



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:50 PM JST

PDB ID : 7XX0  
Title : C281S glycylothricin complex  
Authors : Wang, Y.L.; Li, T.L.  
Deposited on : 2022-05-27  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

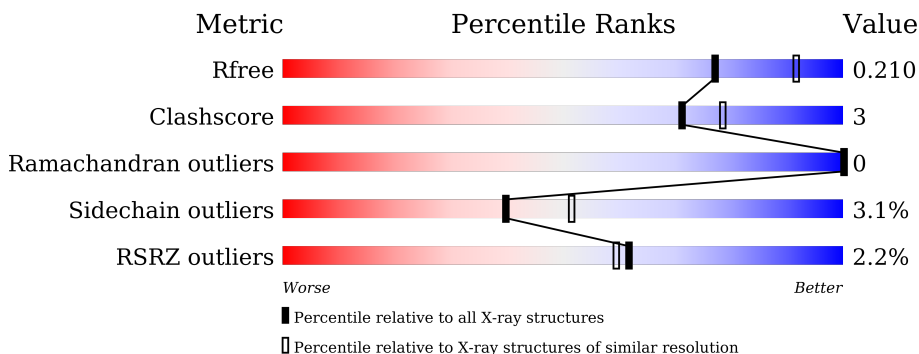
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



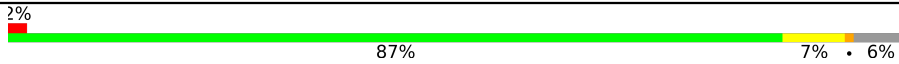

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	512	 87% 6% • 6%
1	B	512	 88% 5% • 6%
1	C	512	 86% 7% • 6%
1	D	512	 85% 8% • 6%
1	E	512	 87% 7% • 6%
1	F	512	 87% 6% • 6%

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Mol	Chain	Length	Quality of chain
1	G	512	 2% 87% 7% • 6%
1	H	512	 5% 85% 8% • 6%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 32001 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
			Total	C	N	O	S			
1	A	482	3654	2293	660	690	11	0	0	0
1	B	482	3662	2298	661	691	12	0	1	0
1	C	482	3662	2298	661	691	12	0	1	0
1	D	480	3638	2284	657	686	11	0	0	0
1	E	481	3645	2288	658	688	11	0	0	0
1	F	482	3662	2298	661	691	12	0	1	0
1	G	482	3662	2298	661	691	12	0	1	0
1	H	479	3630	2280	656	683	11	0	0	0

There are 176 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
A	281	SER	CYS	engineered mutation	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
B	281	SER	CYS	engineered mutation	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
C	-15	HIS	-	expression tag	UNP A0A125SZC1
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	SER	-	expression tag	UNP A0A125SZC1
C	-8	GLY	-	expression tag	UNP A0A125SZC1
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
C	281	SER	CYS	engineered mutation	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
D	281	SER	CYS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	-7	LEU	-	expression tag	UNP A0A125SZC1
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
E	281	SER	CYS	engineered mutation	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
F	281	SER	CYS	engineered mutation	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

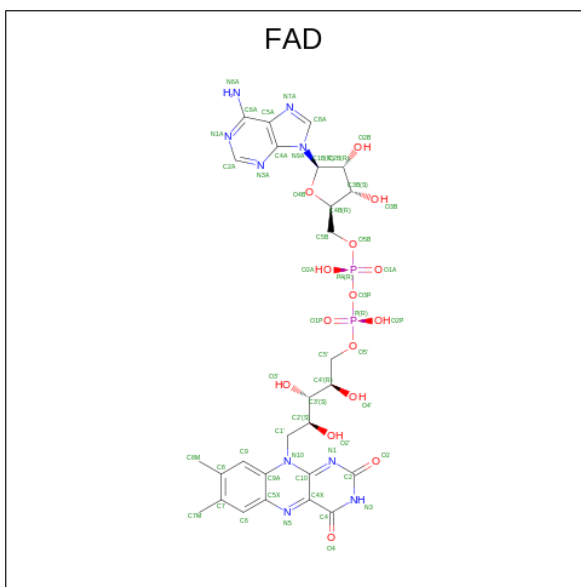
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP A0A125SZC1
G	-12	HIS	-	expression tag	UNP A0A125SZC1
G	-11	HIS	-	expression tag	UNP A0A125SZC1
G	-10	SER	-	expression tag	UNP A0A125SZC1
G	-9	SER	-	expression tag	UNP A0A125SZC1
G	-8	GLY	-	expression tag	UNP A0A125SZC1
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
G	281	SER	CYS	engineered mutation	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
H	281	SER	CYS	engineered mutation	UNP A0A125SZC1

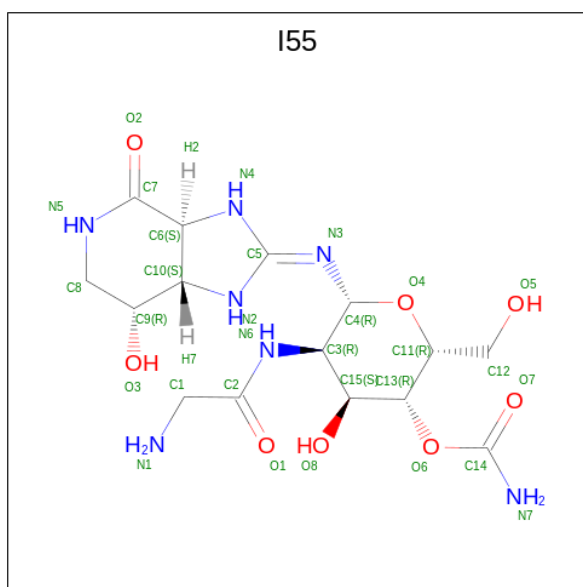
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).





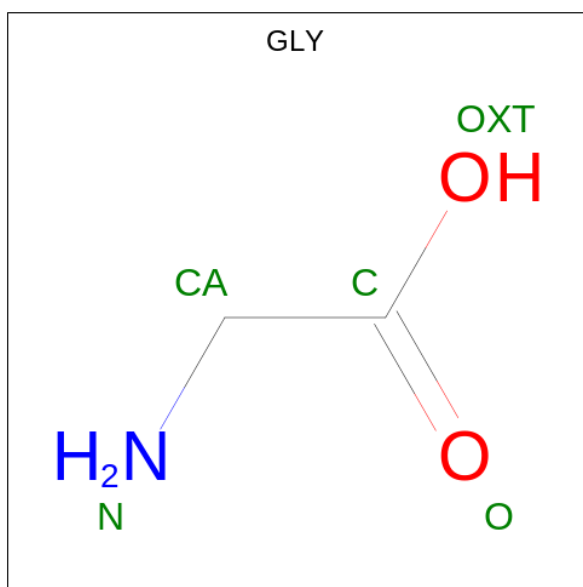
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	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 [(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-(2-azanylethanoylamino)-2-(hydroxymethyl)-4-oxidanyl-oxan-3-yl] carbamate (three-letter code: I55) (formula: C<sub>15</sub>H<sub>25</sub>N<sub>7</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	15	7	8		
3	B	1	Total	C	N	O	0	0
			30	15	7	8		
3	C	1	Total	C	N	O	0	0
			30	15	7	8		
3	D	1	Total	C	N	O	0	0
			30	15	7	8		
3	E	1	Total	C	N	O	0	0
			30	15	7	8		
3	F	1	Total	C	N	O	0	0
			30	15	7	8		
3	G	1	Total	C	N	O	0	0
			30	15	7	8		
3	H	1	Total	C	N	O	0	0
			30	15	7	8		

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	292	Total	O	0	0
			292	292		
5	B	290	Total	O	0	0
			290	290		
5	C	260	Total	O	0	0
			260	260		
5	D	187	Total	O	0	0
			187	187		

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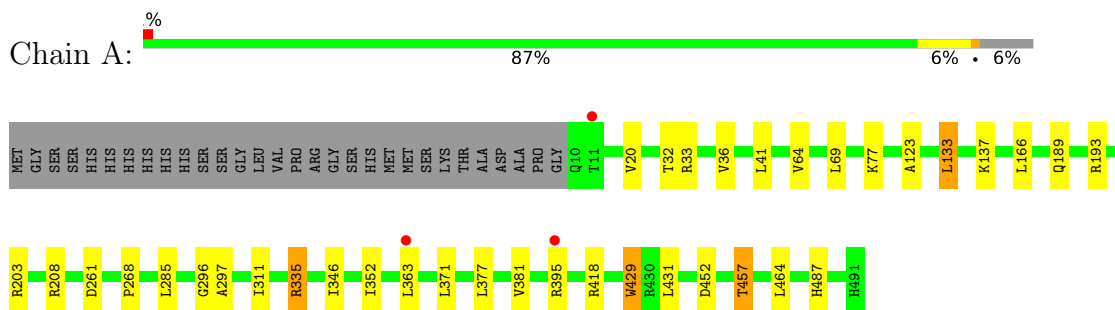
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	E	298	Total 298	O 298	0	0
5	F	302	Total 302	O 302	0	0
5	G	249	Total 249	O 249	0	0
5	H	204	Total 204	O 204	0	0

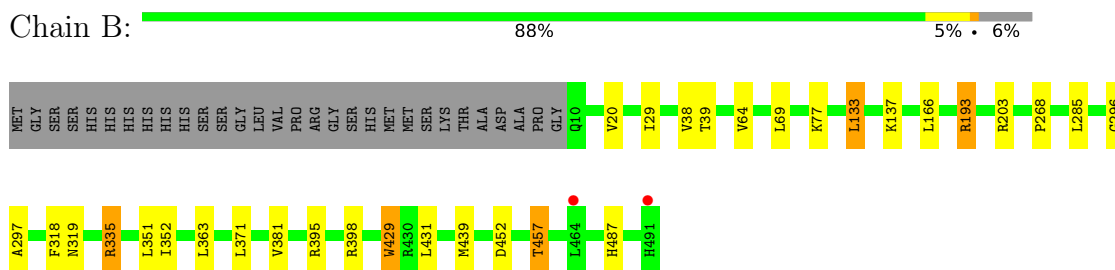
### 3 Residue-property plots

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.

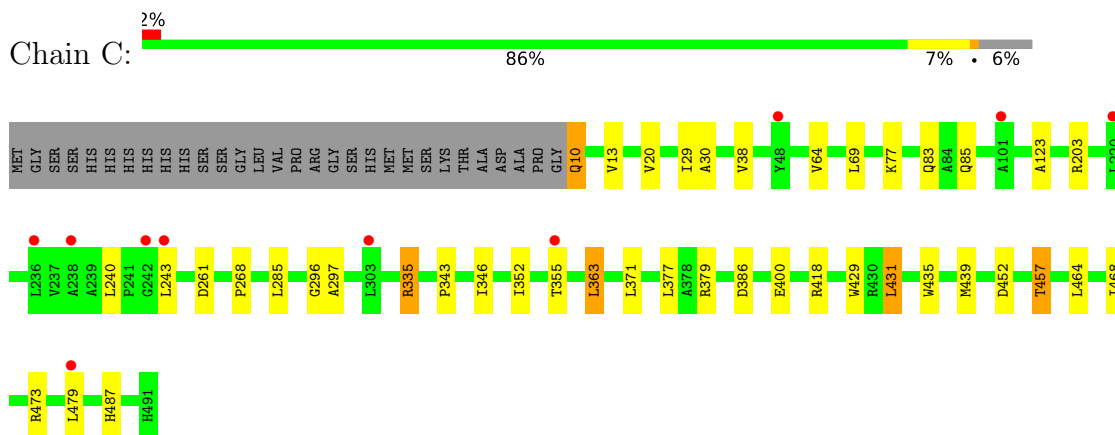
- Molecule 1: N-formimidoyl fortimicin A synthase



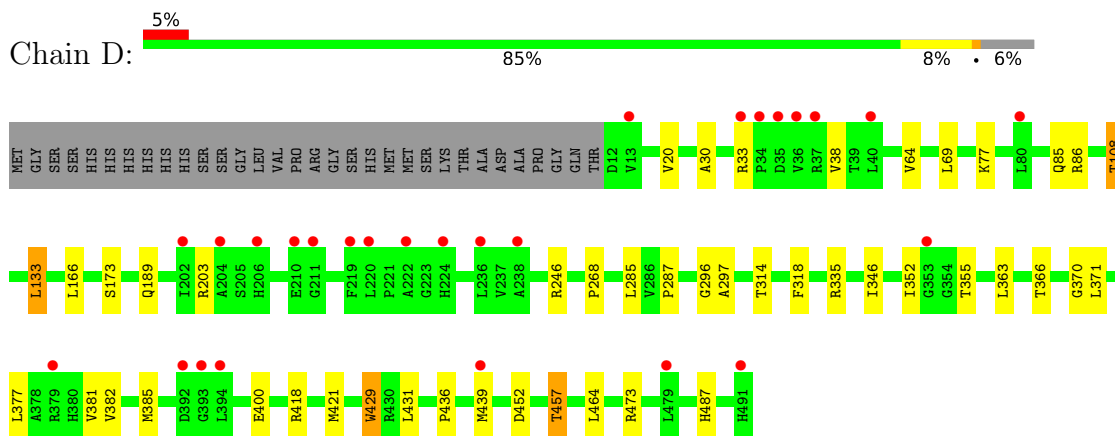
- Molecule 1: N-formimidoyl fortimicin A synthase



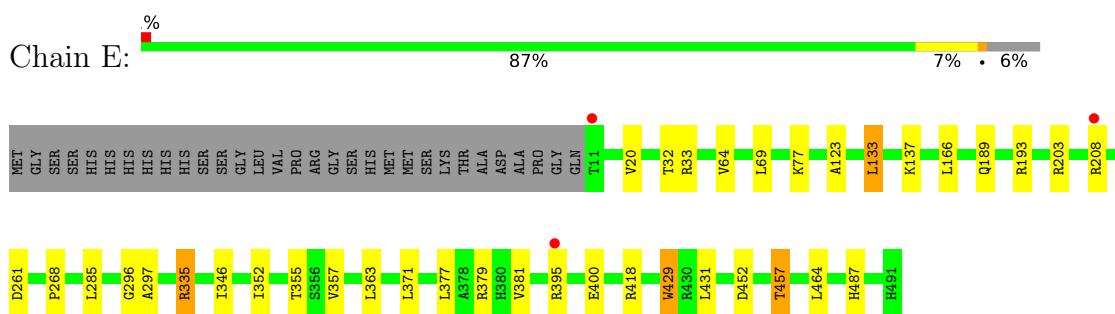
- Molecule 1: N-formimidoyl fortimicin A synthase



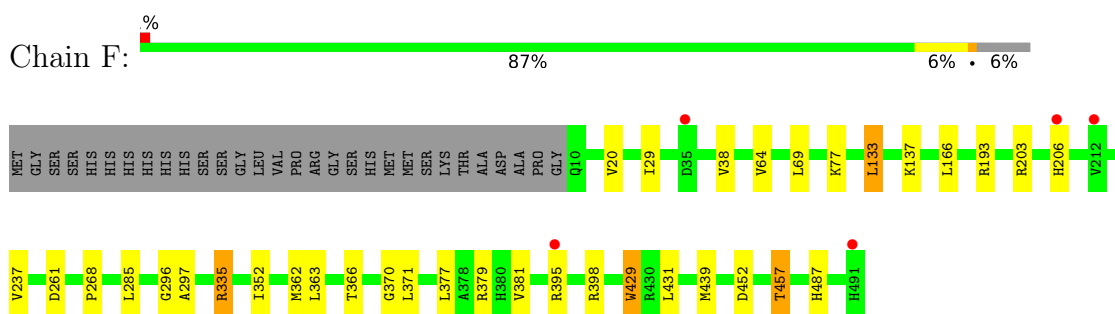
- Molecule 1: N-formimidoyl fortimicin A synthase



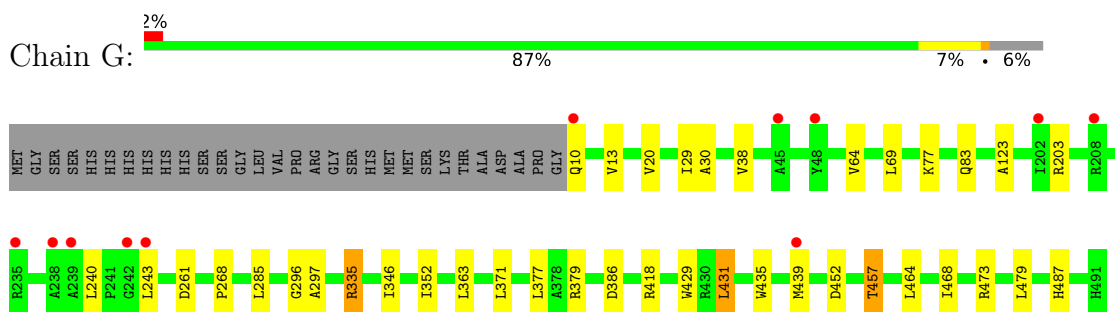
- Molecule 1: N-formimidoyl fortimicin A synthase



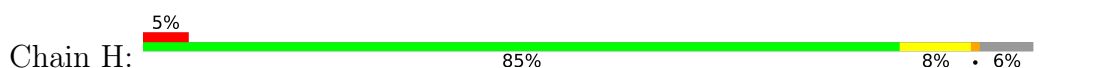
- Molecule 1: N-formimidoyl fortimicin A synthase

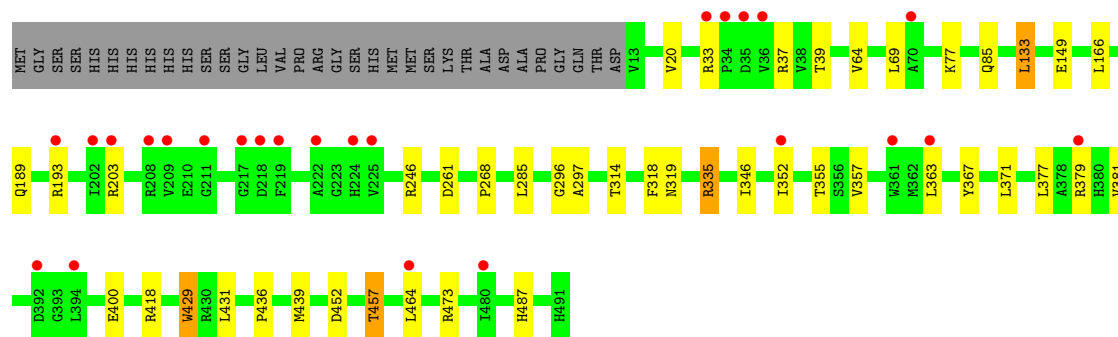


- Molecule 1: N-formimidoyl fortimicin A synthase



- Molecule 1: N-formimidoyl fortimicin A synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.70Å 108.11Å 135.82Å 90.11° 89.95° 96.61°	Depositor
Resolution (Å)	29.85 – 2.20 29.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.85-2.20) 96.9 (29.83-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.184 , 0.206 0.189 , 0.210	Depositor DCC
$R_{free}$ test set	14077 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 20.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.458 for -h,-k,l 0.011 for -k,-h,-l 0.009 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: I55, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	0/3737	0.78	0/5092
1	B	0.65	0/3745	0.78	0/5102
1	C	0.67	0/3745	0.79	0/5102
1	D	0.63	0/3721	0.78	0/5070
1	E	0.64	0/3728	0.78	0/5080
1	F	0.65	0/3745	0.77	0/5102
1	G	0.66	0/3745	0.78	0/5102
1	H	0.63	0/3713	0.77	0/5059
All	All	0.65	0/29879	0.78	0/40709

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	21	0
1	B	3662	0	3592	22	0
1	C	3662	0	3592	29	0
1	D	3638	0	3569	39	0
1	E	3645	0	3576	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3662	0	3592	24	0
1	G	3662	0	3592	27	0
1	H	3630	0	3565	32	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	1	0
2	E	53	0	31	1	0
2	F	53	0	31	1	0
2	G	53	0	31	0	0
2	H	53	0	31	1	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
3	E	30	0	0	0	0
3	F	30	0	0	0	0
3	G	30	0	0	0	0
3	H	30	0	0	0	0
4	A	5	0	2	0	0
4	B	5	0	2	0	0
4	C	5	0	2	0	0
4	D	5	0	2	0	0
4	E	5	0	2	0	0
4	F	5	0	2	0	0
4	G	5	0	2	0	0
4	H	5	0	2	0	0
5	A	292	0	0	4	0
5	B	290	0	0	2	0
5	C	260	0	0	5	0
5	D	187	0	0	0	0
5	E	298	0	0	3	0
5	F	302	0	0	2	0
5	G	249	0	0	3	0
5	H	204	0	0	2	0
All	All	32001	0	28926	204	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 3.

All (204) 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:436:PRO:HA	1:H:439:MET:HE2	1.27	1.13
1:D:436:PRO:HA	1:D:439:MET:HE2	1.27	1.09
1:D:436:PRO:HA	1:D:439:MET:CE	1.94	0.97
1:C:435:TRP:HB3	1:C:439[B]:MET:HE3	1.49	0.94
1:H:436:PRO:HA	1:H:439:MET:CE	2.05	0.86
1:G:435:TRP:HB3	1:G:439[B]:MET:HE3	1.56	0.84
1:B:352:ILE:HD12	1:B:363:LEU:HD12	1.60	0.83
1:H:149:GLU:HG3	5:H:874:HOH:O	1.80	0.81
1:C:435:TRP:HE3	1:C:439[B]:MET:HE2	1.47	0.78
1:C:435:TRP:CE3	1:C:439[B]:MET:HE2	2.18	0.78
1:D:382:VAL:HA	1:D:385:MET:CE	2.18	0.74
1:F:352:ILE:HD13	1:F:377:LEU:HD22	1.71	0.72
1:G:435:TRP:HE3	1:G:439[B]:MET:HE2	1.55	0.71
1:D:246:ARG:NH1	1:D:400:GLU:OE1	2.23	0.71
1:G:435:TRP:CE3	1:G:439[B]:MET:HE2	2.26	0.71
1:H:246:ARG:NH1	1:H:400:GLU:OE1	2.23	0.70
1:D:382:VAL:HA	1:D:385:MET:HE3	1.74	0.68
1:D:108:THR:HG22	1:D:173:SER:OG	1.93	0.68
1:D:429:TRP:CH2	1:D:439:MET:HE3	2.28	0.68
1:D:86:ARG:HD2	1:F:206:HIS:O	1.93	0.68
1:E:352:ILE:HD13	1:E:377:LEU:HD22	1.76	0.66
1:D:352:ILE:HD13	1:D:377:LEU:HD22	1.78	0.66
1:A:352:ILE:HD13	1:A:377:LEU:HD22	1.78	0.65
1:B:335:ARG:HG2	5:B:1073:HOH:O	1.96	0.65
1:H:352:ILE:HD13	1:H:377:LEU:HD22	1.77	0.64
1:C:435:TRP:HB3	1:C:439[B]:MET:CE	2.27	0.64
1:C:355:THR:HG23	1:C:400:GLU:OE2	1.99	0.63
1:D:355:THR:HG23	1:D:400:GLU:OE2	1.99	0.62
1:H:355:THR:HG23	1:H:400:GLU:OE2	1.99	0.62
1:H:436:PRO:CA	1:H:439:MET:HE2	2.18	0.61
1:A:123:ALA:HB1	1:A:418:ARG:HD2	1.83	0.61
1:E:355:THR:HG23	1:E:400:GLU:OE2	2.00	0.61
1:G:431:LEU:HD22	1:G:439[B]:MET:HE3	1.82	0.60
1:E:123:ALA:HB1	1:E:418:ARG:HD2	1.82	0.60
1:D:108:THR:HG21	1:D:287:PRO:O	2.01	0.59
1:B:64:VAL:HG13	1:B:69:LEU:HD22	1.85	0.58
1:C:379:ARG:HD3	5:C:977:HOH:O	2.03	0.58
1:F:133:LEU:HD13	1:F:166:LEU:HD22	1.85	0.58
1:E:64:VAL:HG13	1:E:69:LEU:HD22	1.86	0.58
1:B:133:LEU:HD13	1:B:166:LEU:HD22	1.85	0.57
1:E:133:LEU:HD13	1:E:166:LEU:HD22	1.86	0.57
1:F:64:VAL:HG13	1:F:69:LEU:HD22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:HG13	1:A:69:LEU:HD22	1.86	0.57
1:A:133:LEU:HD13	1:A:166:LEU:HD22	1.86	0.56
1:B:431:LEU:HD11	1:D:431:LEU:HD11	1.86	0.56
1:C:431:LEU:HD22	1:C:439[B]:MET:HE3	1.88	0.56
1:H:64:VAL:HG13	1:H:69:LEU:HD22	1.88	0.55
1:C:352:ILE:HG23	1:C:363:LEU:CD2	2.36	0.55
1:D:382:VAL:HA	1:D:385:MET:HE2	1.87	0.55
1:A:346:ILE:HG13	1:A:464:LEU:CD2	2.36	0.55
1:F:431:LEU:HD11	1:H:431:LEU:HD11	1.88	0.55
1:G:431:LEU:CD1	5:G:1015:HOH:O	2.54	0.55
1:D:346:ILE:HG13	1:D:464:LEU:CD2	2.37	0.55
1:G:431:LEU:CD2	1:G:439[B]:MET:CE	2.85	0.55
1:C:346:ILE:HG13	1:C:464:LEU:CD2	2.37	0.54
1:G:64:VAL:HG13	1:G:69:LEU:HD22	1.90	0.54
1:G:346:ILE:HG13	1:G:464:LEU:CD2	2.37	0.54
1:B:352:ILE:HG23	1:B:363:LEU:CD1	2.37	0.54
1:E:346:ILE:HG13	1:E:464:LEU:CD2	2.38	0.54
1:H:346:ILE:HG13	1:H:464:LEU:CD2	2.37	0.54
1:C:64:VAL:HG13	1:C:69:LEU:HD22	1.89	0.54
1:D:381:VAL:O	1:D:385:MET:HE2	2.07	0.54
1:D:133:LEU:HD13	1:D:166:LEU:HD22	1.90	0.54
1:B:431:LEU:HD11	1:D:431:LEU:CD1	2.38	0.54
1:F:352:ILE:HG23	1:F:363:LEU:CD1	2.38	0.54
1:H:133:LEU:HD13	1:H:166:LEU:HD22	1.89	0.53
1:C:352:ILE:HD13	1:C:377:LEU:HD22	1.91	0.53
1:B:431:LEU:CD1	1:D:431:LEU:HD11	2.38	0.53
1:C:431:LEU:CD1	5:C:1002:HOH:O	2.56	0.53
1:G:352:ILE:HD13	1:G:377:LEU:HD22	1.91	0.53
1:D:429:TRP:HH2	1:D:439:MET:HE3	1.73	0.53
1:G:352:ILE:HG23	1:G:363:LEU:CD1	2.38	0.53
1:D:64:VAL:HG13	1:D:69:LEU:HD22	1.90	0.53
1:A:352:ILE:HG23	1:A:363:LEU:CD1	2.40	0.52
1:D:352:ILE:HG23	1:D:363:LEU:CD1	2.40	0.52
1:C:431:LEU:CD2	1:C:439[B]:MET:HE1	2.40	0.52
1:D:381:VAL:HG12	1:D:385:MET:CE	2.39	0.52
1:C:431:LEU:CD2	1:C:439[B]:MET:CE	2.87	0.52
1:H:352:ILE:HG23	1:H:363:LEU:CD1	2.40	0.52
1:E:363:LEU:HD13	1:E:381:VAL:HG21	1.92	0.51
1:E:352:ILE:HG23	1:E:363:LEU:CD1	2.39	0.51
1:C:431:LEU:HD23	1:C:439[B]:MET:HE1	1.93	0.51
1:F:431:LEU:CD1	1:H:431:LEU:HD11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:ARG:HD3	5:G:1006:HOH:O	2.12	0.50
1:F:431:LEU:HD11	1:H:431:LEU:CD1	2.40	0.50
1:C:343:PRO:HG2	5:C:807:HOH:O	2.10	0.50
1:A:363:LEU:HD13	1:A:381:VAL:HG21	1.93	0.49
1:D:108:THR:CG2	1:D:287:PRO:O	2.60	0.49
1:G:261:ASP:OD2	1:G:335:ARG:HD3	2.13	0.49
1:D:363:LEU:HD13	1:D:381:VAL:HG21	1.94	0.49
1:D:381:VAL:C	1:D:385:MET:HE2	2.33	0.49
1:C:457:THR:HG21	1:C:487:HIS:CE1	2.48	0.49
1:F:457:THR:HG21	1:F:487:HIS:CE1	2.48	0.49
1:H:261:ASP:OD2	1:H:335:ARG:HD3	2.13	0.49
1:H:457:THR:HG21	1:H:487:HIS:CE1	2.48	0.48
1:G:83:GLN:NE2	5:G:802:HOH:O	2.32	0.48
1:C:83:GLN:NE2	5:C:801:HOH:O	2.32	0.48
1:E:261:ASP:OD2	1:E:335:ARG:HD3	2.14	0.48
1:F:261:ASP:OD2	1:F:335:ARG:HD3	2.14	0.48
1:G:457:THR:HG21	1:G:487:HIS:CE1	2.48	0.48
1:C:123:ALA:HB1	1:C:418:ARG:HD3	1.96	0.48
1:C:261:ASP:OD2	1:C:335:ARG:HD3	2.13	0.48
1:B:457:THR:HG21	1:B:487:HIS:CE1	2.48	0.48
1:F:439[B]:MET:HE2	1:H:439:MET:HG2	1.96	0.48
1:D:296:GLY:HA3	1:D:297:ALA:HB2	1.96	0.47
1:F:237:VAL:HG21	1:F:362:MET:HE1	1.96	0.47
1:G:431:LEU:HD23	1:G:439[B]:MET:HE1	1.96	0.47
1:H:363:LEU:HD13	1:H:381:VAL:HG21	1.95	0.47
1:F:379:ARG:HD3	5:F:1046:HOH:O	2.12	0.47
1:D:457:THR:HG21	1:D:487:HIS:CE1	2.49	0.47
1:G:20:VAL:HG11	1:G:371:LEU:HA	1.97	0.47
1:G:431:LEU:CD2	1:G:439[B]:MET:HE3	2.44	0.47
1:H:296:GLY:HA3	1:H:297:ALA:HB2	1.96	0.47
1:A:261:ASP:OD2	1:A:335:ARG:HD3	2.14	0.47
1:C:10:GLN:N	5:C:804:HOH:O	2.46	0.47
1:C:20:VAL:HG11	1:C:371:LEU:HA	1.96	0.47
1:F:296:GLY:HA3	1:F:297:ALA:HB2	1.97	0.47
1:C:296:GLY:HA3	1:C:297:ALA:HB2	1.97	0.46
1:C:30:ALA:HB2	1:C:38:VAL:HG11	1.97	0.46
1:B:431:LEU:CD1	1:D:431:LEU:CD1	2.94	0.46
1:F:363:LEU:HD13	1:F:381:VAL:HG21	1.97	0.46
1:G:296:GLY:HA3	1:G:297:ALA:HB2	1.97	0.46
1:E:296:GLY:HA3	1:E:297:ALA:HB2	1.98	0.46
1:E:457:THR:HG21	1:E:487:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:431:LEU:CD2	1:G:439[B]:MET:HE1	2.46	0.46
1:B:439[B]:MET:HE2	1:D:439:MET:HG2	1.98	0.46
1:B:296:GLY:HA3	1:B:297:ALA:HB2	1.97	0.46
1:G:30:ALA:HB2	1:G:38:VAL:HG11	1.98	0.46
1:A:296:GLY:HA3	1:A:297:ALA:HB2	1.97	0.45
1:A:208:ARG:HG2	5:A:810:HOH:O	2.16	0.45
2:E:701:FAD:H9	2:E:701:FAD:H1'2	1.78	0.45
1:B:29:ILE:HG22	1:B:38:VAL:HG21	1.98	0.45
1:A:457:THR:HG21	1:A:487:HIS:CE1	2.51	0.45
1:C:13:VAL:HG11	1:C:29:ILE:HD13	1.99	0.45
1:C:268:PRO:HG3	1:C:285:LEU:HD22	1.99	0.45
1:G:123:ALA:HB1	1:G:418:ARG:HD3	1.98	0.45
1:G:268:PRO:HG3	1:G:285:LEU:HD22	1.99	0.45
1:H:20:VAL:HG11	1:H:371:LEU:HA	1.99	0.45
1:B:351:LEU:O	1:B:352:ILE:HD13	2.17	0.44
1:B:363:LEU:HD13	1:B:381:VAL:HG21	1.98	0.44
1:A:268:PRO:HG3	1:A:285:LEU:HD22	2.00	0.44
1:A:363:LEU:HD12	1:A:363:LEU:HA	1.86	0.44
1:D:20:VAL:HG11	1:D:371:LEU:HA	1.98	0.44
1:A:20:VAL:HG11	1:A:371:LEU:HA	1.99	0.44
1:A:137:LYS:NZ	5:A:818:HOH:O	2.51	0.44
1:D:421:MET:HE3	1:D:439:MET:HE3	1.99	0.44
1:F:398:ARG:HB2	5:F:892:HOH:O	2.17	0.44
1:E:137:LYS:NZ	5:E:808:HOH:O	2.50	0.44
1:H:246:ARG:NH1	1:H:400:GLU:HG2	2.33	0.43
2:H:701:FAD:H9	2:H:701:FAD:H1'2	1.78	0.43
2:A:701:FAD:H9	2:A:701:FAD:H1'2	1.80	0.43
1:G:13:VAL:HG11	1:G:29:ILE:HD13	1.99	0.43
1:C:431:LEU:HD22	1:C:439[B]:MET:CE	2.48	0.43
1:D:268:PRO:HG3	1:D:285:LEU:HD22	2.00	0.43
1:F:431:LEU:CD1	1:H:431:LEU:CD1	2.96	0.43
1:F:20:VAL:HG11	1:F:371:LEU:HA	2.00	0.43
1:F:29:ILE:HG22	1:F:38:VAL:HG21	2.00	0.43
1:H:268:PRO:HG3	1:H:285:LEU:HD22	2.00	0.43
1:D:246:ARG:NH1	1:D:400:GLU:HG2	2.33	0.43
1:E:379:ARG:HD3	5:E:1040:HOH:O	2.17	0.43
1:F:297:ALA:HB1	2:F:701:FAD:HM73	2.01	0.43
1:G:363:LEU:HD11	1:G:377:LEU:HB3	2.00	0.43
1:B:429:TRP:CG	1:B:431:LEU:HD13	2.54	0.43
1:G:240:LEU:HB2	1:G:243:LEU:HD22	2.01	0.43
1:H:314:THR:CG2	1:H:318:PHE:CE2	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:379:ARG:NH2	5:H:806:HOH:O	2.50	0.43
1:B:268:PRO:HG3	1:B:285:LEU:HD22	2.01	0.43
1:D:314:THR:CG2	1:D:318:PHE:CE2	3.02	0.43
1:E:268:PRO:HG3	1:E:285:LEU:HD22	2.00	0.43
1:H:429:TRP:CH2	1:H:439:MET:HE3	2.54	0.43
1:A:311:ILE:HG23	1:B:318:PHE:HB3	2.00	0.42
1:B:352:ILE:CD1	1:B:363:LEU:HD12	2.39	0.42
1:D:363:LEU:HD12	1:D:363:LEU:HA	1.87	0.42
1:F:439[A]:MET:HE2	1:H:439:MET:SD	2.59	0.42
1:G:435:TRP:HB3	1:G:439[B]:MET:CE	2.38	0.42
1:B:20:VAL:HG11	1:B:371:LEU:HA	2.00	0.42
1:E:208:ARG:HG2	5:E:810:HOH:O	2.20	0.42
1:A:457:THR:CG2	5:A:1065:HOH:O	2.68	0.42
1:F:429:TRP:CG	1:F:431:LEU:HD13	2.54	0.42
1:E:20:VAL:HG11	1:E:371:LEU:HA	2.00	0.42
1:E:429:TRP:CG	1:E:431:LEU:HD13	2.54	0.42
1:A:429:TRP:CG	1:A:431:LEU:HD13	2.55	0.42
1:H:39:THR:OG1	1:H:193:ARG:NH1	2.52	0.42
1:D:429:TRP:CG	1:D:431:LEU:HD13	2.55	0.41
1:H:429:TRP:CG	1:H:431:LEU:HD13	2.55	0.41
1:A:208:ARG:NH2	5:A:821:HOH:O	2.53	0.41
1:C:240:LEU:HB2	1:C:243:LEU:HD22	2.01	0.41
1:D:366:THR:HB	1:D:370:GLY:CA	2.51	0.41
1:F:268:PRO:HG3	1:F:285:LEU:HD22	2.01	0.41
1:G:468:ILE:HD13	1:G:479:LEU:CD2	2.51	0.41
1:H:314:THR:HG22	1:H:318:PHE:CE2	2.55	0.41
1:D:314:THR:HG22	1:D:318:PHE:CE2	2.56	0.41
1:A:32:THR:HG22	1:A:33:ARG:HG2	2.02	0.41
1:C:468:ILE:HD13	1:C:479:LEU:CD2	2.50	0.41
1:A:33:ARG:HB3	1:A:36:VAL:HG13	2.03	0.41
1:B:398:ARG:HB2	5:B:898:HOH:O	2.19	0.41
1:E:355:THR:HG22	1:E:357:VAL:H	1.86	0.41
1:H:363:LEU:HD12	1:H:363:LEU:HA	1.89	0.40
1:B:39:THR:HG23	1:B:193:ARG:HG2	2.03	0.40
2:D:701:FAD:O4'	2:D:701:FAD:H1'1	2.21	0.40
1:F:366:THR:HB	1:F:370:GLY:CA	2.52	0.40
1:D:30:ALA:HB2	1:D:38:VAL:HG11	2.04	0.40
1:E:32:THR:HG22	1:E:33:ARG:HG2	2.03	0.40
1:H:355:THR:HG22	1:H:357:VAL:H	1.86	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%)	466 (97%)	14 (3%)	0	100	100
1	B	481/512 (94%)	467 (97%)	14 (3%)	0	100	100
1	C	481/512 (94%)	467 (97%)	14 (3%)	0	100	100
1	D	478/512 (93%)	464 (97%)	14 (3%)	0	100	100
1	E	479/512 (94%)	465 (97%)	14 (3%)	0	100	100
1	F	481/512 (94%)	467 (97%)	14 (3%)	0	100	100
1	G	481/512 (94%)	467 (97%)	14 (3%)	0	100	100
1	H	477/512 (93%)	463 (97%)	14 (3%)	0	100	100
All	All	3838/4096 (94%)	3726 (97%)	112 (3%)	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%)	365 (97%)	11 (3%)	42	54
1	B	377/400 (94%)	366 (97%)	11 (3%)	42	54
1	C	377/400 (94%)	365 (97%)	12 (3%)	39	50
1	D	374/400 (94%)	361 (96%)	13 (4%)	36	46
1	E	375/400 (94%)	365 (97%)	10 (3%)	44	57
1	F	377/400 (94%)	367 (97%)	10 (3%)	44	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	377/400 (94%)	367 (97%)	10 (3%)	44	57
1	H	373/400 (93%)	358 (96%)	15 (4%)	31	40
All	All	3006/3200 (94%)	2914 (97%)	92 (3%)	40	51

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	77	LYS
1	A	133	LEU
1	A	189	GLN
1	A	193	ARG
1	A	203	ARG
1	A	335	ARG
1	A	395	ARG
1	A	429	TRP
1	A	452	ASP
1	A	457	THR
1	B	77	LYS
1	B	133	LEU
1	B	137	LYS
1	B	193	ARG
1	B	203	ARG
1	B	319	ASN
1	B	335	ARG
1	B	395	ARG
1	B	429	TRP
1	B	452	ASP
1	B	457	THR
1	C	10	GLN
1	C	77	LYS
1	C	85	GLN
1	C	203	ARG
1	C	335	ARG
1	C	363	LEU
1	C	386	ASP
1	C	429	TRP
1	C	431	LEU
1	C	452	ASP
1	C	457	THR
1	C	473	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	33	ARG
1	D	77	LYS
1	D	85	GLN
1	D	108	THR
1	D	133	LEU
1	D	189	GLN
1	D	203	ARG
1	D	335	ARG
1	D	418	ARG
1	D	429	TRP
1	D	452	ASP
1	D	457	THR
1	D	473	ARG
1	E	77	LYS
1	E	133	LEU
1	E	189	GLN
1	E	193	ARG
1	E	203	ARG
1	E	335	ARG
1	E	395	ARG
1	E	429	TRP
1	E	452	ASP
1	E	457	THR
1	F	77	LYS
1	F	133	LEU
1	F	137	LYS
1	F	193	ARG
1	F	203	ARG
1	F	335	ARG
1	F	395	ARG
1	F	429	TRP
1	F	452	ASP
1	F	457	THR
1	G	10	GLN
1	G	77	LYS
1	G	203	ARG
1	G	335	ARG
1	G	386	ASP
1	G	429	TRP
1	G	431	LEU
1	G	452	ASP
1	G	457	THR

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Mol	Chain	Res	Type
1	G	473	ARG
1	H	33	ARG
1	H	37	ARG
1	H	77	LYS
1	H	85	GLN
1	H	133	LEU
1	H	189	GLN
1	H	203	ARG
1	H	319	ASN
1	H	335	ARG
1	H	367	TYR
1	H	418	ARG
1	H	429	TRP
1	H	452	ASP
1	H	457	THR
1	H	473	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	GLN
1	D	319	ASN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	I55	G	702	-	28,32,32	0.67	0	31,46,46	1.06	2 (6%)
4	GLY	A	703	-	4,4,4	1.10	0	3,4,4	0.73	0
4	GLY	B	703	-	4,4,4	0.71	0	3,4,4	1.85	1 (33%)
4	GLY	F	703	-	4,4,4	0.64	0	3,4,4	1.71	1 (33%)
2	FAD	D	701	-	53,58,58	0.60	0	68,89,89	0.80	1 (1%)
3	I55	E	702	-	28,32,32	1.00	1 (3%)	31,46,46	1.12	2 (6%)
4	GLY	C	703	-	4,4,4	0.91	0	3,4,4	2.20	2 (66%)
2	FAD	F	701	-	53,58,58	0.68	0	68,89,89	0.79	3 (4%)
3	I55	F	702	-	28,32,32	1.33	1 (3%)	31,46,46	1.18	3 (9%)
4	GLY	E	703	-	4,4,4	1.05	0	3,4,4	0.81	0
2	FAD	B	701	-	53,58,58	0.68	1 (1%)	68,89,89	0.81	2 (2%)
2	FAD	E	701	-	53,58,58	0.72	1 (1%)	68,89,89	0.90	3 (4%)
4	GLY	H	703	-	4,4,4	1.04	0	3,4,4	0.87	0
2	FAD	H	701	-	53,58,58	0.62	0	68,89,89	0.85	3 (4%)
4	GLY	D	703	-	4,4,4	0.97	0	3,4,4	1.16	0
3	I55	H	702	-	28,32,32	0.79	1 (3%)	31,46,46	1.18	2 (6%)
3	I55	B	702	-	28,32,32	1.34	1 (3%)	31,46,46	1.16	2 (6%)
3	I55	A	702	-	28,32,32	1.08	1 (3%)	31,46,46	1.14	2 (6%)
2	FAD	G	701	-	53,58,58	0.60	0	68,89,89	0.85	2 (2%)
4	GLY	G	703	-	4,4,4	1.00	0	3,4,4	2.00	2 (66%)
2	FAD	A	701	-	53,58,58	0.71	0	68,89,89	0.88	3 (4%)
3	I55	D	702	-	28,32,32	1.03	2 (7%)	31,46,46	1.14	1 (3%)
3	I55	C	702	-	28,32,32	0.74	2 (7%)	31,46,46	1.01	1 (3%)
2	FAD	C	701	-	53,58,58	0.60	0	68,89,89	0.84	3 (4%)

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	I55	G	702	-	-	1/14/61/61	0/3/3/3
4	GLY	A	703	-	-	0/2/2/2	-
4	GLY	B	703	-	-	0/2/2/2	-
4	GLY	F	703	-	-	0/2/2/2	-
2	FAD	D	701	-	-	2/30/50/50	0/6/6/6
3	I55	E	702	-	-	1/14/61/61	0/3/3/3
4	GLY	C	703	-	-	0/2/2/2	-
2	FAD	F	701	-	-	3/30/50/50	0/6/6/6
3	I55	F	702	-	-	1/14/61/61	0/3/3/3
4	GLY	E	703	-	-	0/2/2/2	-
2	FAD	B	701	-	-	1/30/50/50	0/6/6/6
2	FAD	E	701	-	-	2/30/50/50	0/6/6/6
4	GLY	H	703	-	-	0/2/2/2	-
2	FAD	H	701	-	-	2/30/50/50	0/6/6/6
4	GLY	D	703	-	-	0/2/2/2	-
3	I55	H	702	-	-	1/14/61/61	0/3/3/3
3	I55	B	702	-	-	1/14/61/61	0/3/3/3
3	I55	A	702	-	-	1/14/61/61	0/3/3/3
2	FAD	G	701	-	-	2/30/50/50	0/6/6/6
4	GLY	G	703	-	-	0/2/2/2	-
2	FAD	A	701	-	-	2/30/50/50	0/6/6/6
3	I55	D	702	-	-	0/14/61/61	0/3/3/3
3	I55	C	702	-	-	1/14/61/61	0/3/3/3
2	FAD	C	701	-	-	4/30/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	I55	C4-C3	-6.34	1.49	1.53
3	F	702	I55	C4-C3	-6.30	1.49	1.53
3	A	702	I55	C4-C3	-5.01	1.50	1.53
3	E	702	I55	C4-C3	-4.26	1.50	1.53
3	D	702	I55	C4-C3	-4.09	1.50	1.53
3	H	702	I55	C4-C3	-2.80	1.51	1.53
2	E	701	FAD	C1'-C2'	-2.25	1.49	1.52
3	D	702	I55	C8-C9	2.19	1.54	1.52
3	C	702	I55	C8-C9	2.07	1.54	1.52
2	B	701	FAD	O2'-C2'	-2.04	1.39	1.43
3	C	702	I55	C4-C3	-2.04	1.52	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	702	I55	C10-N6-C5	-4.84	107.92	112.56
3	B	702	I55	C10-N6-C5	-4.29	108.45	112.56
3	F	702	I55	C10-N6-C5	-4.27	108.47	112.56
3	D	702	I55	C10-N6-C5	-4.17	108.56	112.56
3	A	702	I55	C10-N6-C5	-4.02	108.70	112.56
3	E	702	I55	C10-N6-C5	-3.97	108.76	112.56
3	G	702	I55	C10-N6-C5	-3.80	108.91	112.56
3	C	702	I55	C10-N6-C5	-3.60	109.11	112.56
4	C	703	GLY	OXT-C-CA	2.69	124.17	113.45
2	H	701	FAD	O2P-P-O1P	2.59	125.05	112.24
3	B	702	I55	C9-C8-N5	2.56	112.48	109.83
4	C	703	GLY	OXT-C-O	-2.55	116.94	123.30
2	E	701	FAD	C5A-C6A-N6A	2.54	124.22	120.35
4	B	703	GLY	OXT-C-CA	2.53	123.54	113.45
2	G	701	FAD	O2P-P-O1P	2.51	124.67	112.24
2	A	701	FAD	O2A-PA-O1A	2.51	124.65	112.24
4	G	703	GLY	OXT-C-CA	2.47	123.28	113.45
2	E	701	FAD	O2A-PA-O1A	2.46	124.41	112.24
3	F	702	I55	C9-C8-N5	2.45	112.36	109.83
2	B	701	FAD	C4'-C3'-C2'	2.42	118.40	113.36
2	C	701	FAD	O2P-P-O1P	2.39	124.07	112.24
2	D	701	FAD	O2P-P-O1P	2.39	124.06	112.24
4	F	703	GLY	OXT-C-CA	2.36	122.84	113.45
2	A	701	FAD	C5A-C6A-N6A	2.33	123.89	120.35
2	G	701	FAD	C5A-C6A-N6A	2.31	123.86	120.35
2	F	701	FAD	O2A-PA-O1A	2.30	123.62	112.24
4	G	703	GLY	OXT-C-O	-2.29	117.58	123.30
2	A	701	FAD	C4'-C3'-C2'	2.29	118.12	113.36
3	F	702	I55	O3-C9-C10	2.27	115.00	109.77
2	E	701	FAD	C4'-C3'-C2'	2.24	118.03	113.36
3	A	702	I55	C9-C8-N5	2.22	112.13	109.83
2	H	701	FAD	O2A-PA-O1A	2.16	122.94	112.24
2	H	701	FAD	C5A-C6A-N6A	2.15	123.61	120.35
3	E	702	I55	C9-C8-N5	2.12	112.03	109.83
2	F	701	FAD	C4'-C3'-C2'	2.11	117.75	113.36
2	B	701	FAD	O2A-PA-O1A	2.10	122.64	112.24
3	G	702	I55	O3-C9-C10	2.09	114.59	109.77
2	C	701	FAD	C5A-C6A-N6A	2.06	123.48	120.35
2	C	701	FAD	C4-N3-C2	-2.04	121.87	125.64
3	H	702	I55	C9-C8-N5	2.03	111.93	109.83
2	F	701	FAD	C5A-C6A-N6A	2.02	123.43	120.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C3B-C4B-C5B-O5B
2	E	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C5B-O5B-PA-O2A
3	A	702	I55	C15-C13-O6-C14
3	B	702	I55	C15-C13-O6-C14
3	C	702	I55	C15-C13-O6-C14
3	E	702	I55	C15-C13-O6-C14
3	F	702	I55	C15-C13-O6-C14
3	G	702	I55	C15-C13-O6-C14
3	H	702	I55	C15-C13-O6-C14
2	B	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	C2'-C1'-N10-C10
2	F	701	FAD	C2'-C1'-N10-C10
2	H	701	FAD	C2'-C1'-N10-C10
2	H	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	C3B-C4B-C5B-O5B
2	E	701	FAD	C3B-C4B-C5B-O5B
2	F	701	FAD	C3B-C4B-C5B-O5B
2	C	701	FAD	N10-C1'-C2'-O2'
2	G	701	FAD	N10-C1'-C2'-O2'

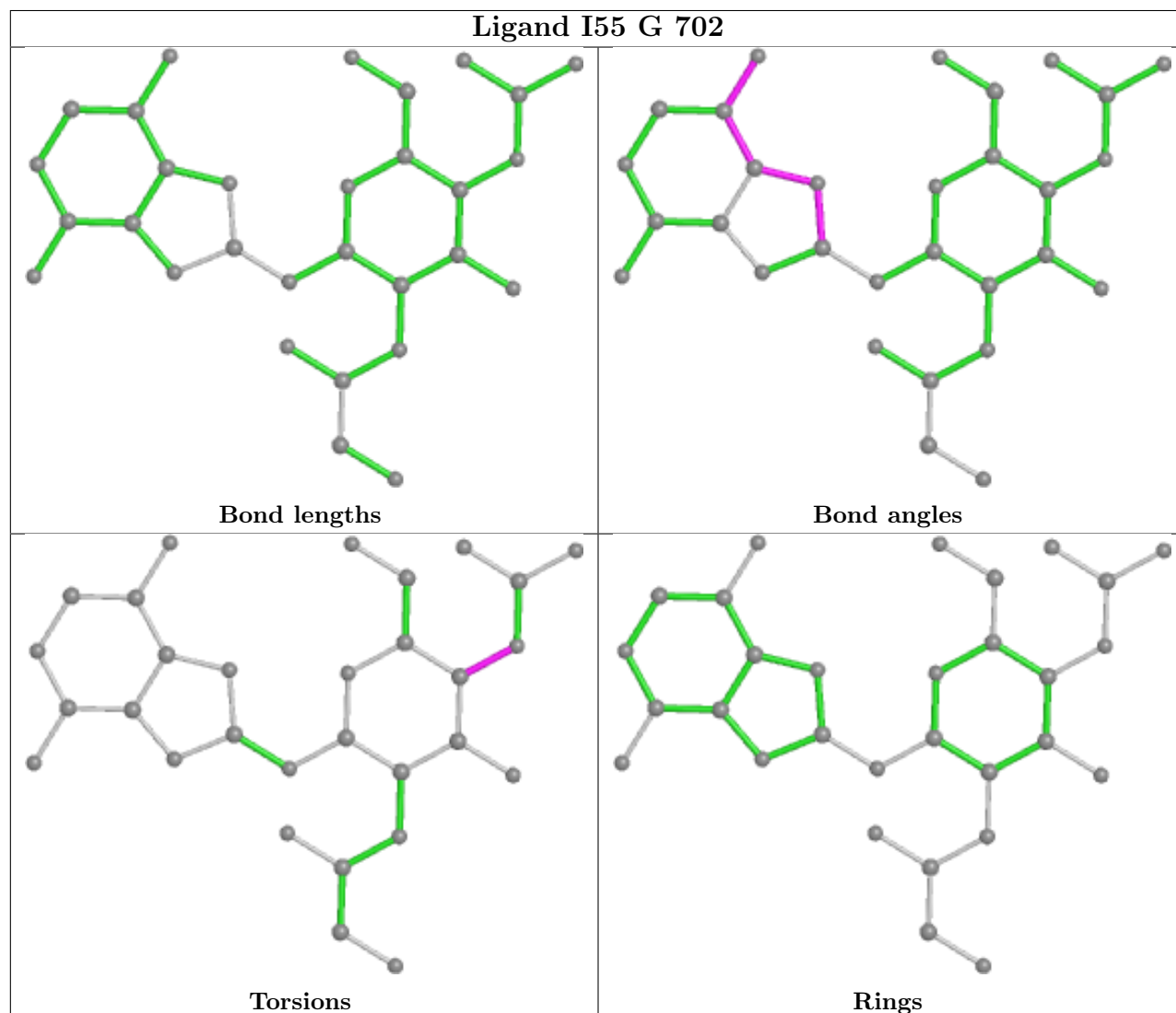
There are no ring outliers.

5 monomers are involved in 5 short contacts:

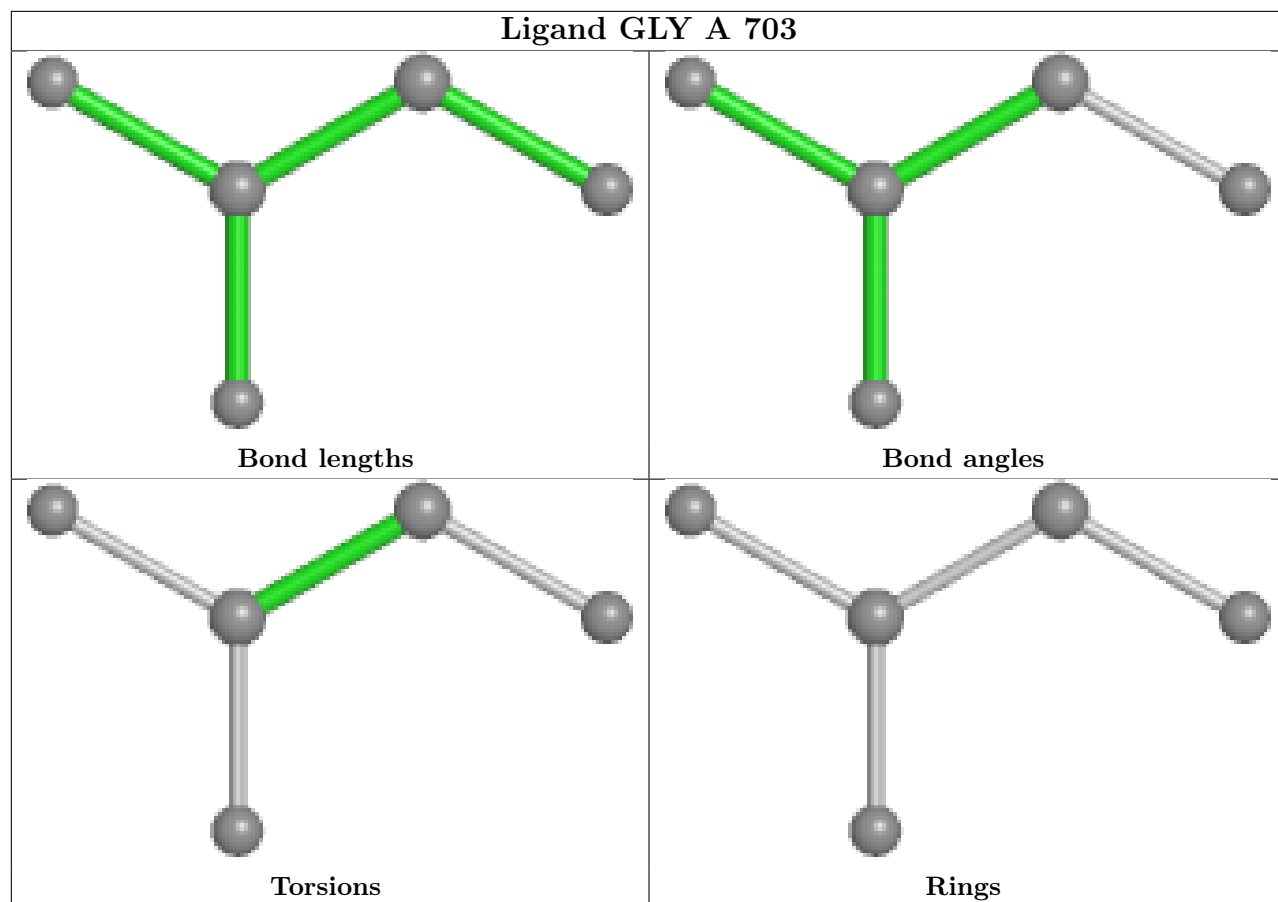
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	FAD	1	0
2	F	701	FAD	1	0
2	E	701	FAD	1	0
2	H	701	FAD	1	0
2	A	701	FAD	1	0

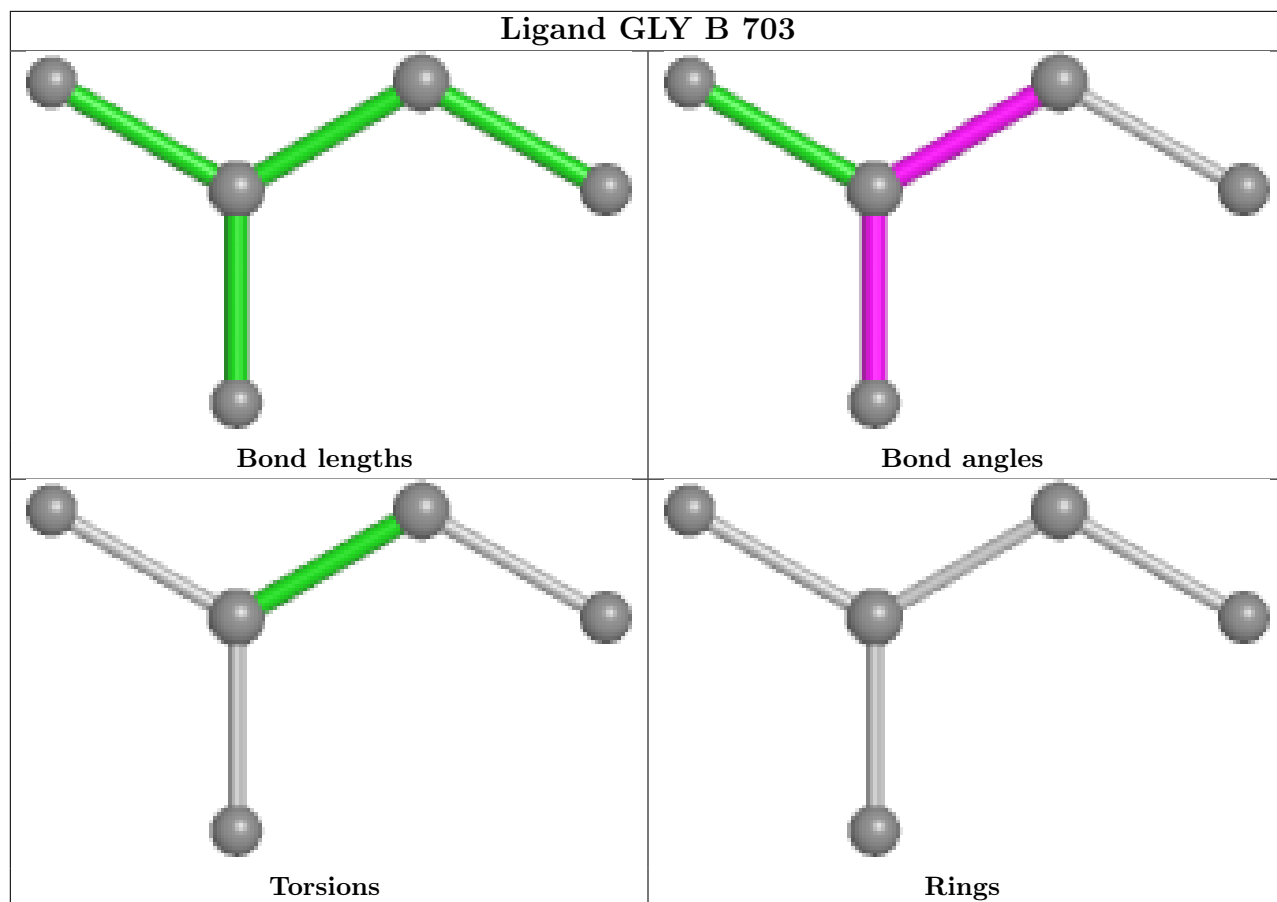
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

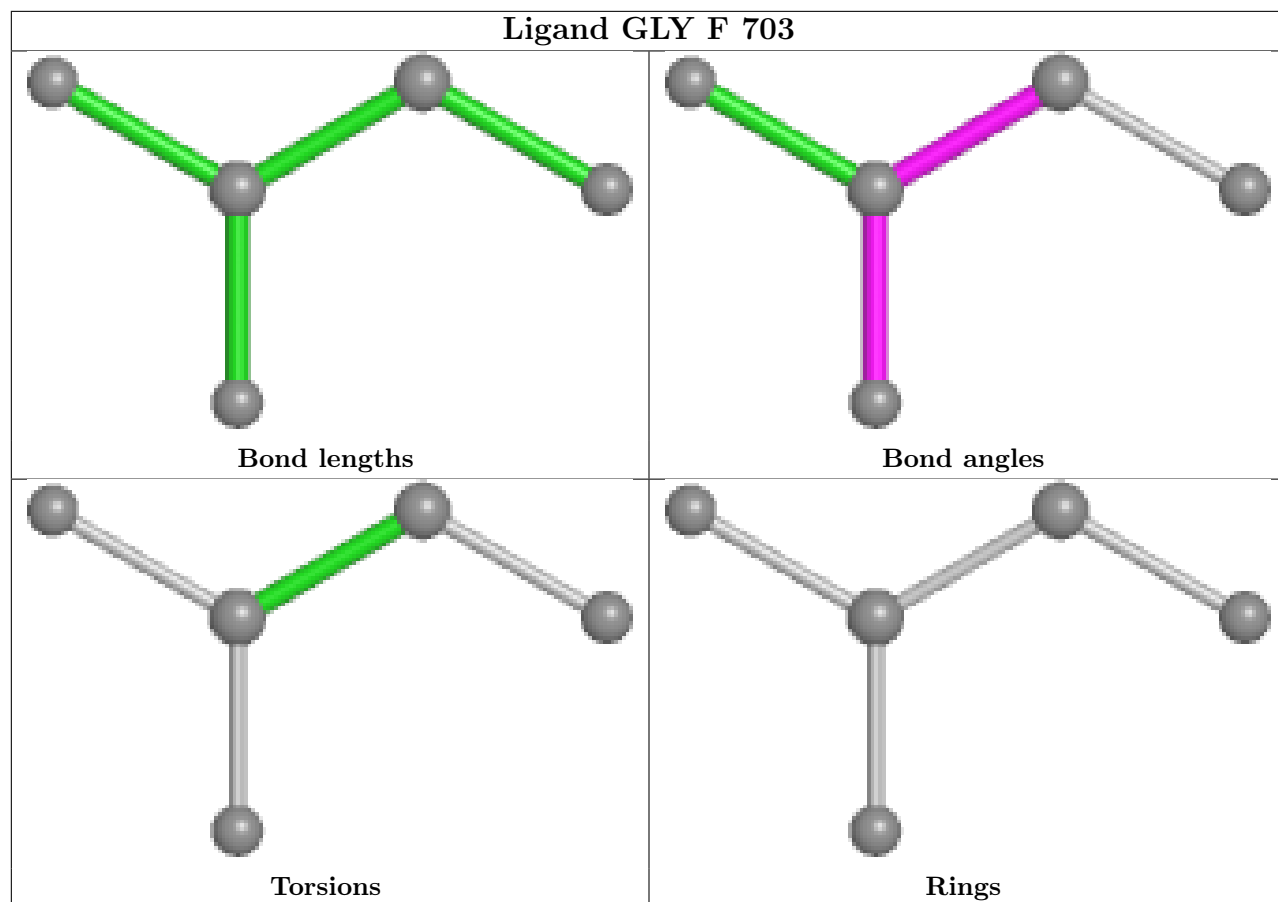
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

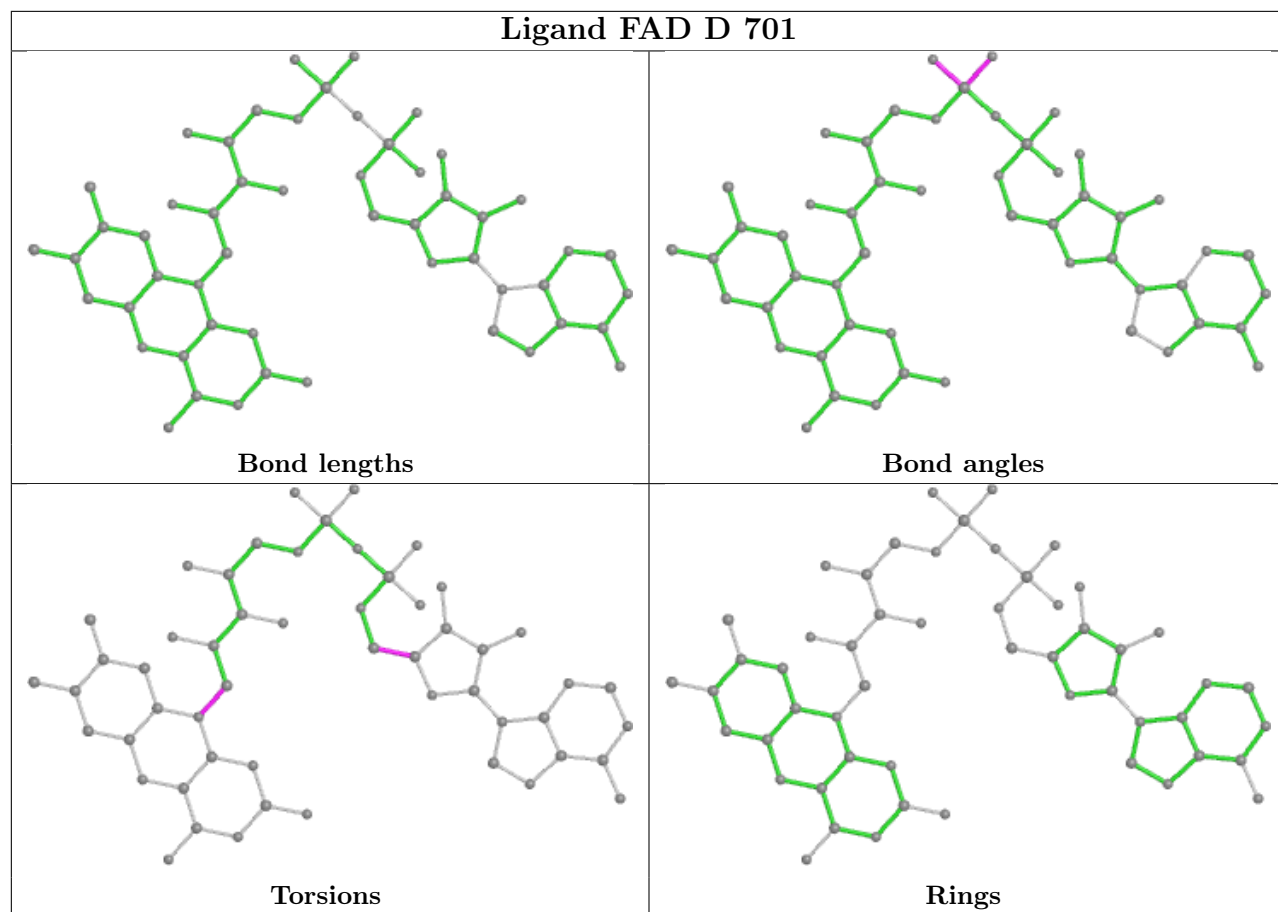


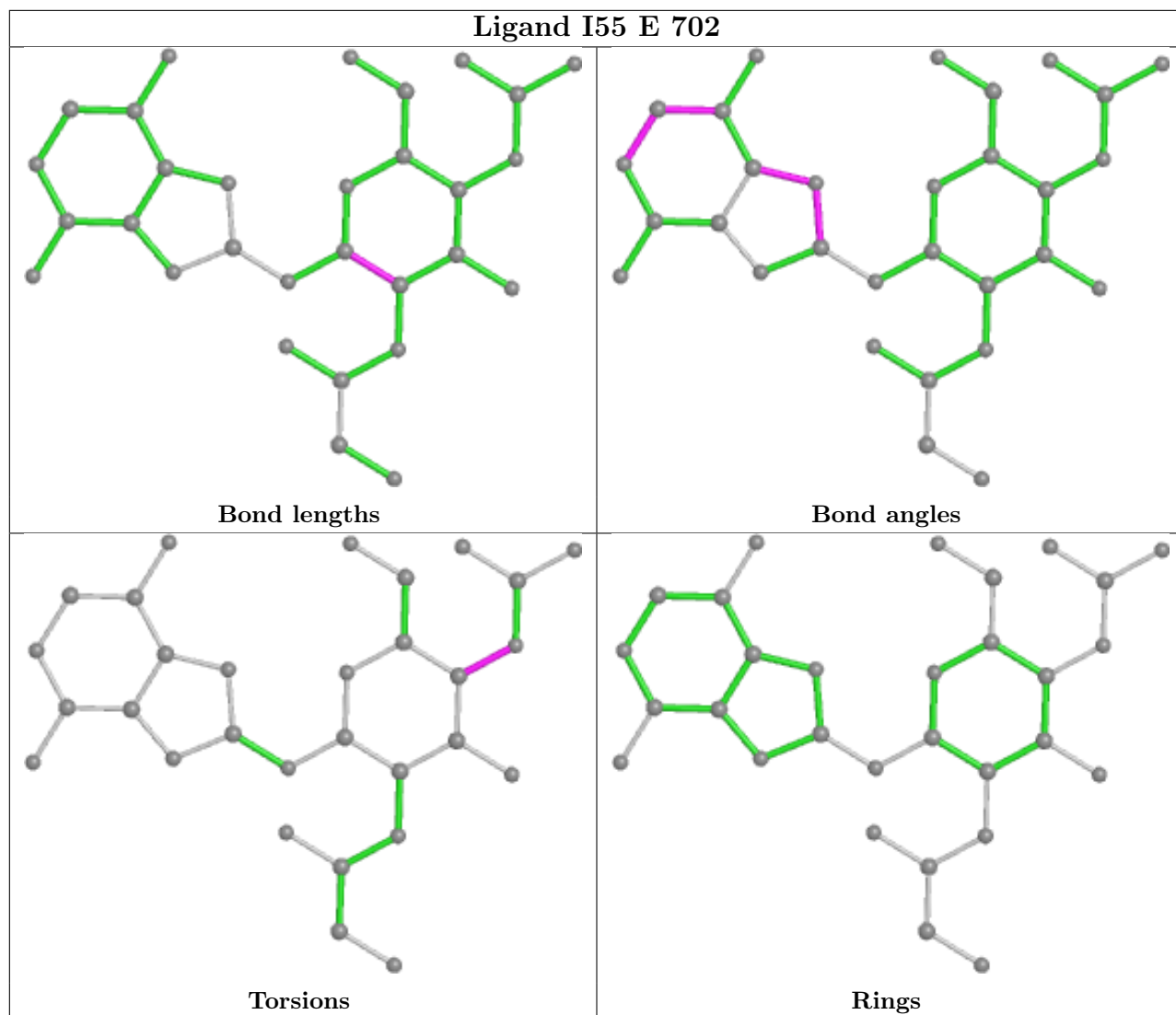


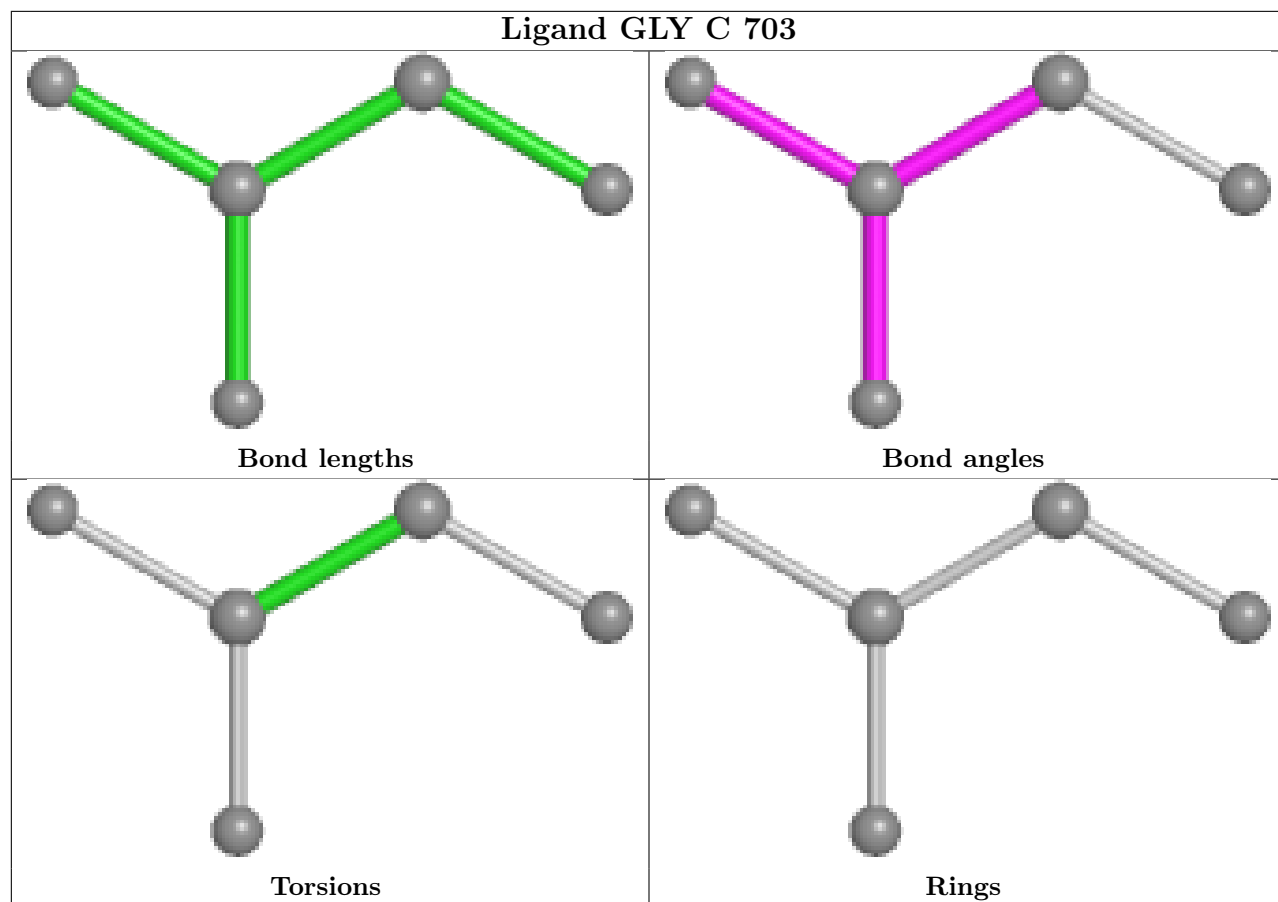


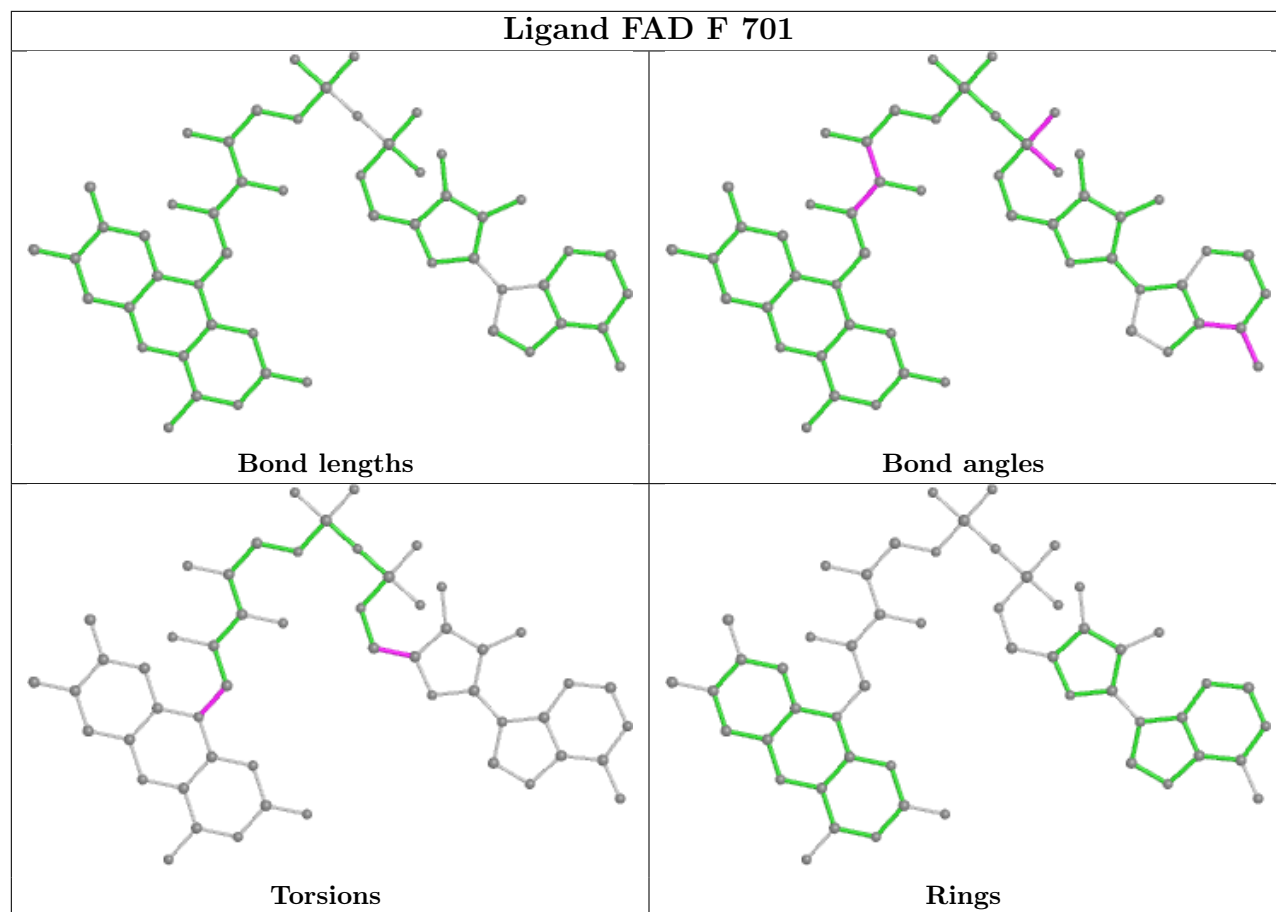


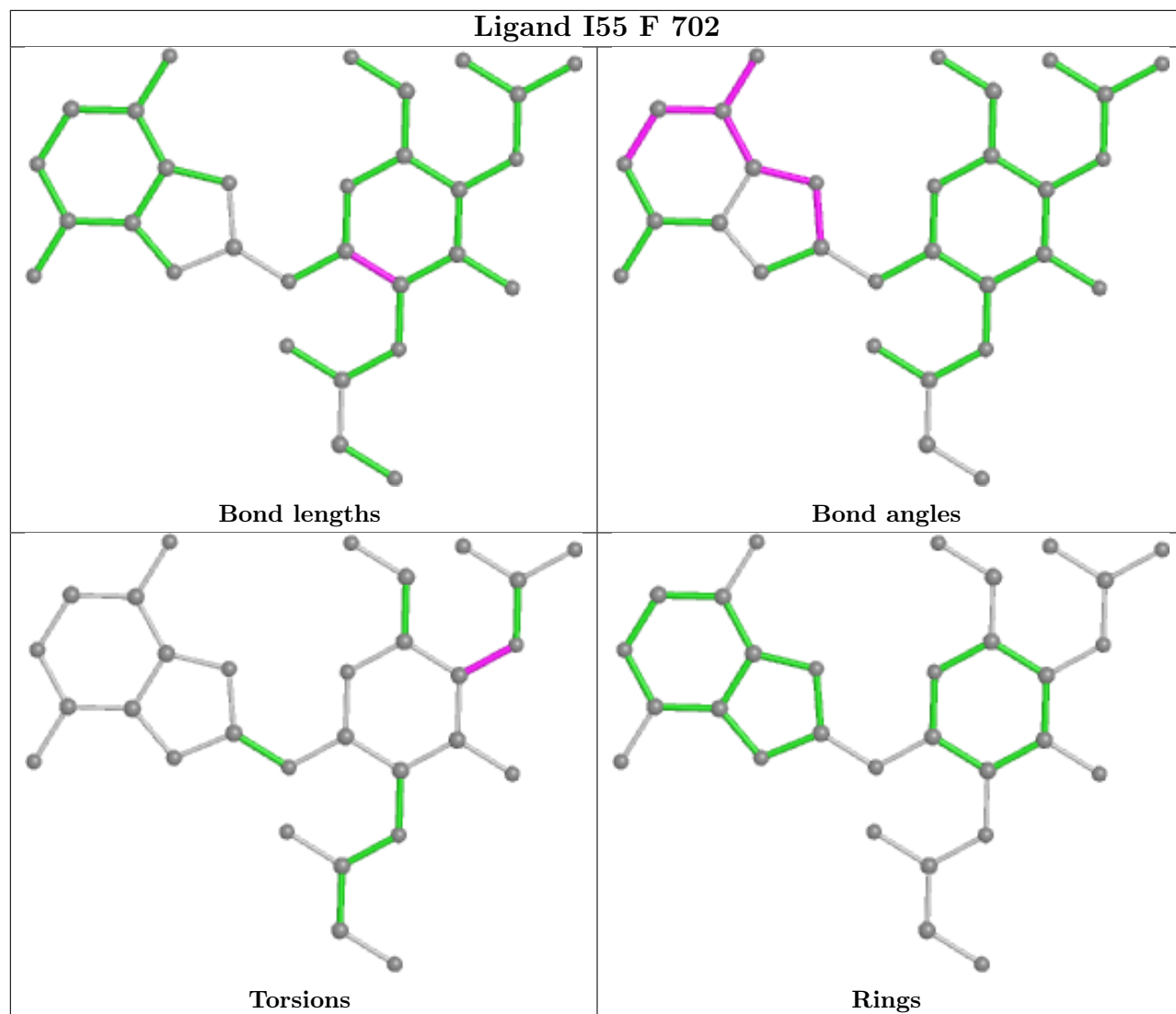




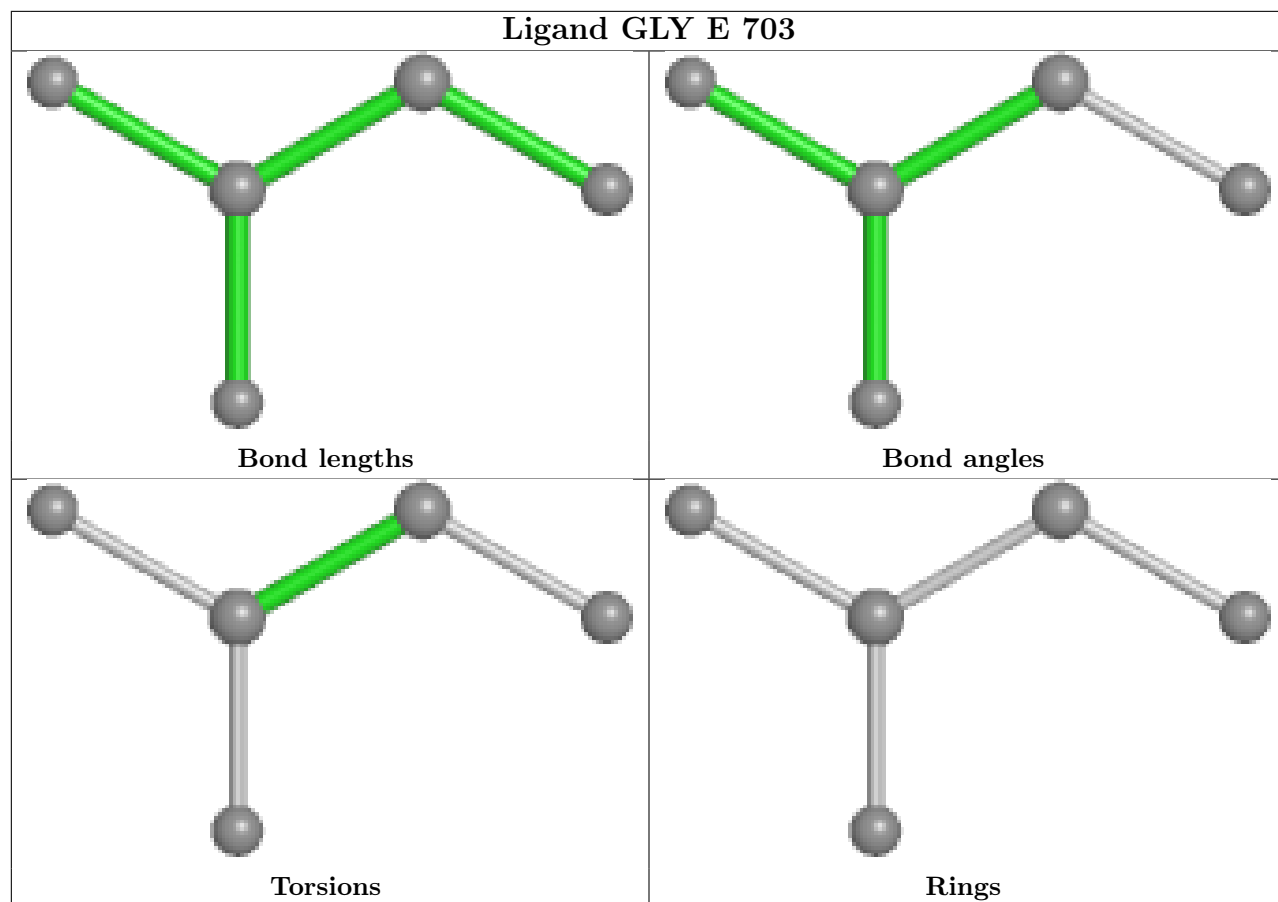


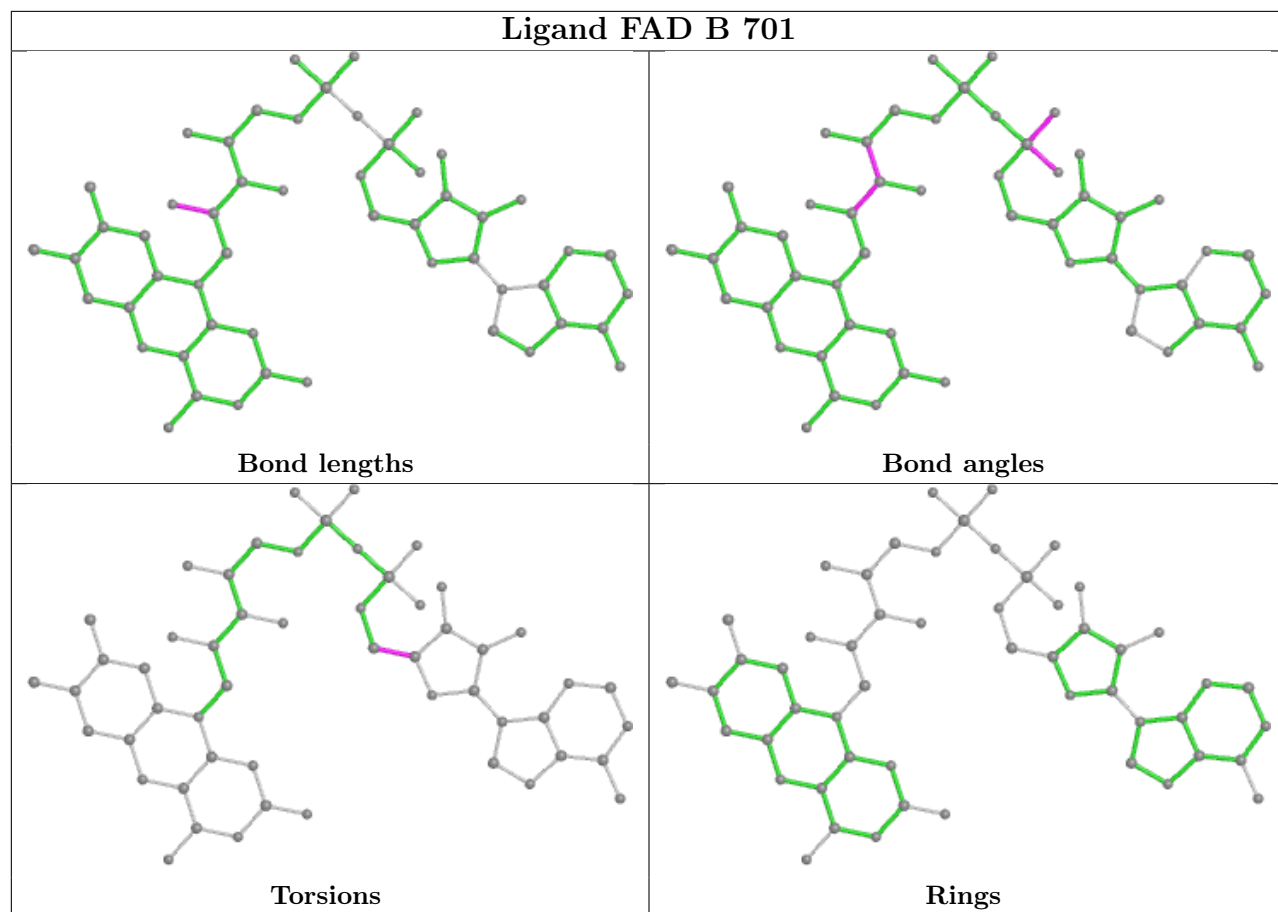


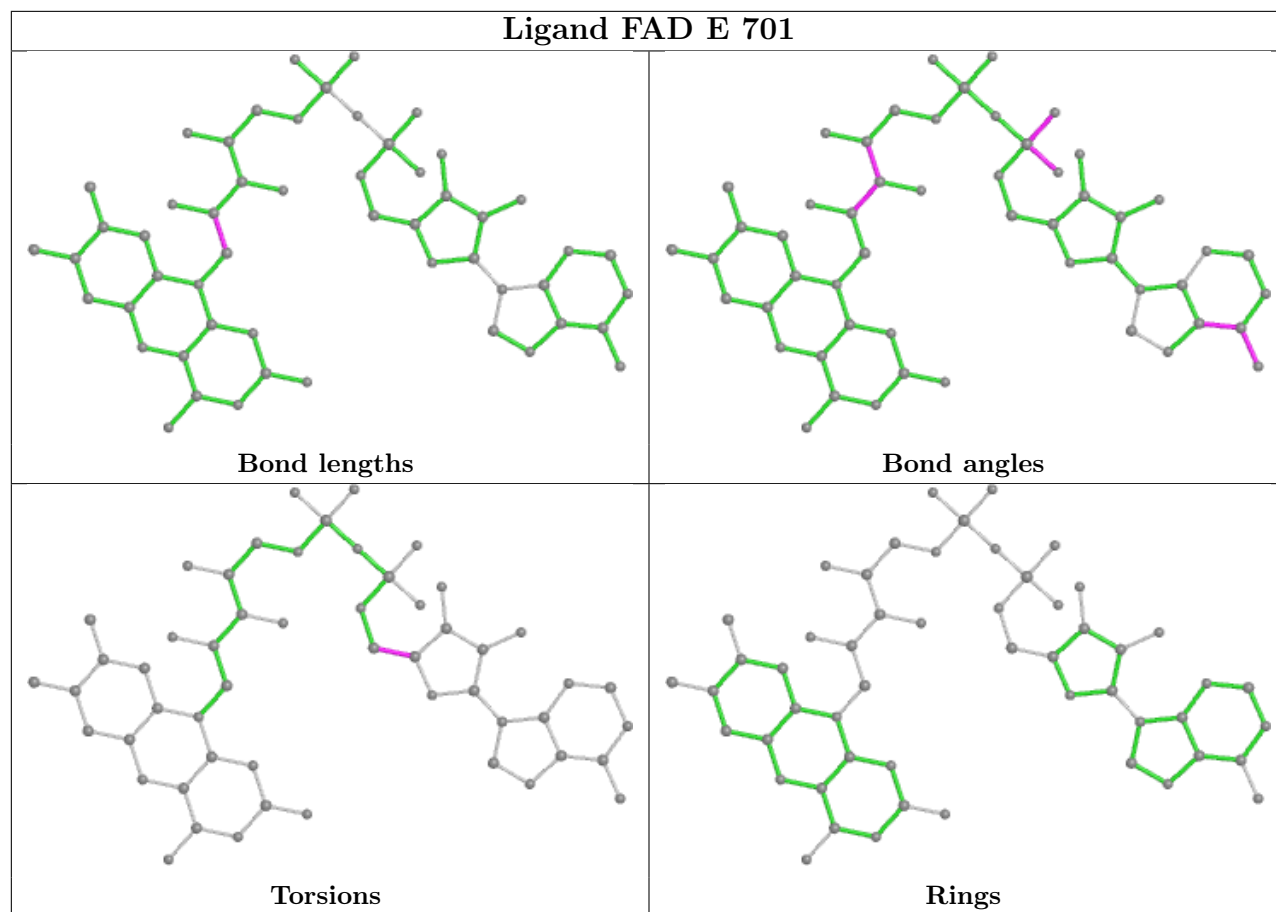


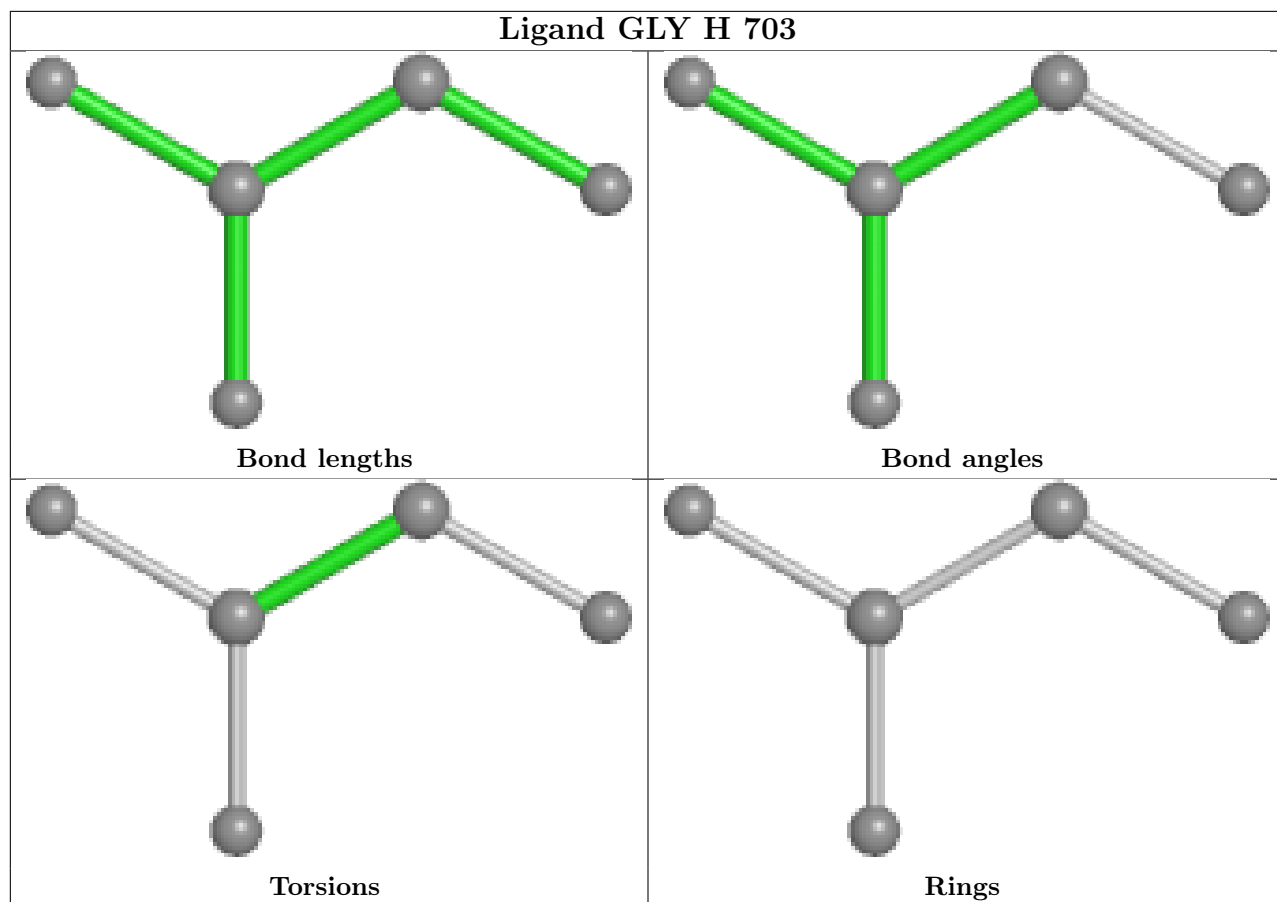


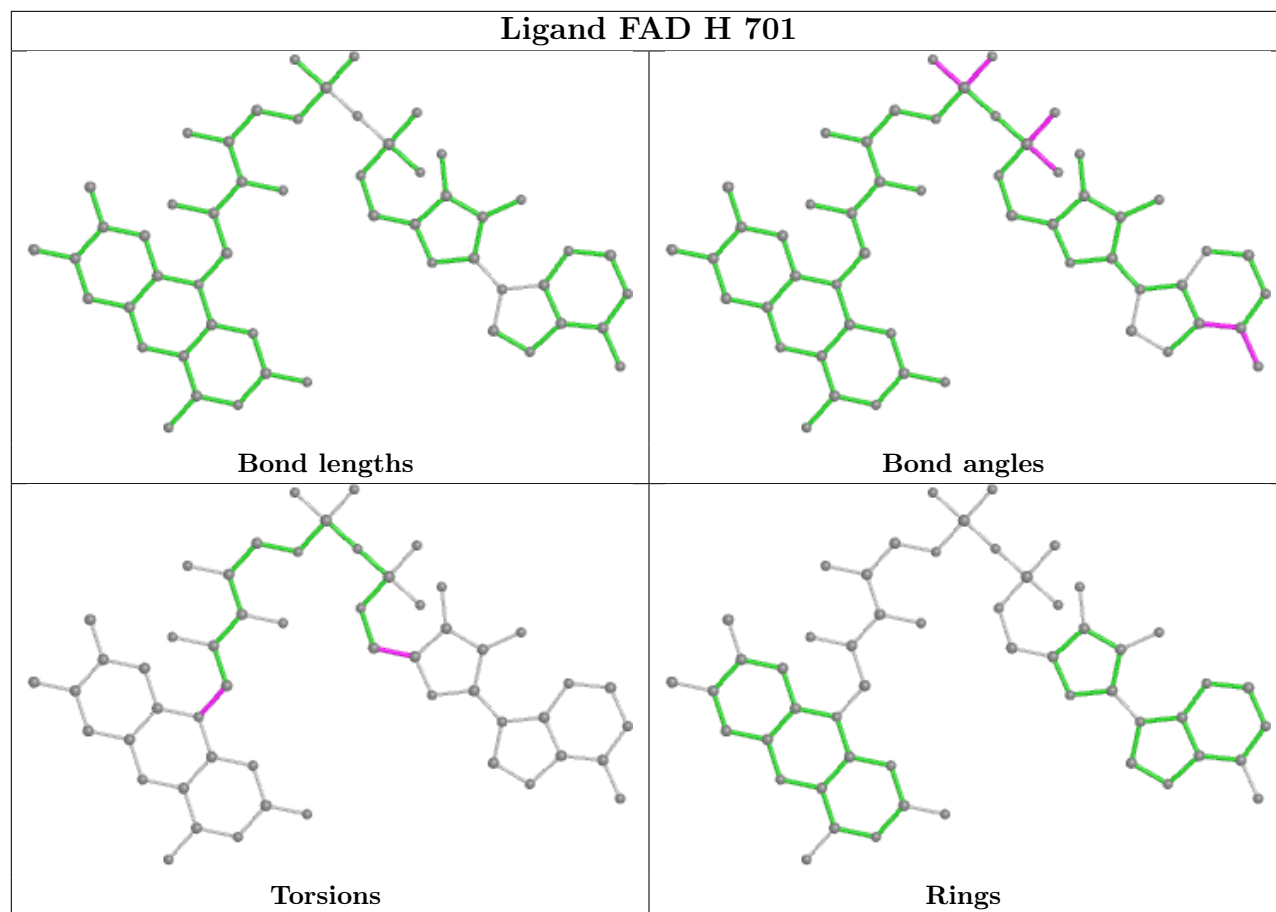


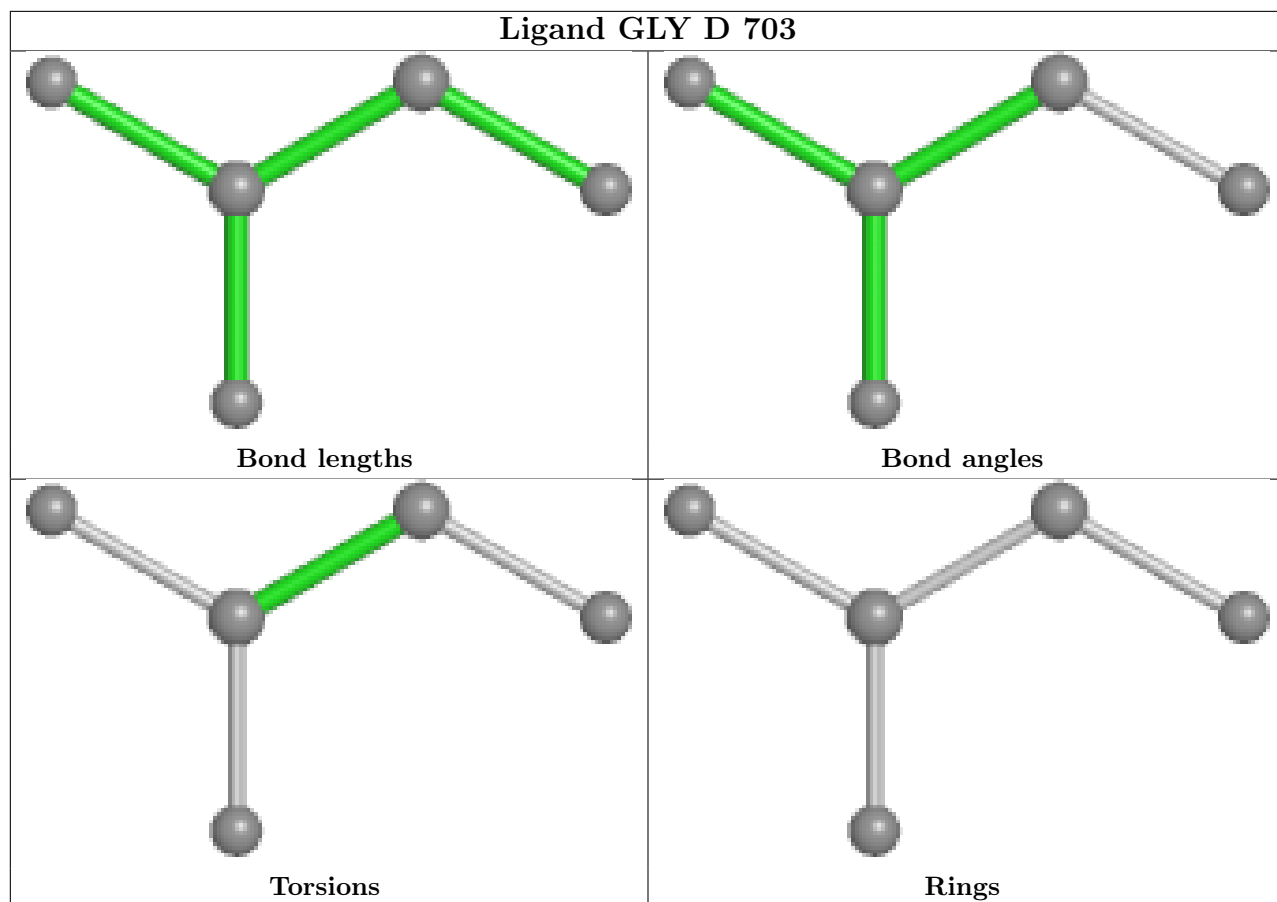


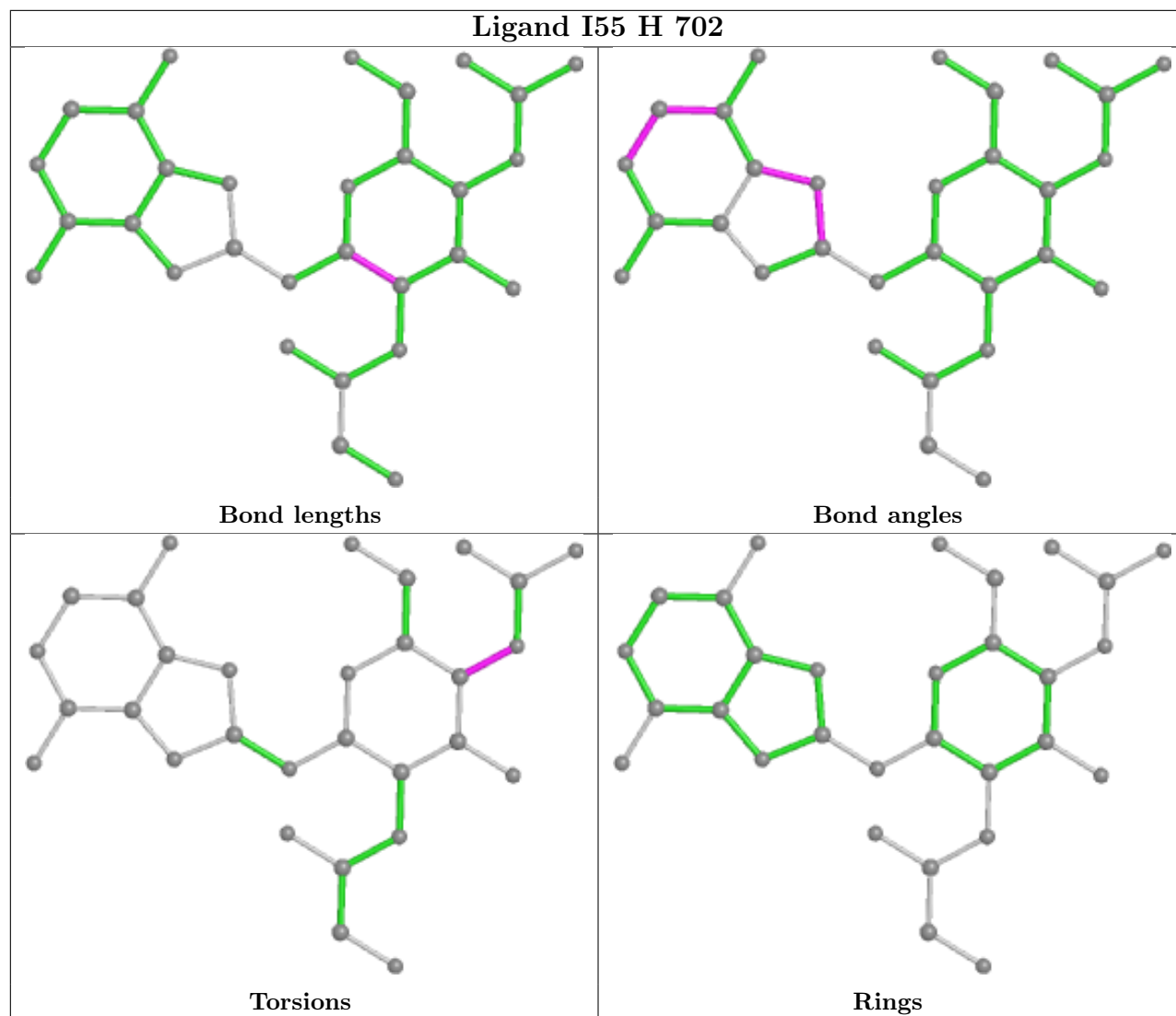


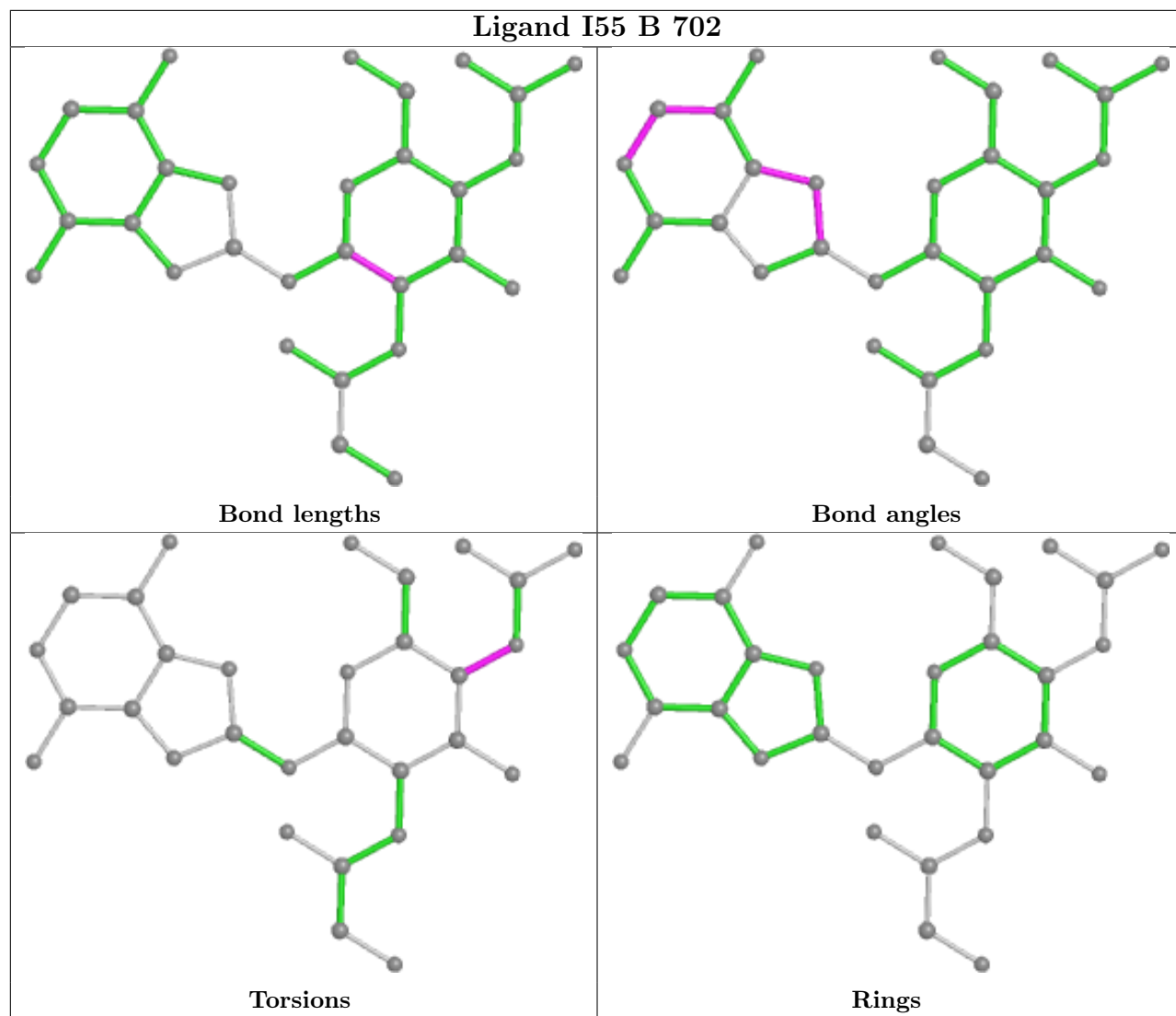




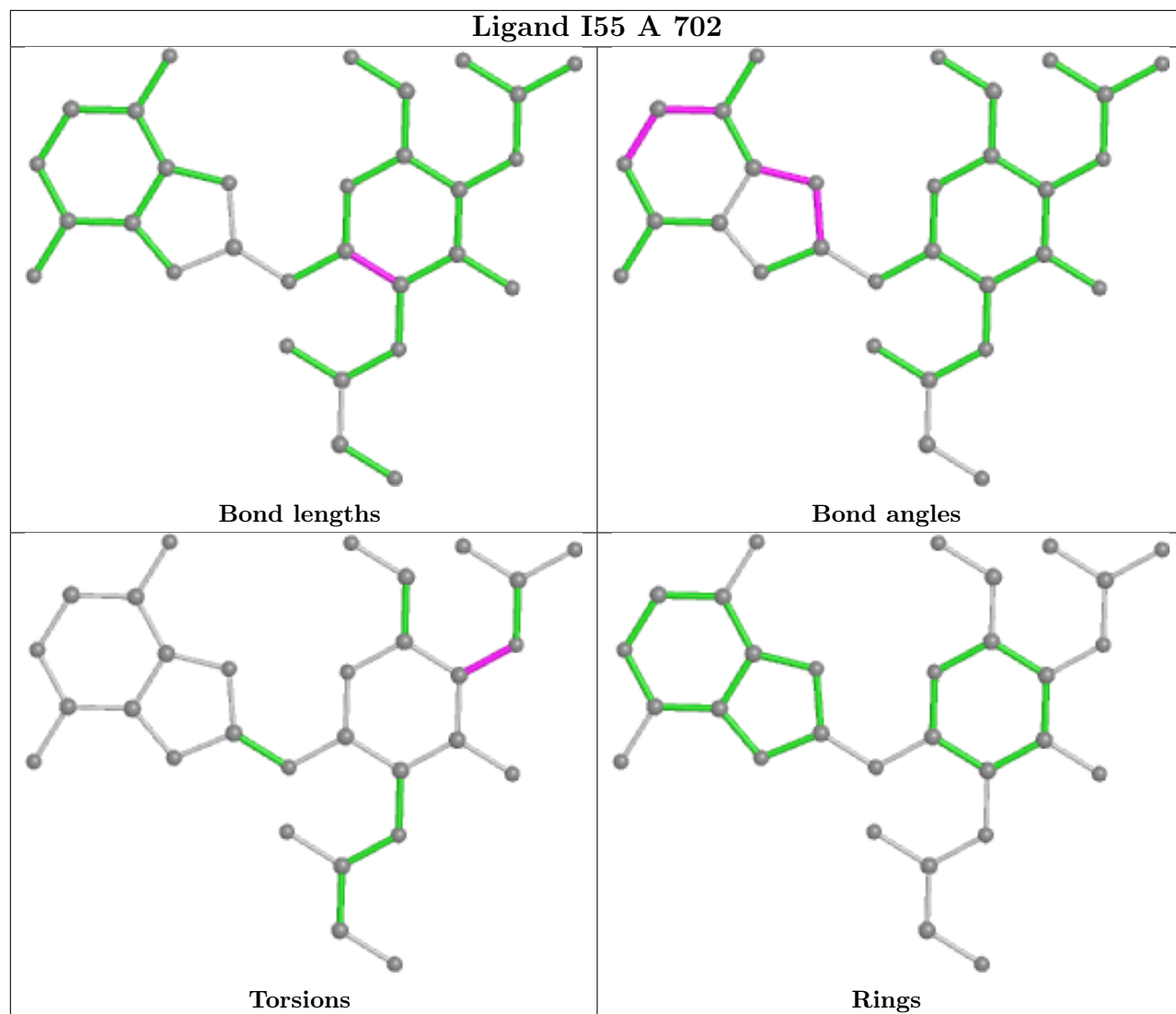


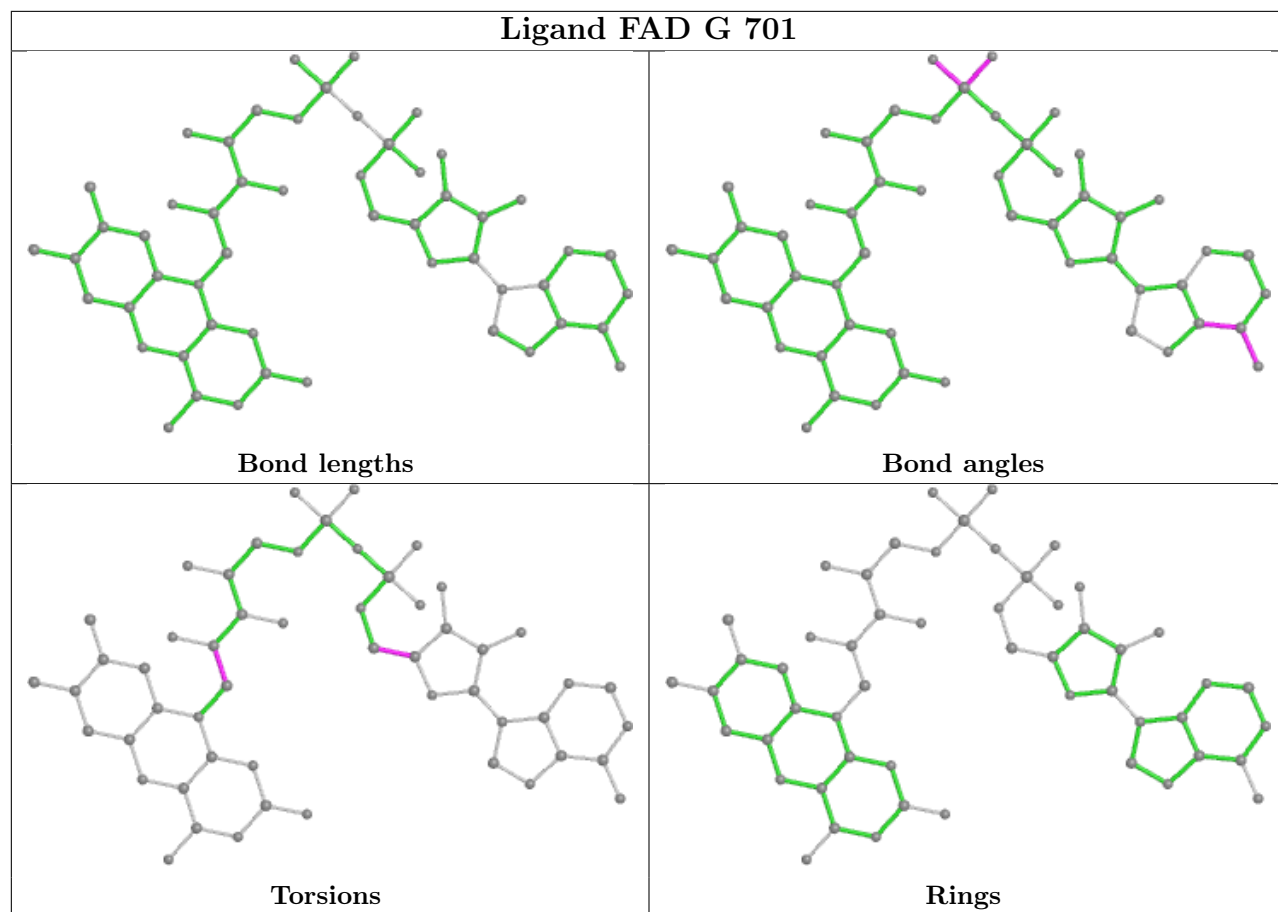


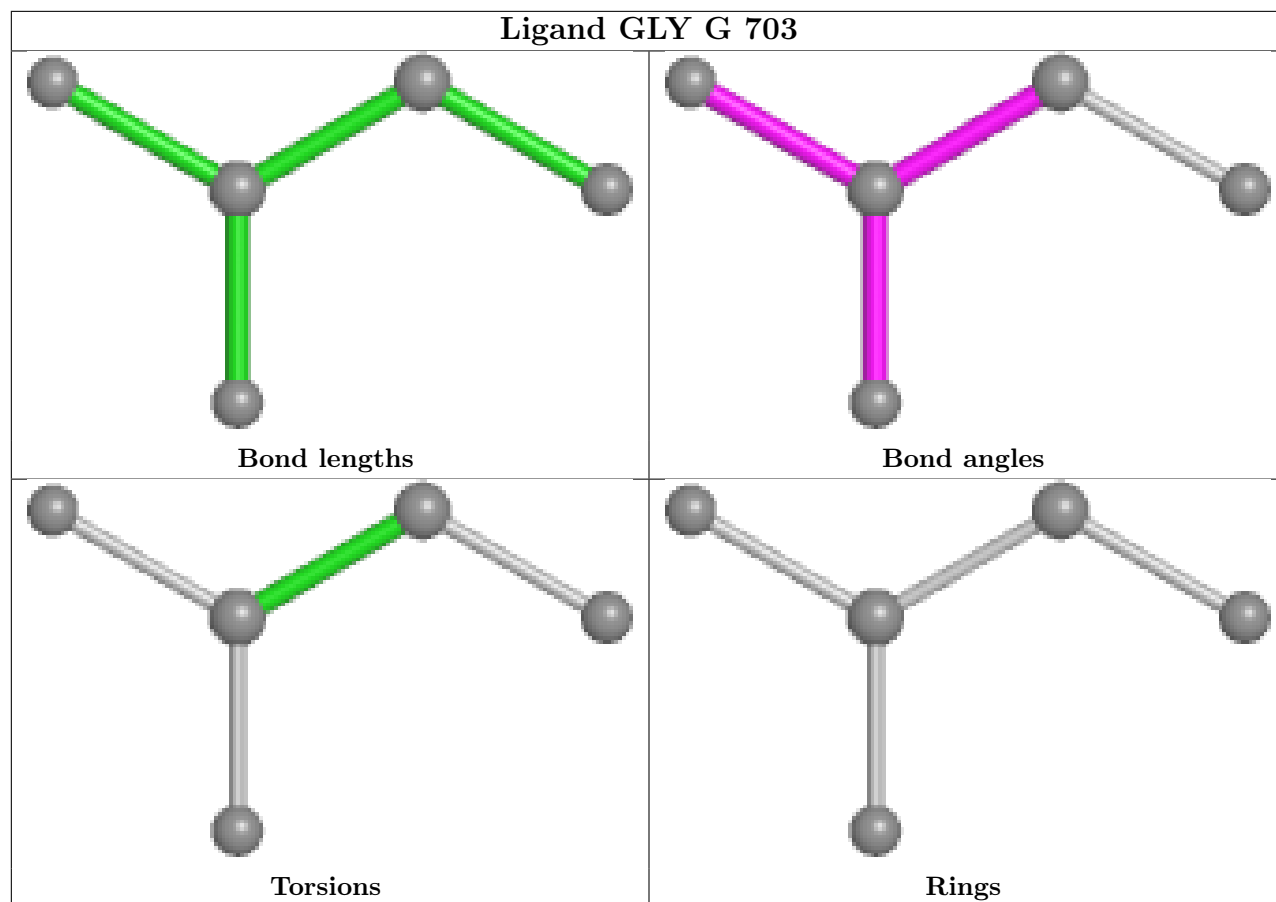


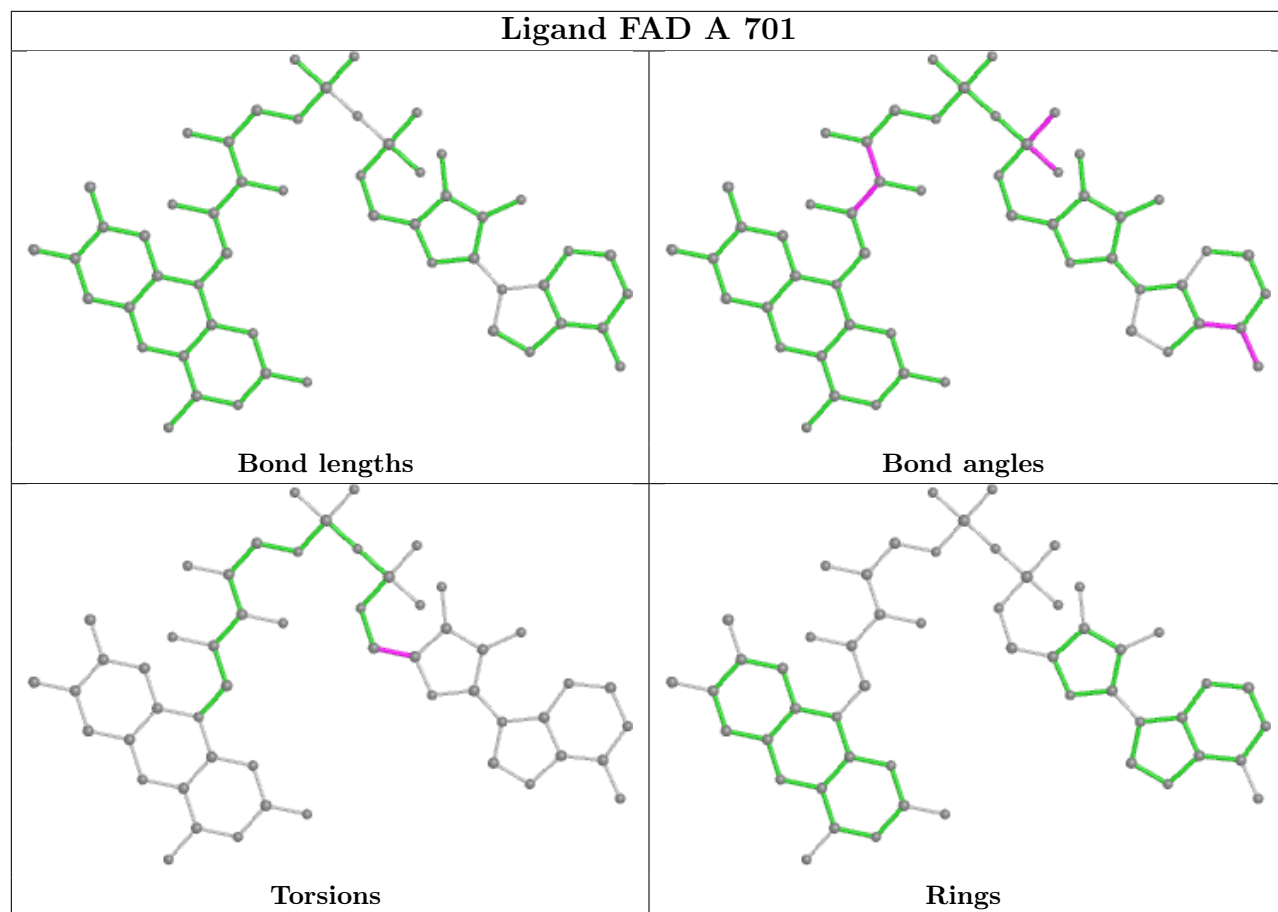


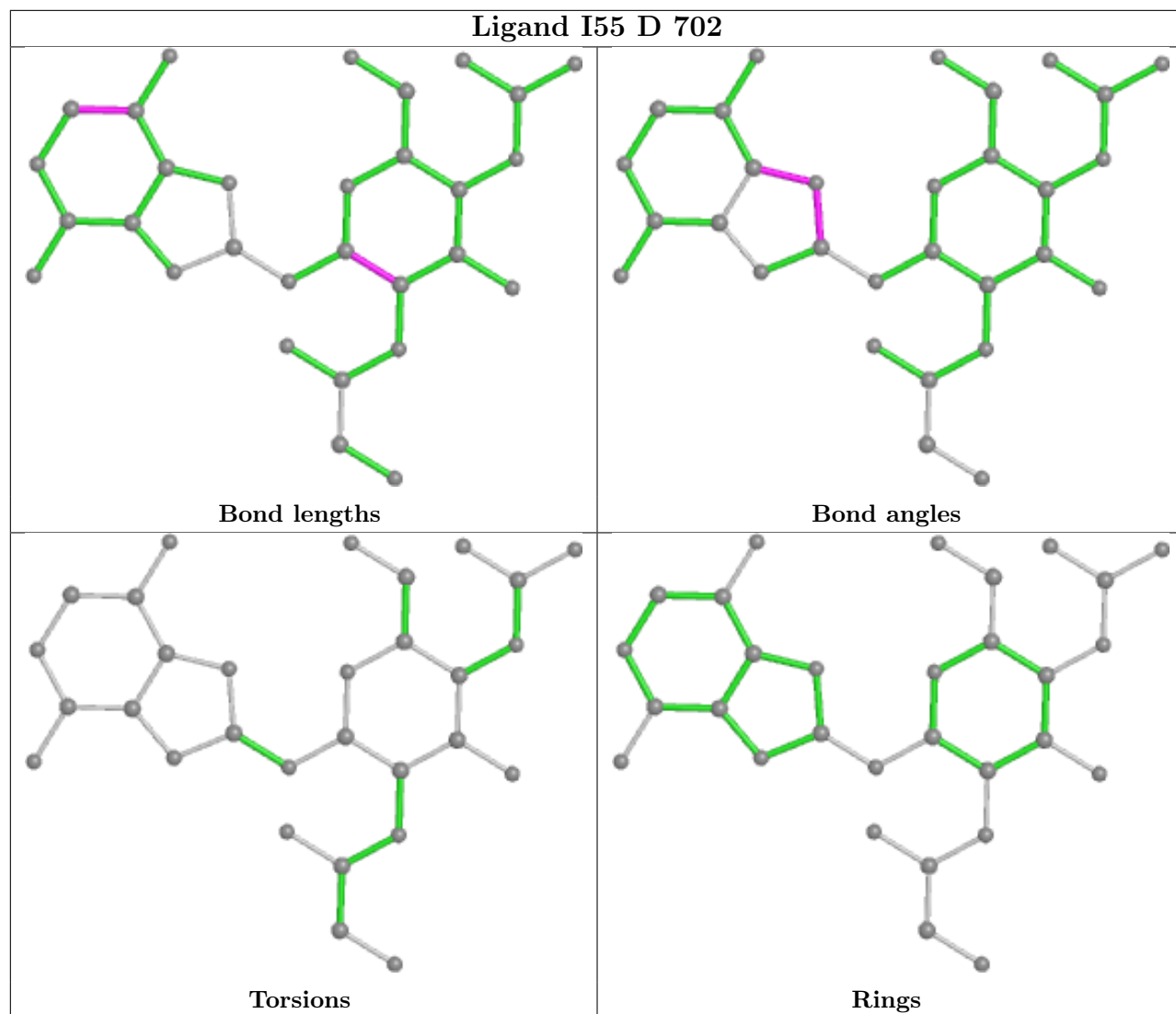


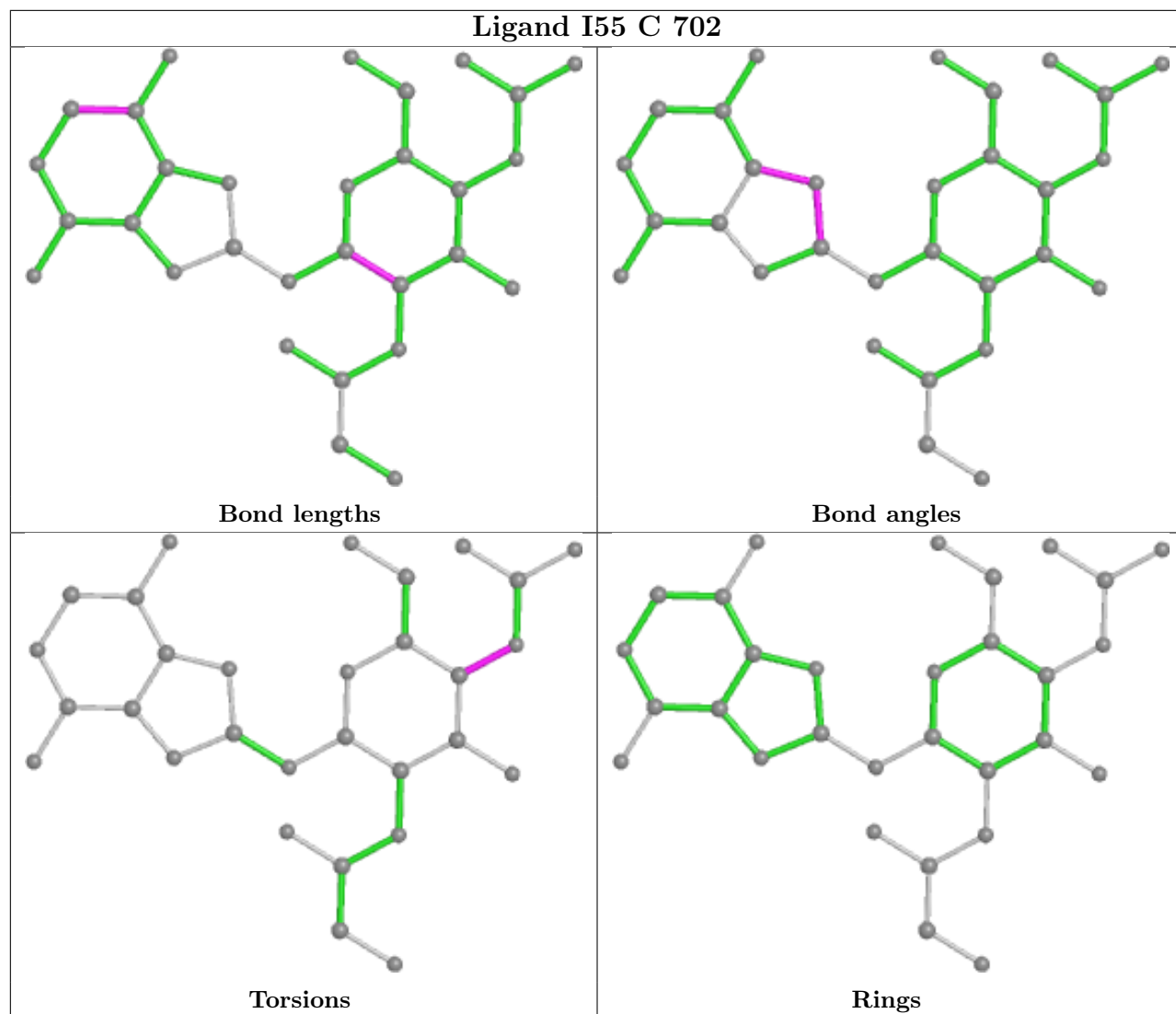


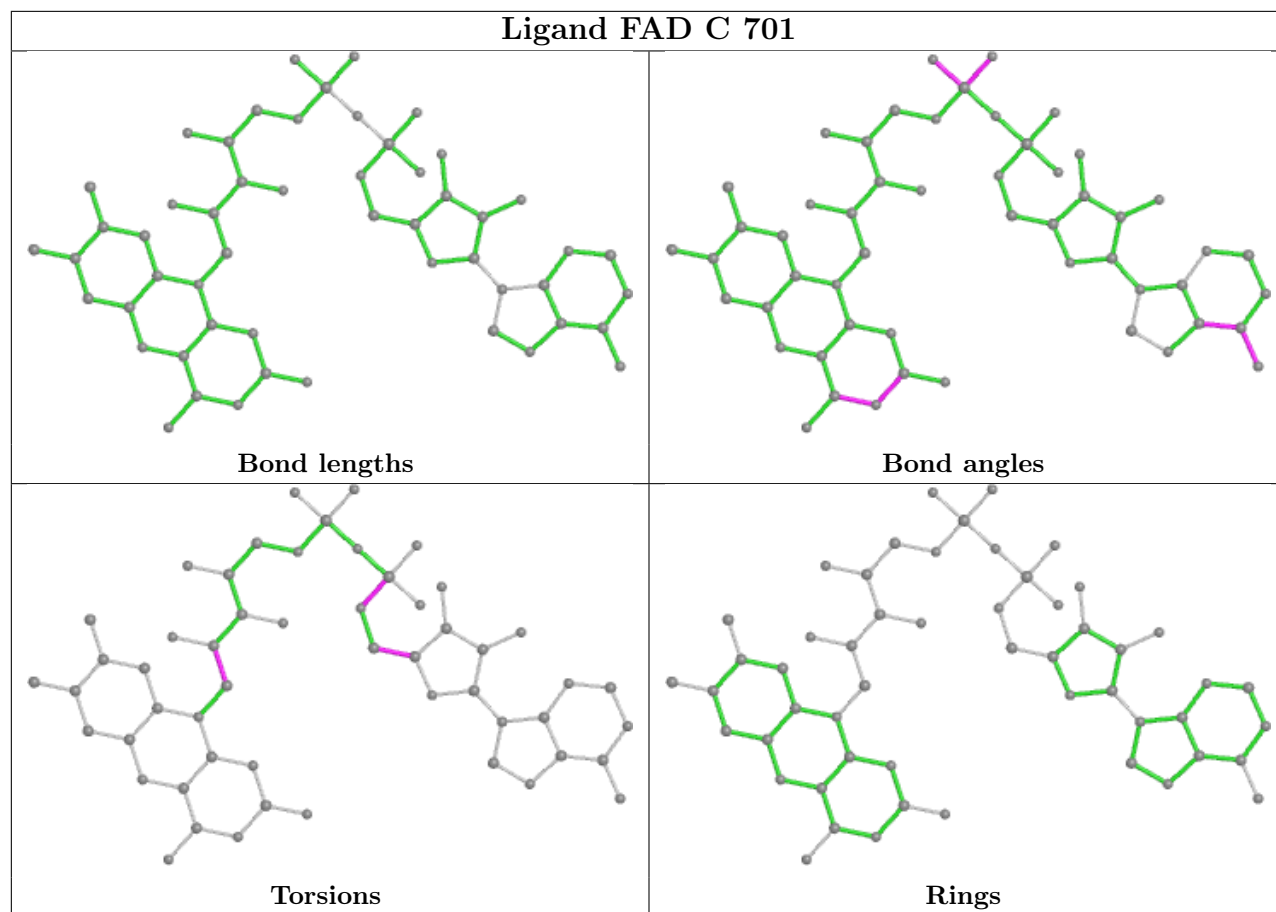












## 5.7 Other polymers [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	482/512 (94%)	0.24	3 (0%) 89 88	20, 30, 52, 76	0
1	B	482/512 (94%)	0.20	2 (0%) 92 91	19, 29, 50, 71	0
1	C	482/512 (94%)	0.37	10 (2%) 63 61	19, 32, 60, 82	0
1	D	480/512 (93%)	0.50	27 (5%) 24 23	21, 39, 77, 99	0
1	E	481/512 (93%)	0.21	3 (0%) 89 88	19, 30, 51, 79	0
1	F	482/512 (94%)	0.20	5 (1%) 82 81	19, 29, 49, 77	0
1	G	482/512 (94%)	0.37	11 (2%) 60 58	20, 32, 60, 84	0
1	H	479/512 (93%)	0.46	25 (5%) 27 26	22, 39, 75, 97	0
All	All	3850/4096 (93%)	0.32	86 (2%) 62 59	19, 32, 63, 99	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	45	ALA	3.8
1	D	202	ILE	3.8
1	H	219	PHE	3.6
1	D	36	VAL	3.6
1	D	220	LEU	3.5
1	D	393	GLY	3.4
1	E	395	ARG	3.3
1	G	242	GLY	3.3
1	H	217	GLY	3.2
1	D	236	LEU	3.2
1	H	202	ILE	3.2
1	H	394	LEU	3.1
1	D	491	HIS	3.1
1	H	34	PRO	3.1
1	H	211	GLY	3.0
1	C	236	LEU	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	208	ARG	3.0
1	D	40	LEU	2.9
1	C	479	LEU	2.9
1	D	34	PRO	2.9
1	G	243	LEU	2.9
1	G	238	ALA	2.8
1	D	37	ARG	2.8
1	G	48	TYR	2.8
1	C	303	LEU	2.7
1	D	394	LEU	2.7
1	G	10	GLN	2.7
1	C	101	ALA	2.6
1	G	439[A]	MET	2.6
1	F	491	HIS	2.6
1	H	203	ARG	2.6
1	H	35	ASP	2.6
1	D	353	GLY	2.6
1	D	479	LEU	2.6
1	H	225	VAL	2.5
1	C	48	TYR	2.5
1	D	80	LEU	2.5
1	H	224	HIS	2.5
1	D	392	ASP	2.5
1	H	222	ALA	2.5
1	D	222	ALA	2.5
1	D	211	GLY	2.5
1	C	220	LEU	2.4
1	H	36	VAL	2.4
1	H	352	ILE	2.4
1	C	355	THR	2.4
1	H	193	ARG	2.4
1	E	11	THR	2.4
1	D	206	HIS	2.4
1	H	464	LEU	2.4
1	D	13	VAL	2.4
1	H	480	ILE	2.4
1	A	11	THR	2.4
1	D	219	PHE	2.3
1	H	209	VAL	2.3
1	A	395	ARG	2.3
1	C	242	GLY	2.3
1	G	202	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	35	ASP	2.3
1	H	392	ASP	2.3
1	D	379	ARG	2.2
1	D	439	MET	2.2
1	G	239	ALA	2.2
1	H	33	ARG	2.2
1	H	361	TRP	2.2
1	G	208	ARG	2.2
1	H	379	ARG	2.2
1	H	363	LEU	2.1
1	C	238	ALA	2.1
1	A	363	LEU	2.1
1	D	224	HIS	2.1
1	D	204	ALA	2.1
1	B	491	HIS	2.1
1	F	206	HIS	2.1
1	B	464	LEU	2.1
1	D	33	ARG	2.1
1	E	208	ARG	2.1
1	H	218	ASP	2.1
1	G	235	ARG	2.1
1	C	243	LEU	2.0
1	F	35	ASP	2.0
1	F	395	ARG	2.0
1	D	210	GLU	2.0
1	D	238	ALA	2.0
1	H	70	ALA	2.0
1	F	212	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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,

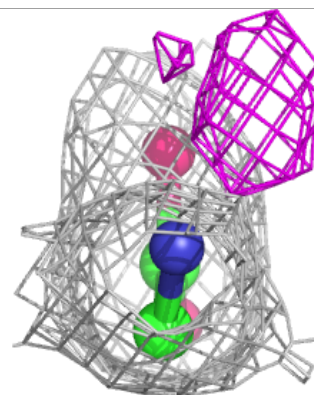
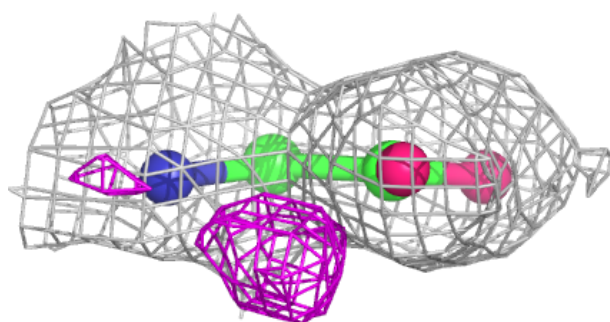
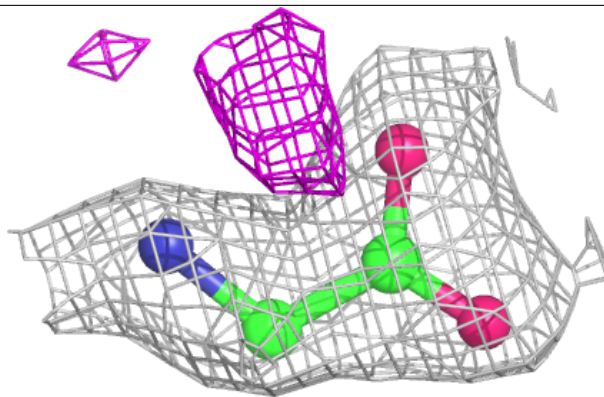
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GLY	C	703	5/5	0.86	0.18	42,46,47,47	0
2	FAD	G	701	53/53	0.87	0.17	34,46,56,58	0
2	FAD	C	701	53/53	0.88	0.17	34,47,55,56	0
3	I55	D	702	30/30	0.89	0.16	27,33,61,62	0
3	I55	A	702	30/30	0.90	0.18	20,30,56,58	0
3	I55	F	702	30/30	0.90	0.15	21,31,51,52	0
3	I55	C	702	30/30	0.90	0.16	23,33,60,61	0
3	I55	G	702	30/30	0.92	0.16	23,34,59,60	0
3	I55	E	702	30/30	0.93	0.14	20,29,55,56	0
3	I55	B	702	30/30	0.93	0.14	22,30,52,54	0
3	I55	H	702	30/30	0.94	0.15	26,34,62,63	0
2	FAD	H	701	53/53	0.94	0.12	31,37,52,54	0
4	GLY	E	703	5/5	0.94	0.12	25,26,30,30	0
2	FAD	A	701	53/53	0.95	0.11	21,25,27,28	0
4	GLY	D	703	5/5	0.95	0.11	33,33,37,37	0
2	FAD	D	701	53/53	0.95	0.12	32,38,56,58	0
4	GLY	A	703	5/5	0.96	0.11	24,25,29,29	0
4	GLY	B	703	5/5	0.96	0.10	27,27,29,31	0
2	FAD	E	701	53/53	0.96	0.12	20,24,28,29	0
2	FAD	F	701	53/53	0.96	0.11	17,22,25,26	0
2	FAD	B	701	53/53	0.96	0.11	19,22,25,26	0
4	GLY	G	703	5/5	0.96	0.22	43,45,49,49	0
4	GLY	F	703	5/5	0.97	0.12	27,27,31,32	0
4	GLY	H	703	5/5	0.97	0.12	35,35,38,40	0

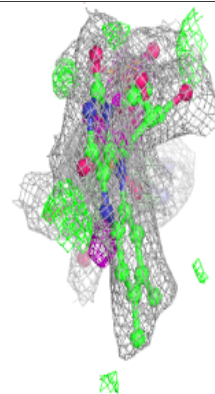
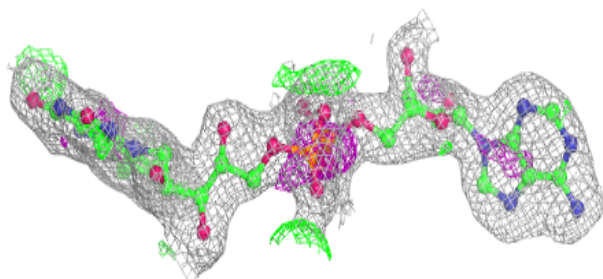
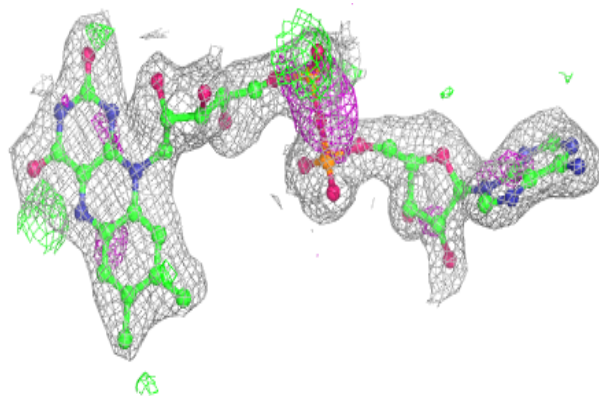
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GLY 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)

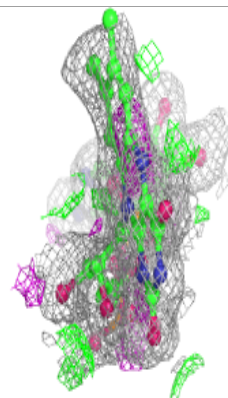
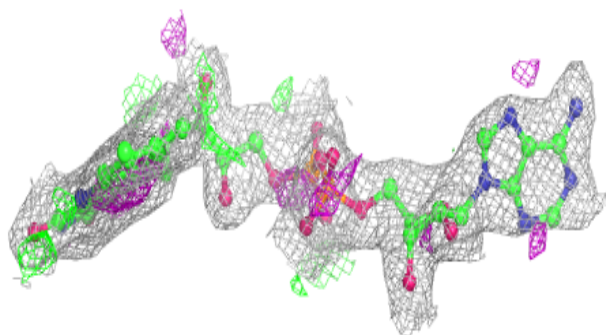
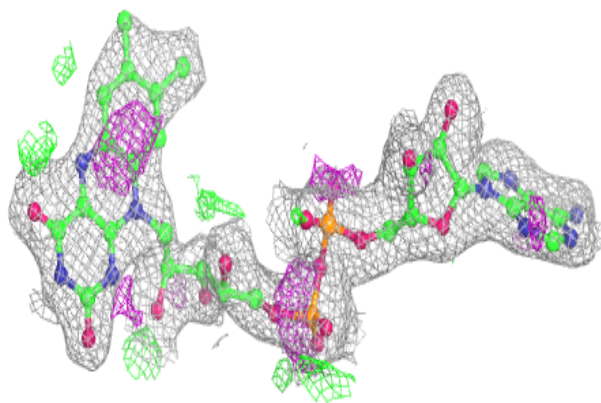
**Electron density around FAD G 701:**

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



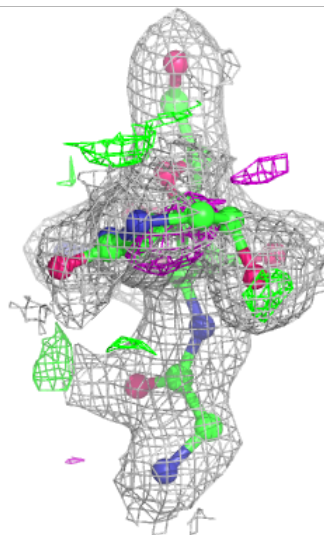
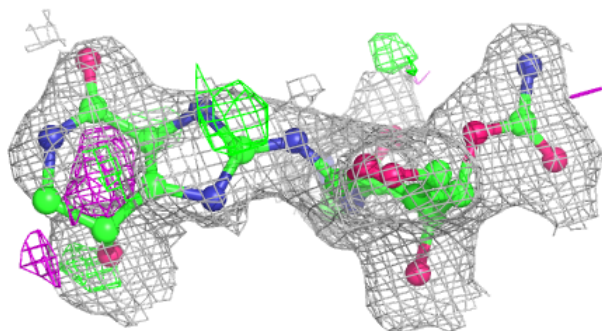
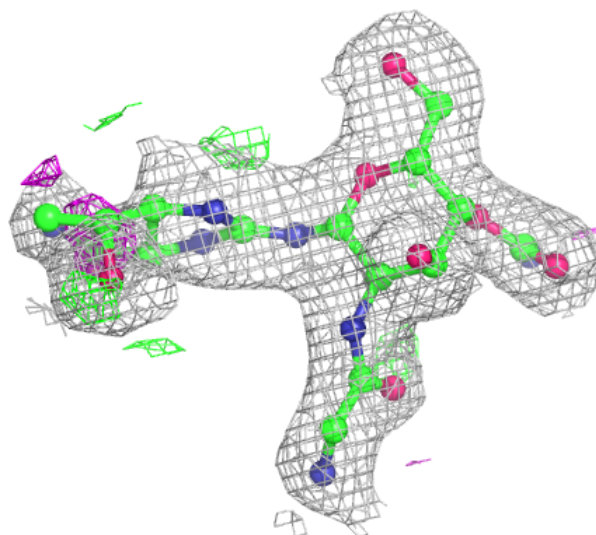
**Electron density around FAD C 701:**

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



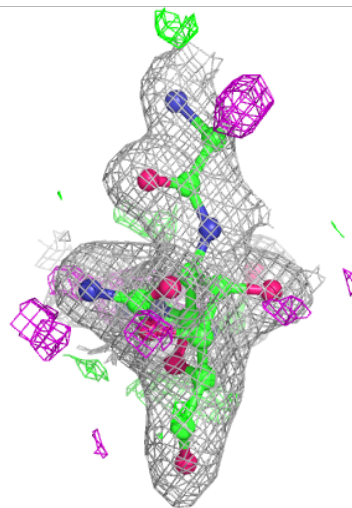
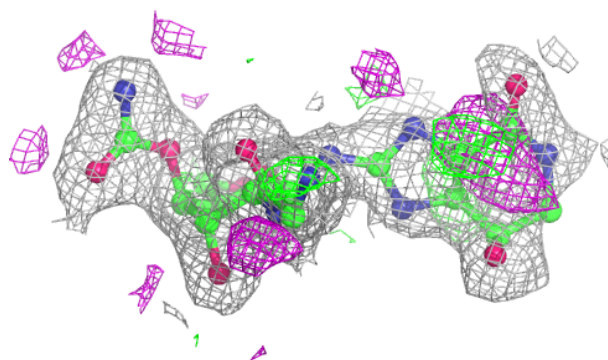
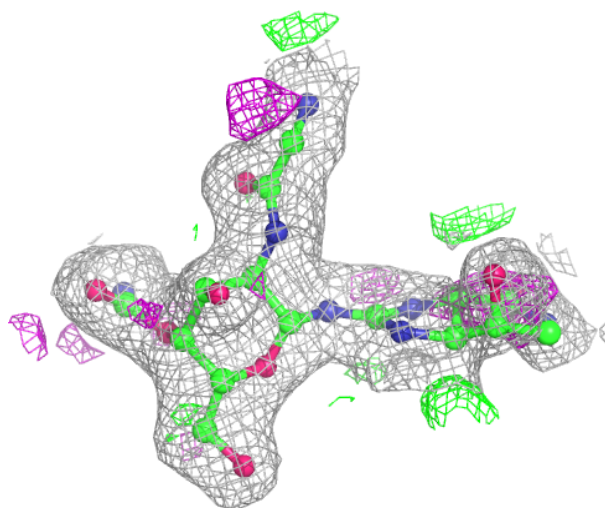
**Electron density around I55 D 702:**

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



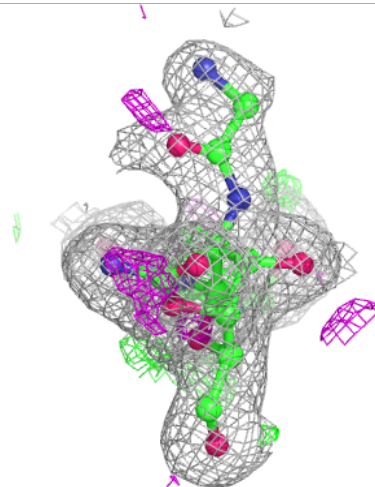
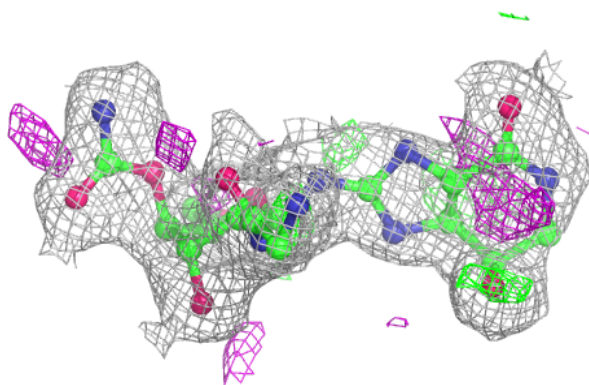
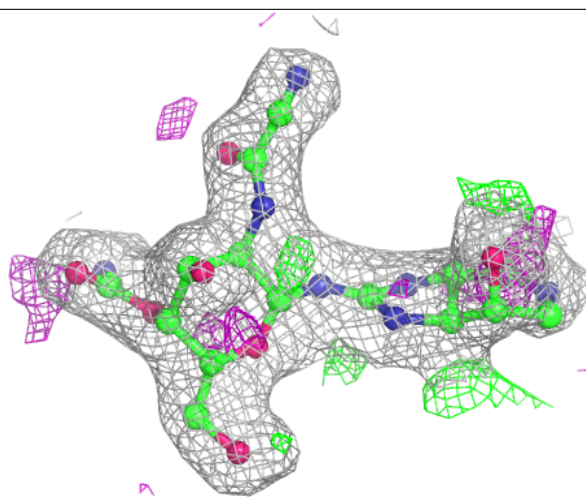
**Electron density around I55 A 702:**

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



**Electron density around I55 F 702:**

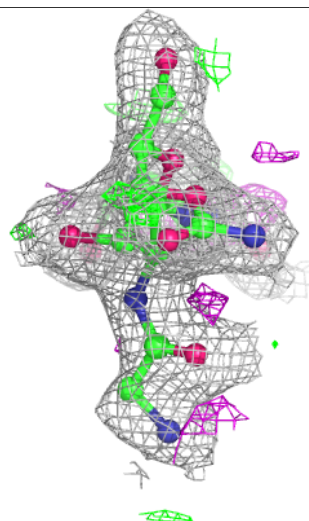
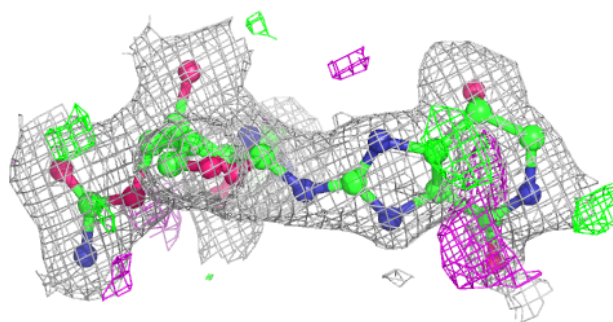
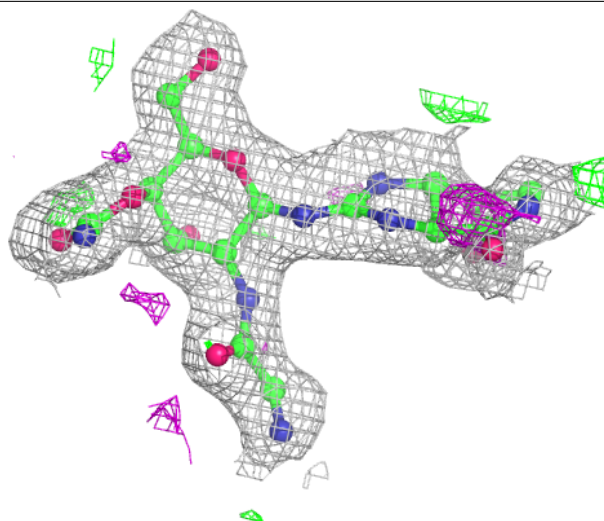
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





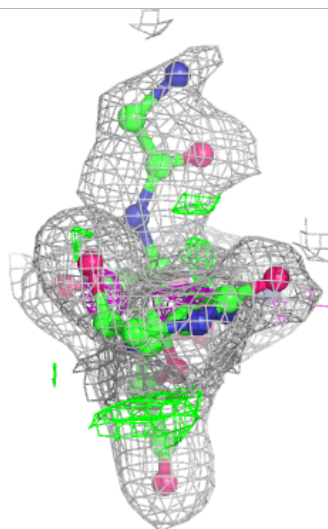
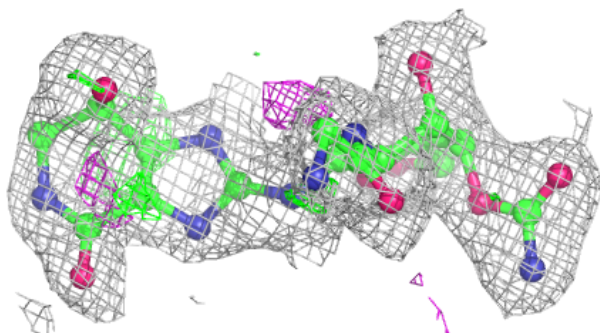
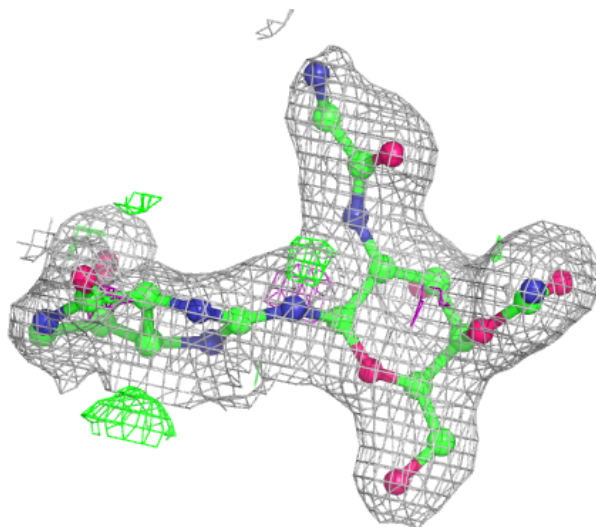
**Electron density around I55 C 702:**

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



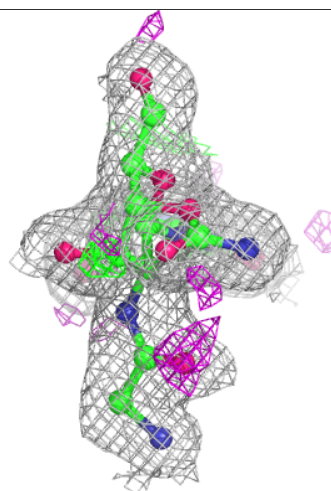
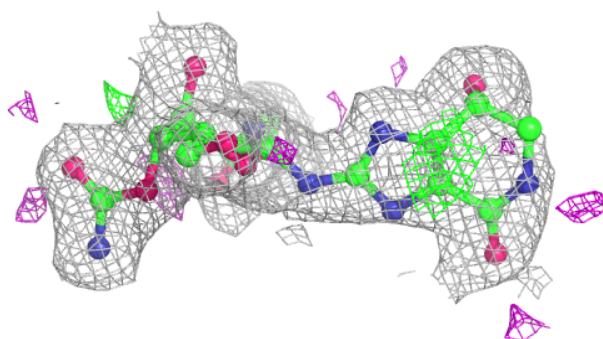
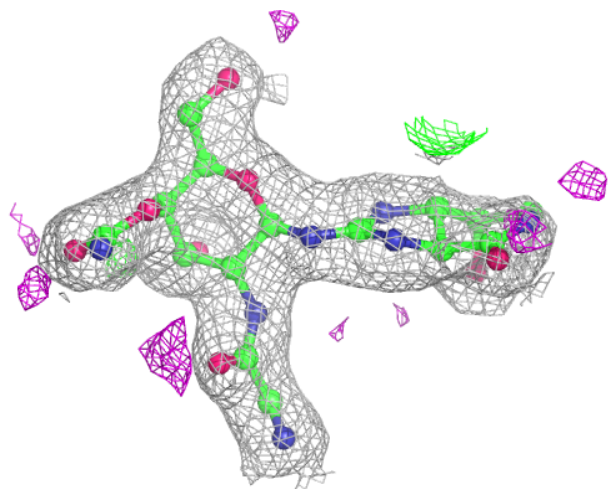
**Electron density around I55 G 702:**

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



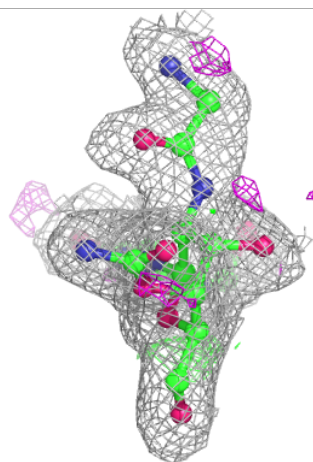
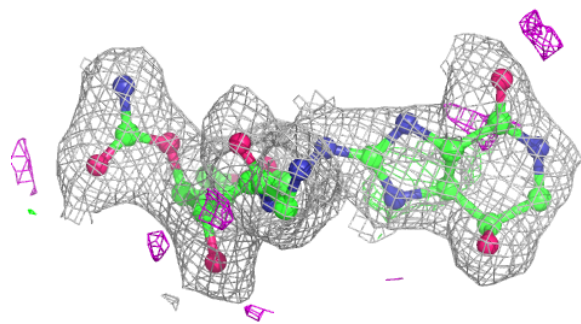
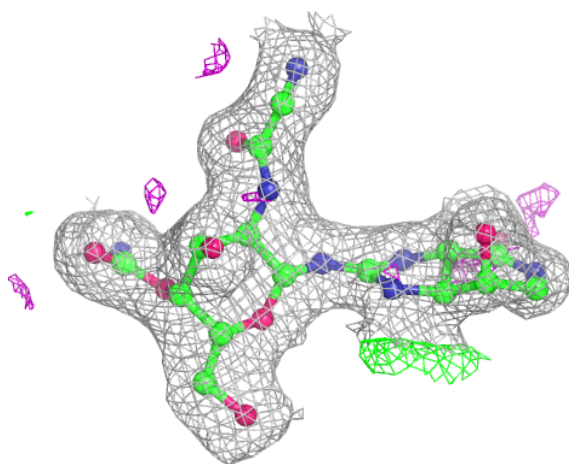
**Electron density around I55 E 702:**

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



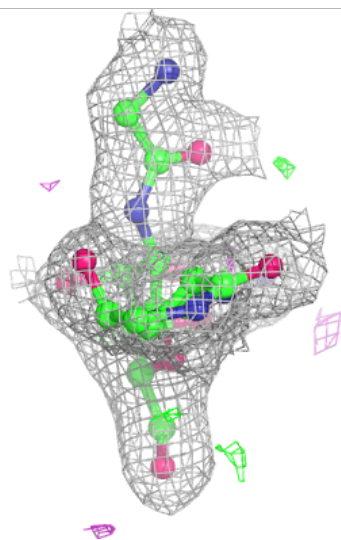
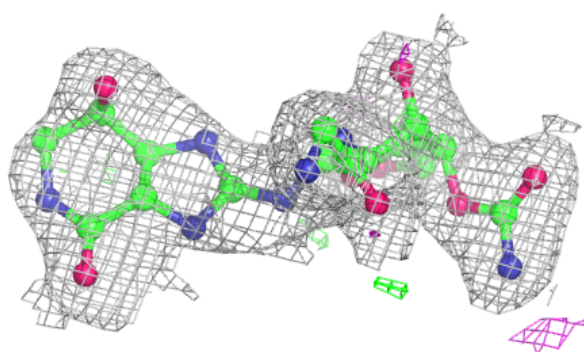
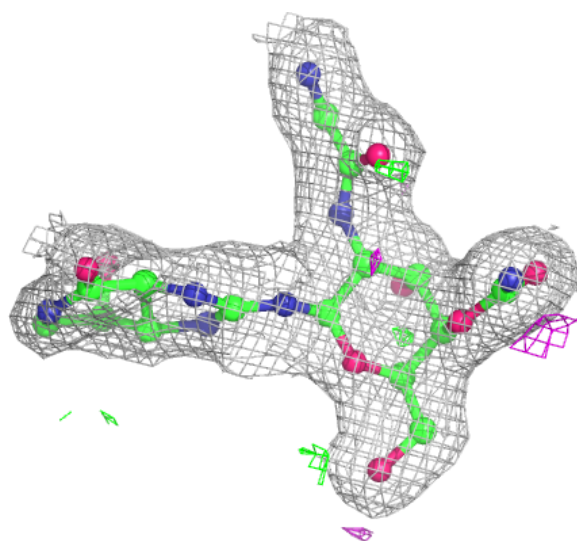
**Electron density around I55 B 702:**

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



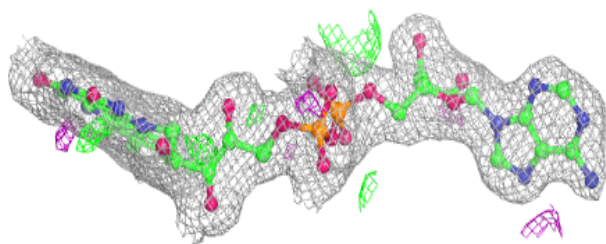
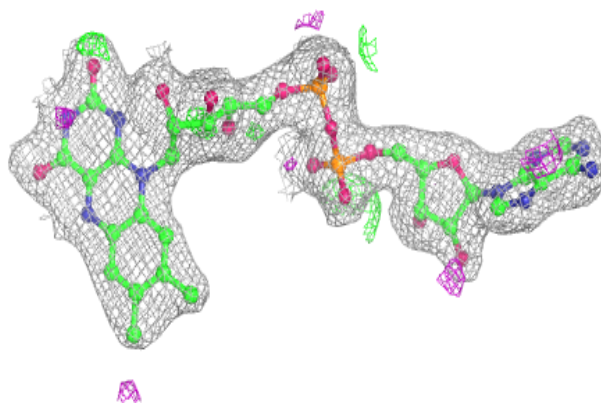
**Electron density around I55 H 702:**

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

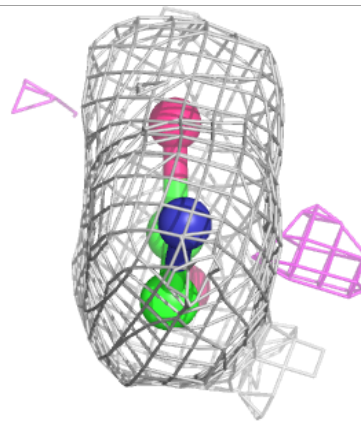
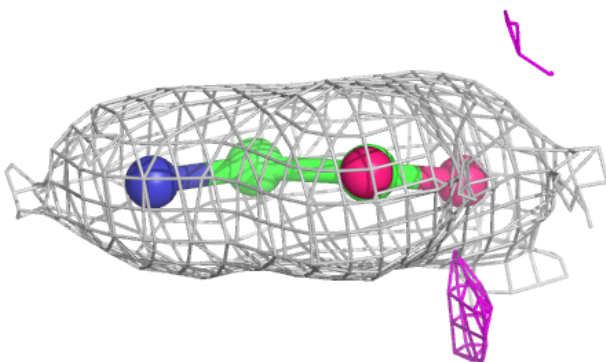
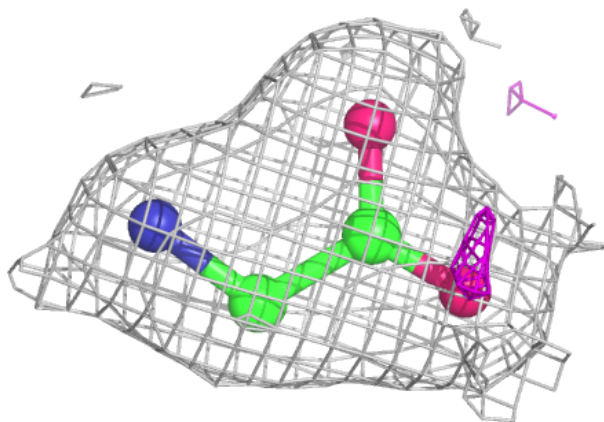


**Electron density around FAD H 701:**

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

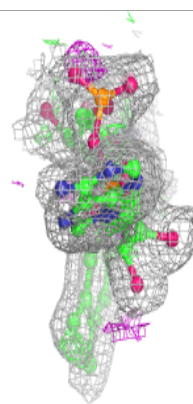
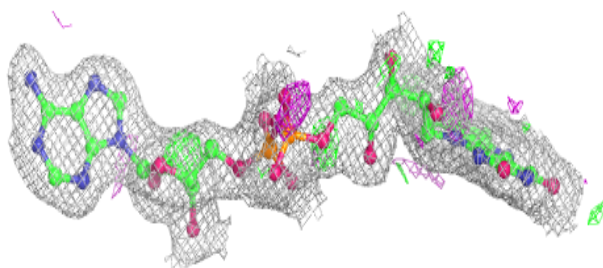
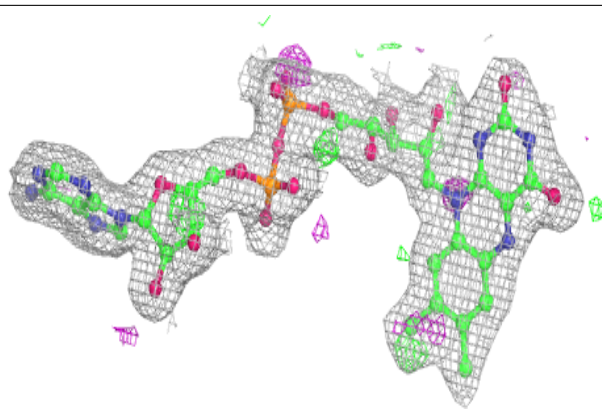
**Electron density around GLY E 703:**

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

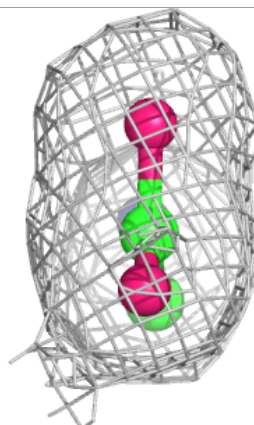
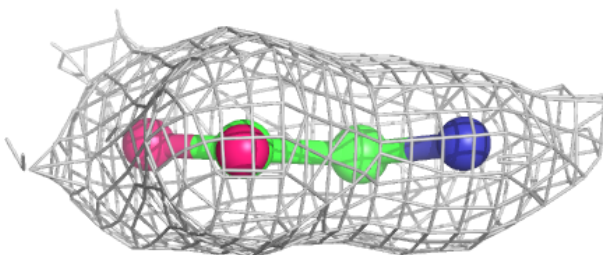
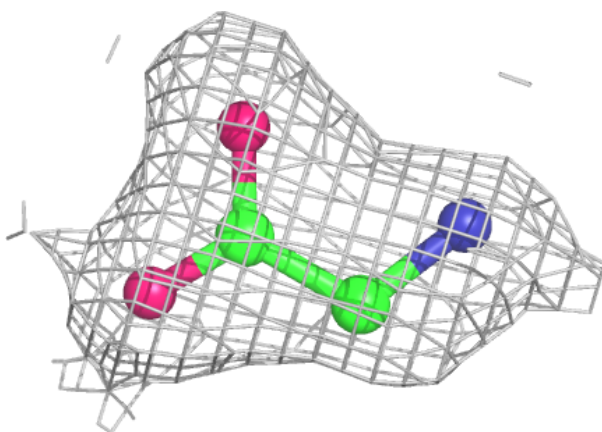


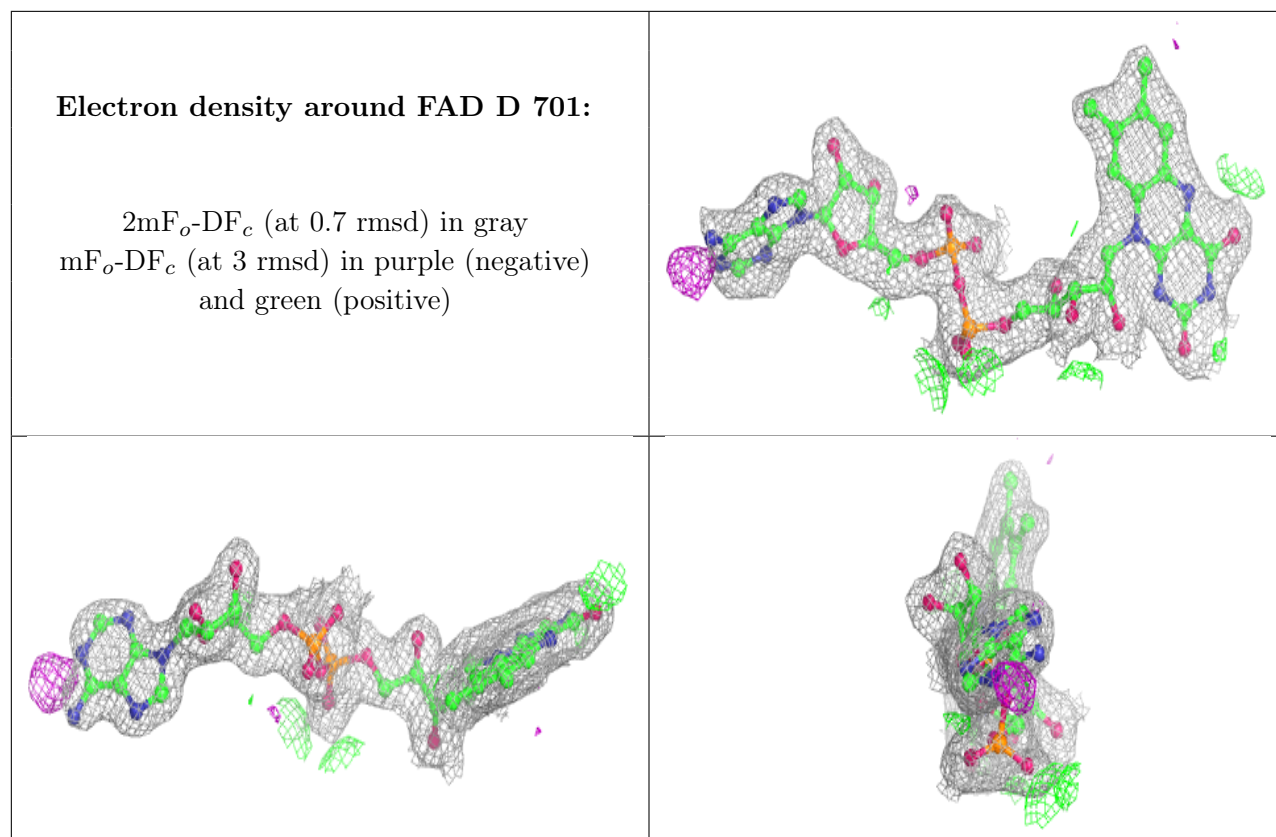
**Electron density around FAD A 701:**

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

**Electron density around GLY 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)

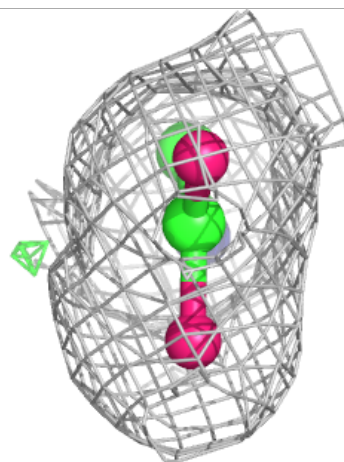
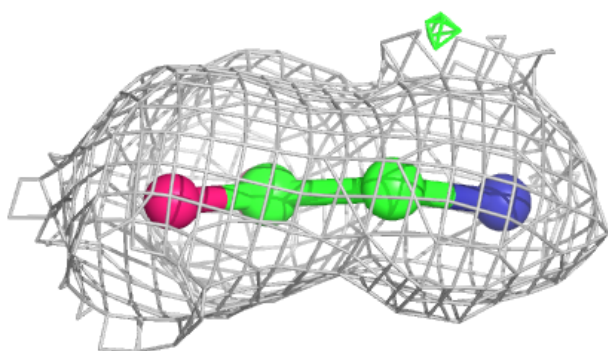
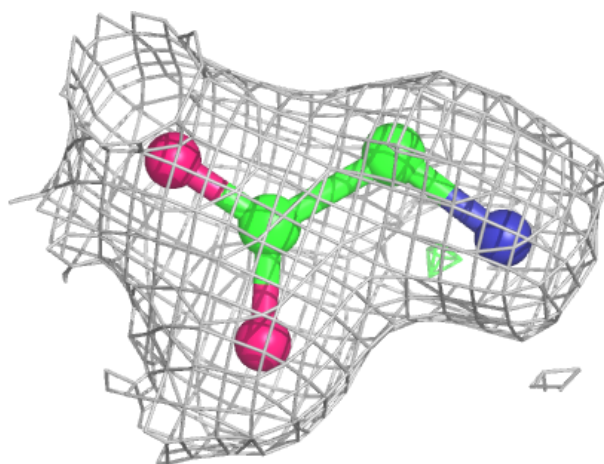






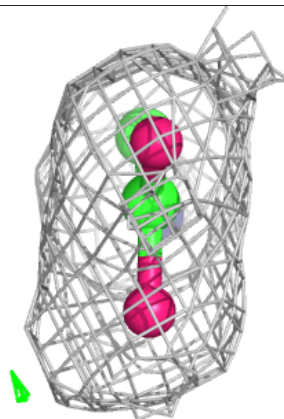
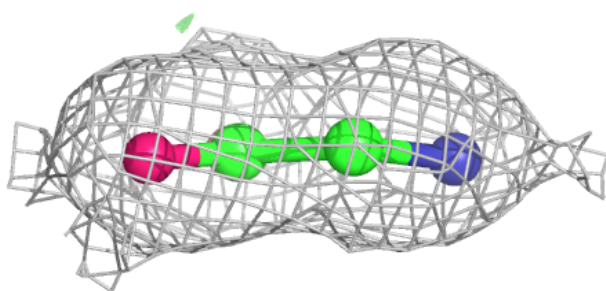
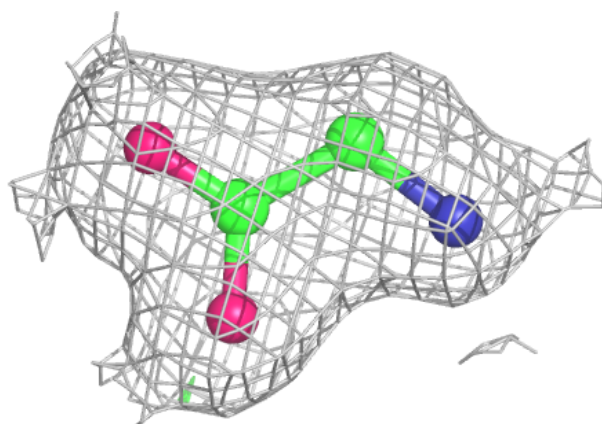
**Electron density around GLY A 703:**

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

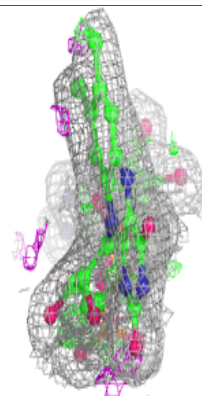
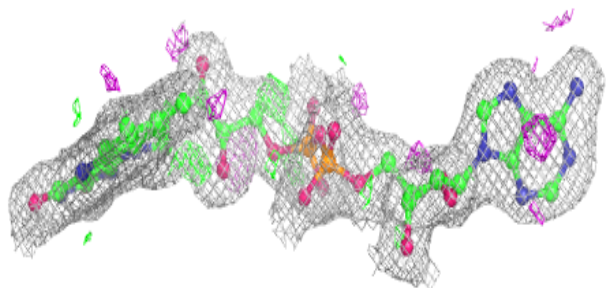
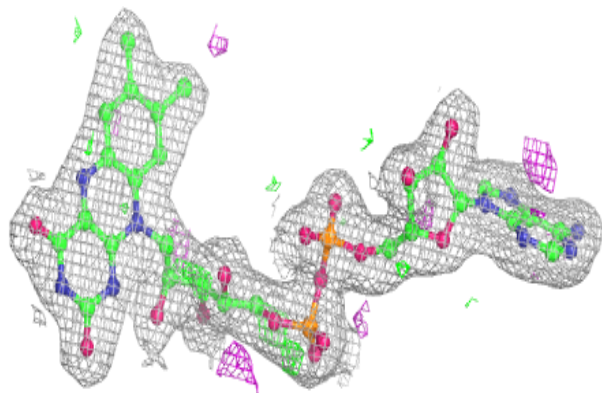


**Electron density around GLY B 703:**

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

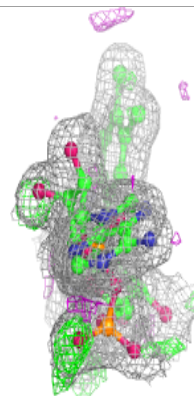
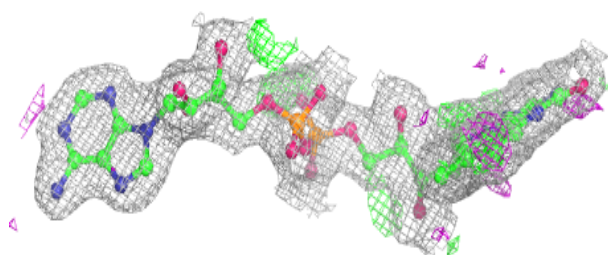
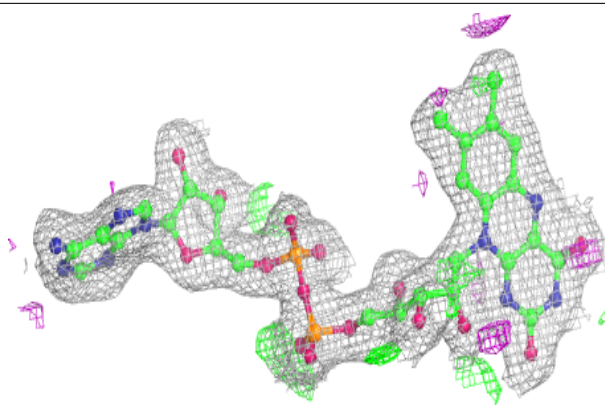
**Electron density around FAD E 701:**

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

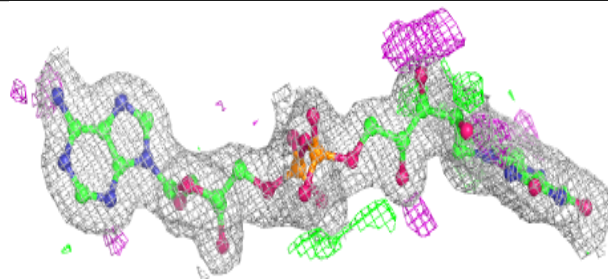
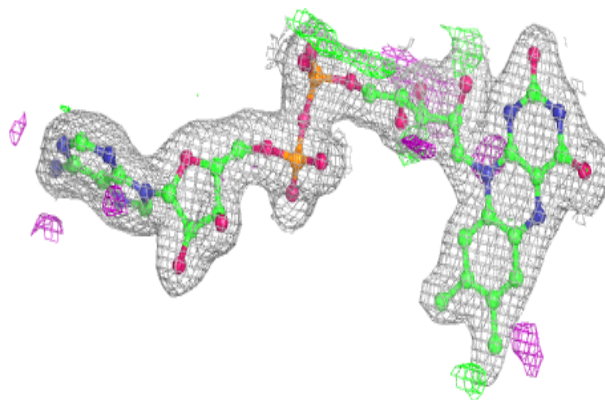


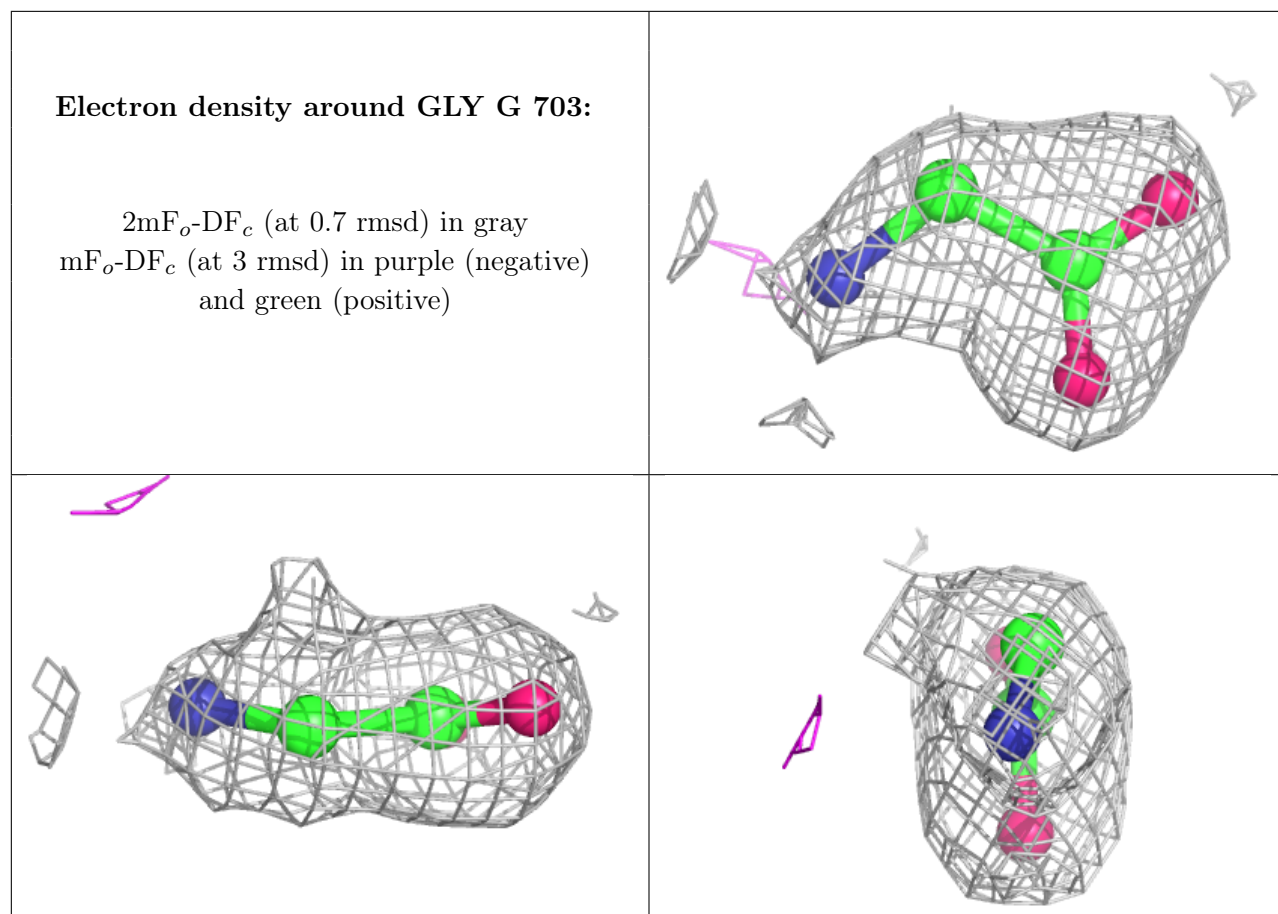
**Electron density around FAD F 701:**

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

**Electron density around FAD B 701:**

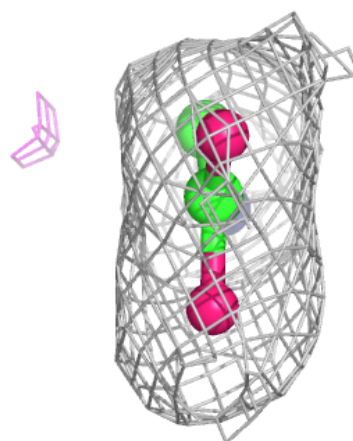
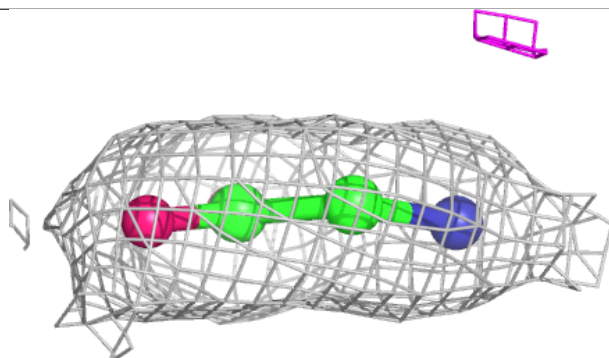
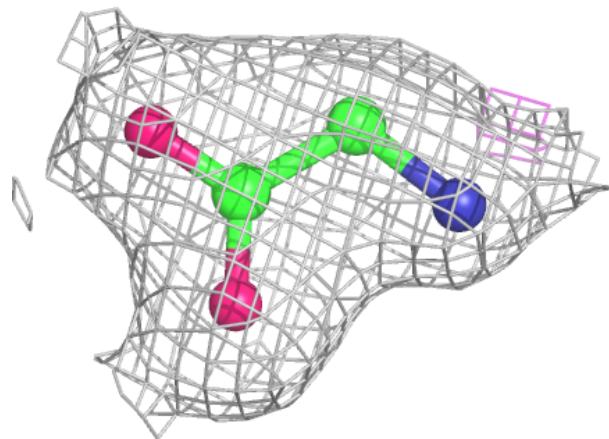
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

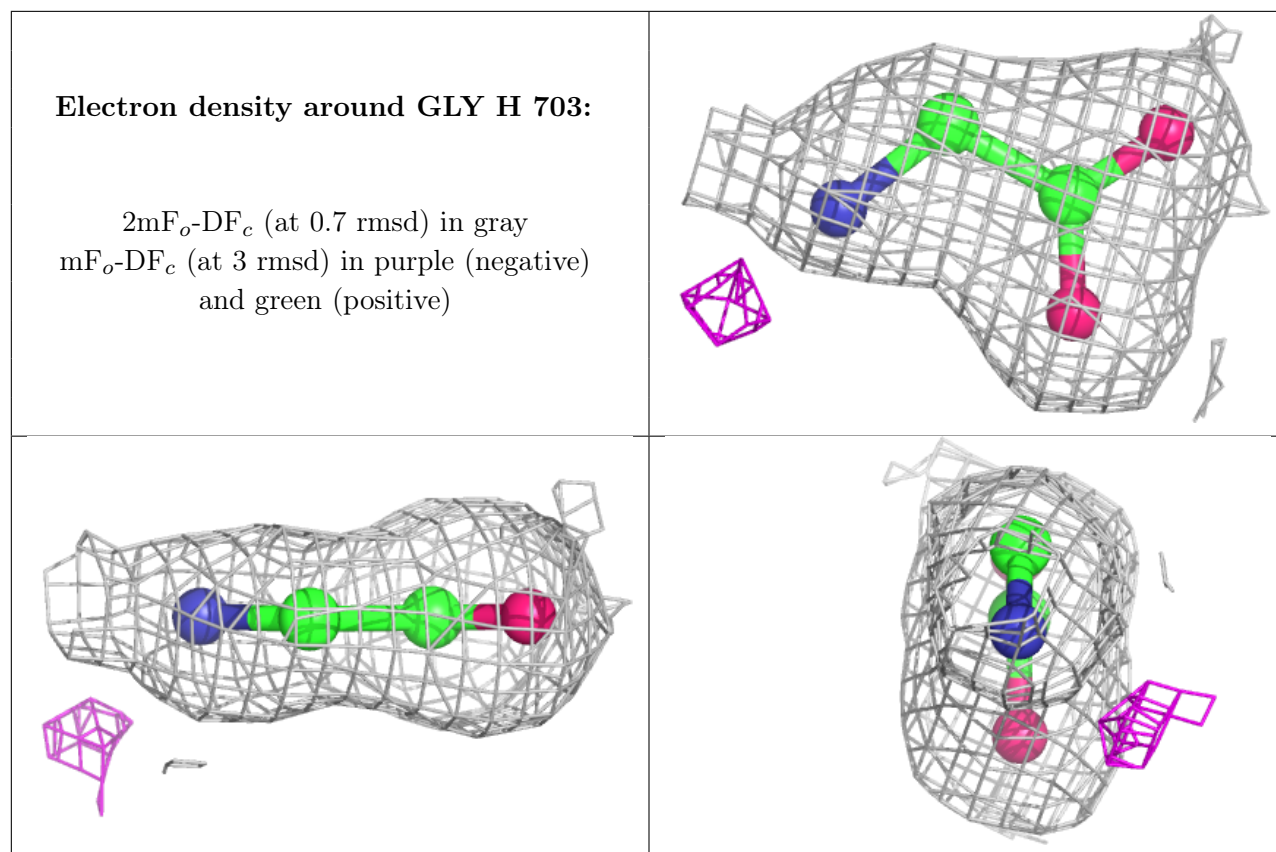




**Electron density around GLY F 703:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.