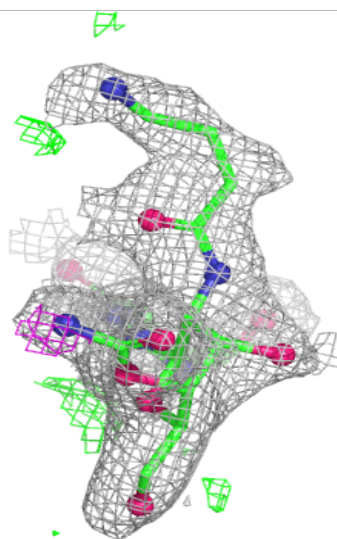
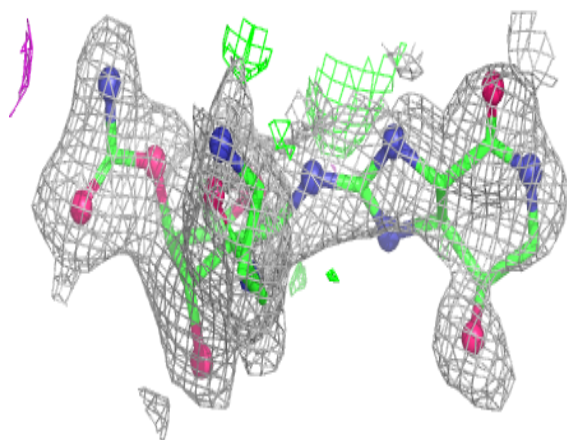
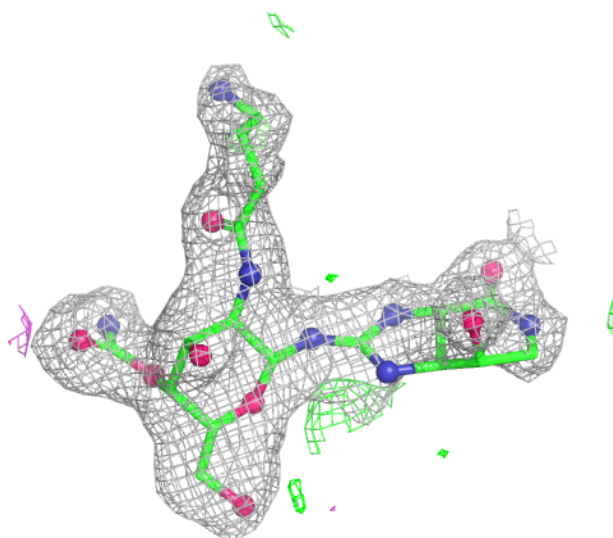
Electron density around I60 G 703:

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



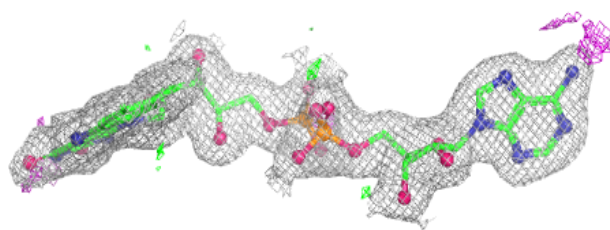
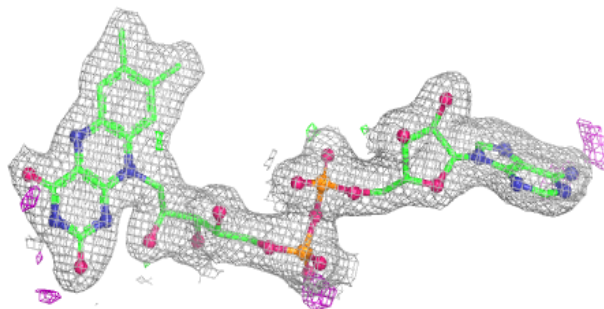
Electron density around I60 H 703:

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



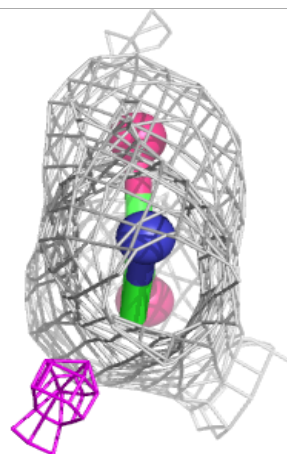
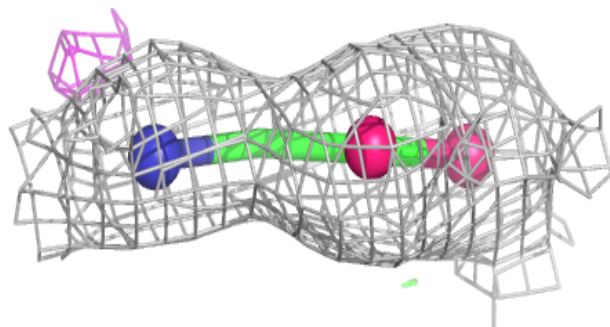
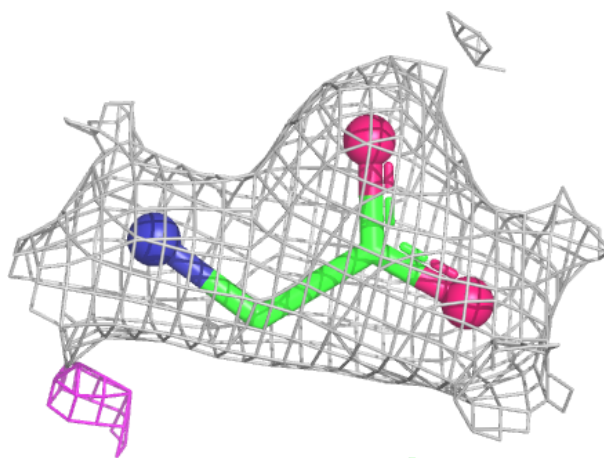
Electron density around FAD E 701:

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



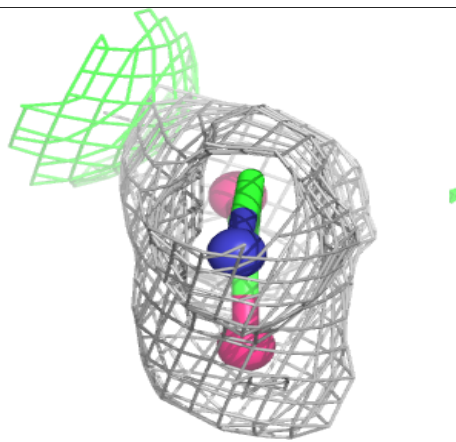
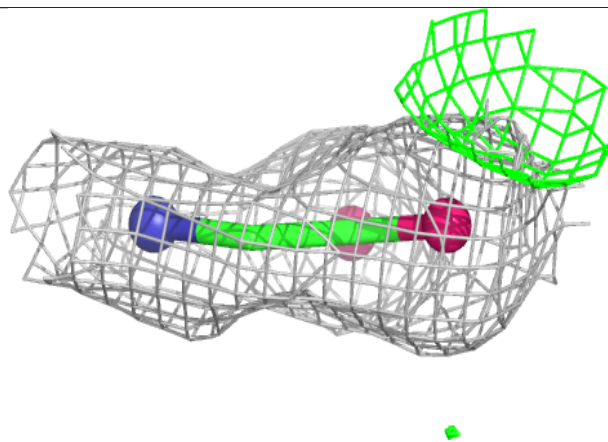
Electron density around GLY F 702:

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



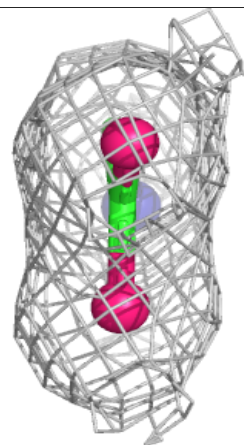
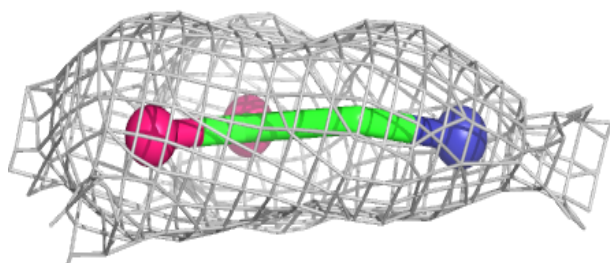
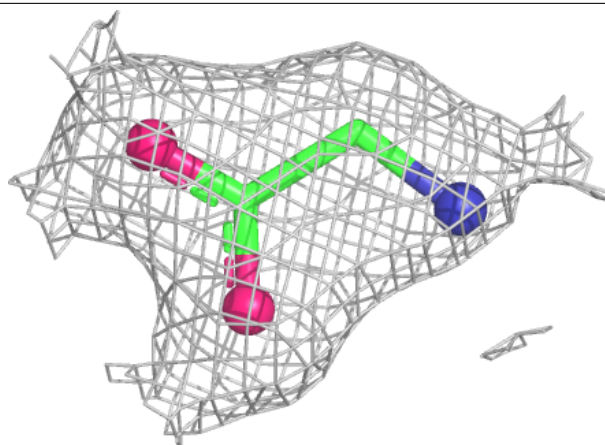
Electron density around GLY A 702:

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

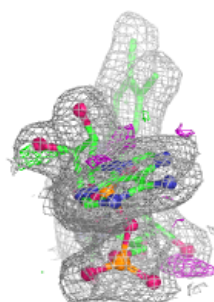
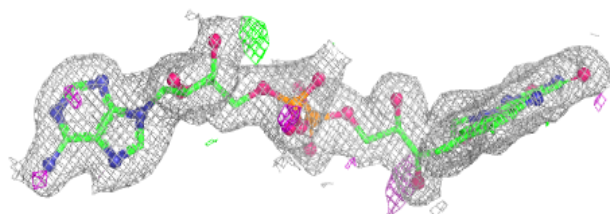
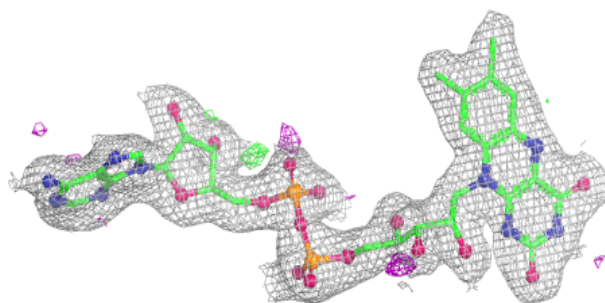


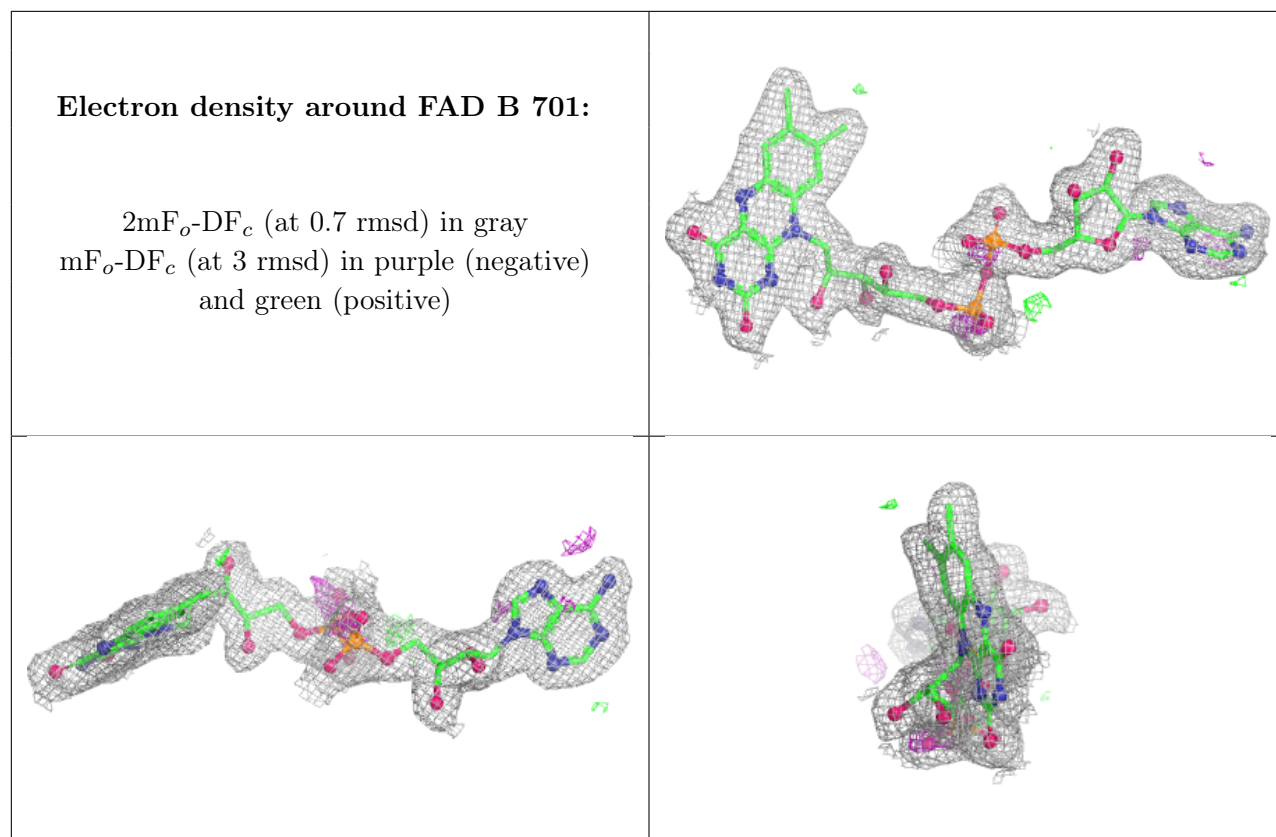
Electron density around GLY B 702:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.