Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 01:39 AM JST

PDB ID	:	7XXM
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:

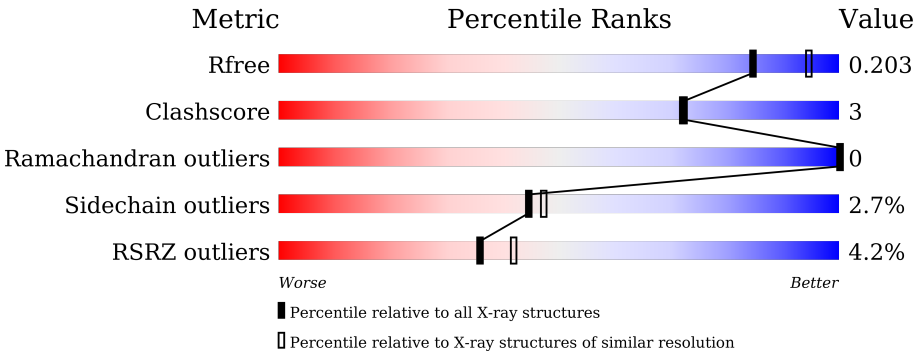
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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 <=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	88% 5% • 6%
1	B	512	87% 6% • 6%
1	C	512	3% 83% 8% 8%
1	D	512	11% 82% 9% • 9%
1	E	512	% 88% 6% 6%
1	F	512	% 88% 6% • 6%

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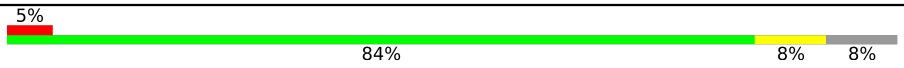
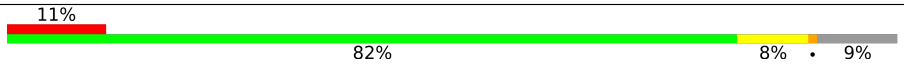
Mol	Chain	Length	Quality of chain
1	G	512	
1	H	512	

2 Entry composition (i)

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
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
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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Chain	Residue	Modelled	Actual	Comment	Reference
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
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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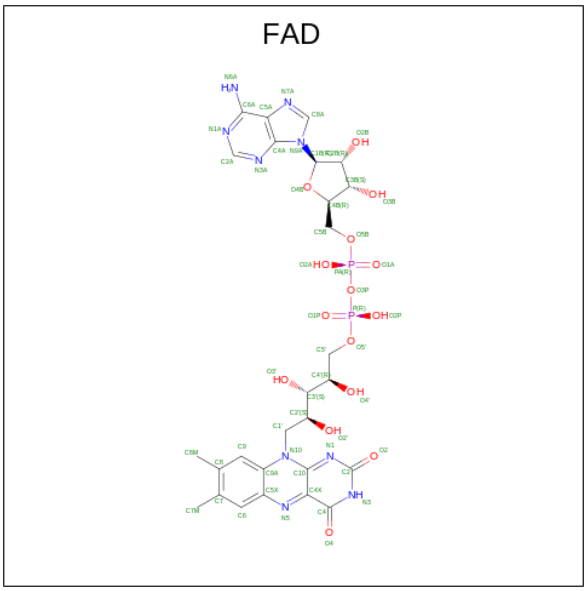
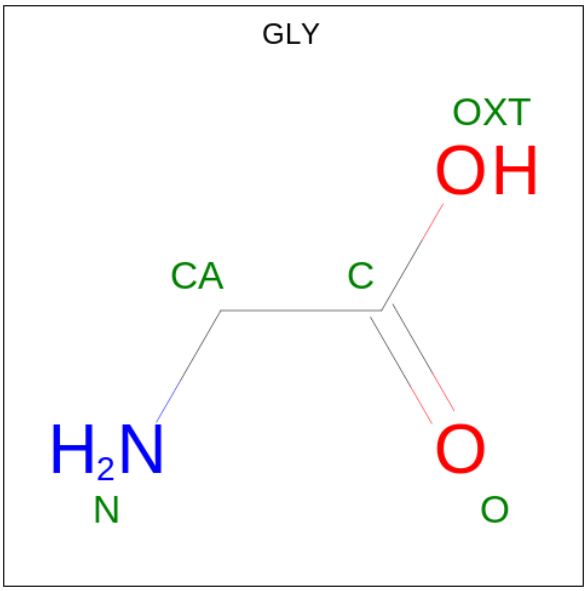
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	LEU	-	expression tag	UNP A0A125SZC1
G	-6	VAL	-	expression tag	UNP A0A125SZC1
G	-5	PRO	-	expression tag	UNP A0A125SZC1
G	-4	ARG	-	expression tag	UNP A0A125SZC1
G	-3	GLY	-	expression tag	UNP A0A125SZC1
G	-2	SER	-	expression tag	UNP A0A125SZC1
G	-1	HIS	-	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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



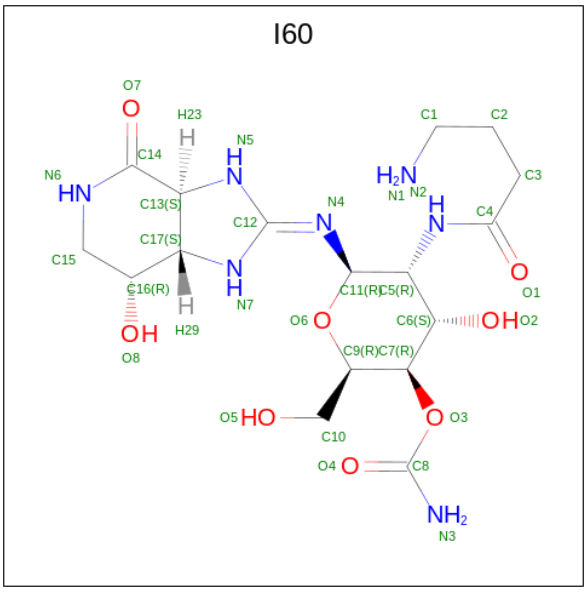
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	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 GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$) (labeled as "Ligand of Interest" by depositor).



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

- 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 (three-letter code: I60) (formula: $C_{17}H_{29}N_7O_8$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

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

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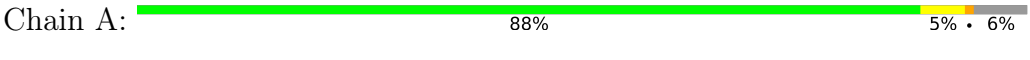
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	330	Total O 330 330	0	0
5	F	352	Total O 352 352	0	0
5	G	310	Total O 310 310	0	0
5	H	193	Total O 193 193	0	0

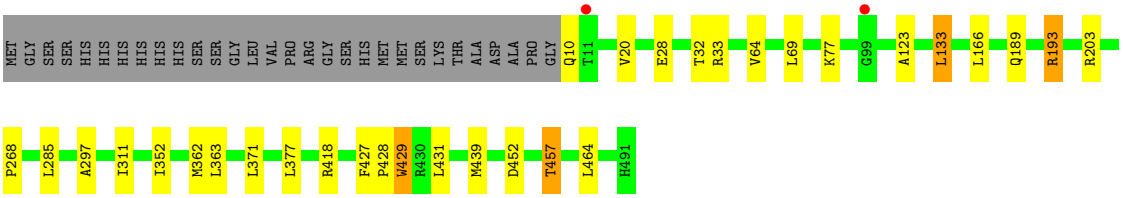
3 Residue-property plots (i)

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

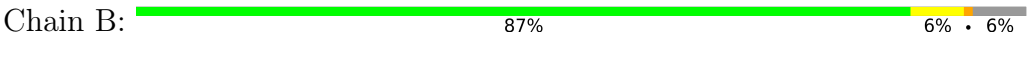
Chain A:

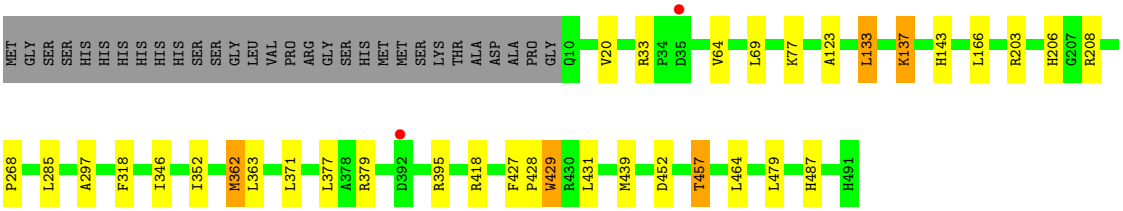




• Molecule 1: N-formimidoyl fortimicin A synthase

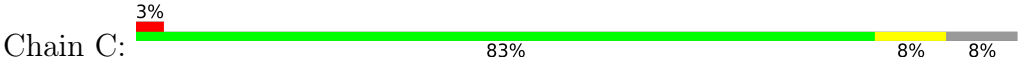
Chain B:

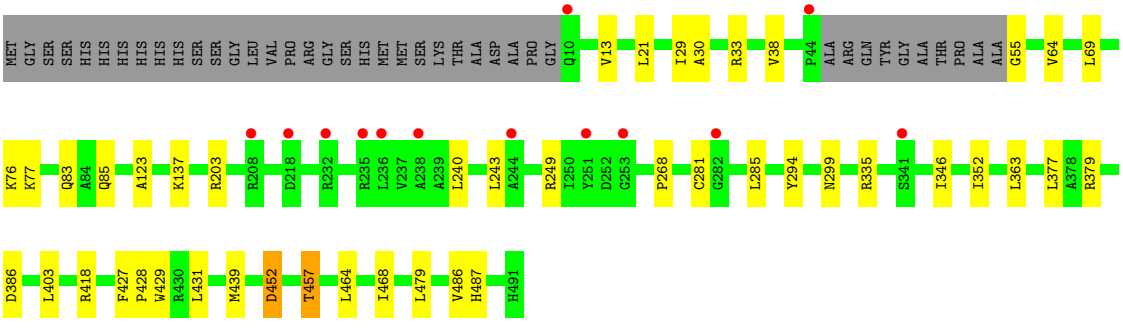




• Molecule 1: N-formimidoyl fortimicin A synthase

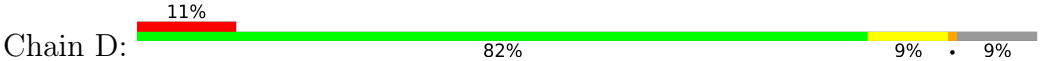
Chain C:

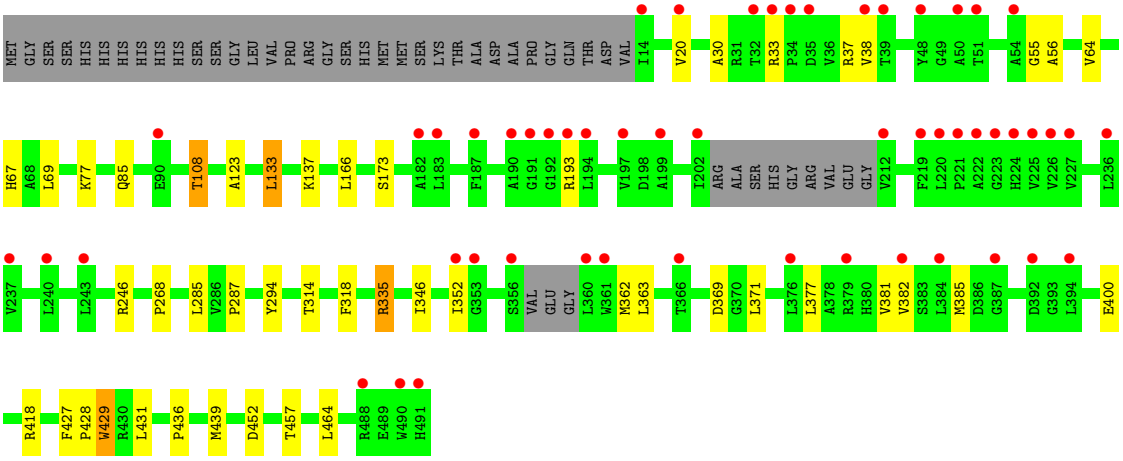




• Molecule 1: N-formimidoyl fortimicin A synthase

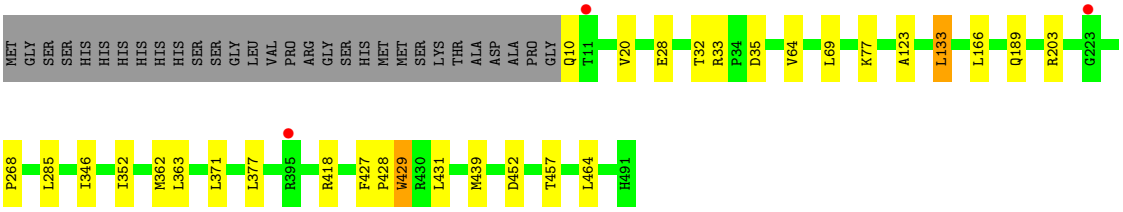
Chain D:





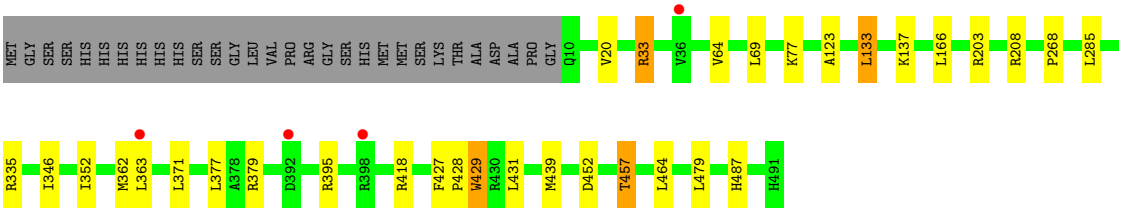
• Molecule 1: N-formimidoyl fortimicin A synthase

Chain E:



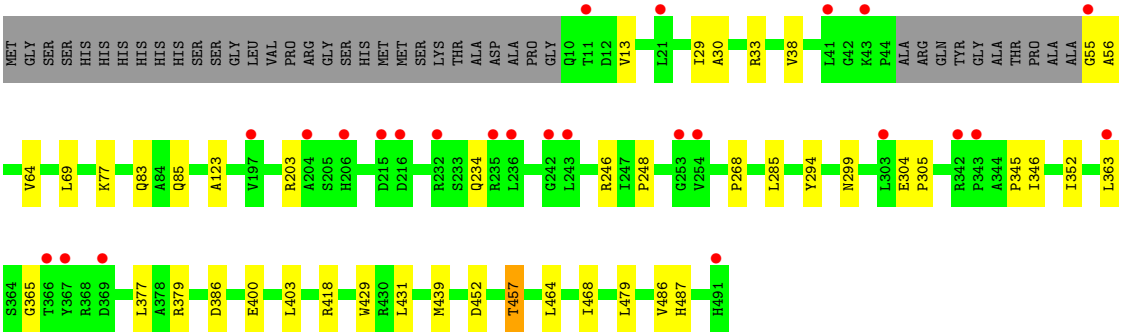
• Molecule 1: N-formimidoyl fortimicin A synthase

Chain F:



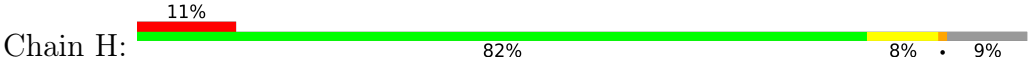
• Molecule 1: N-formimidoyl fortimicin A synthase

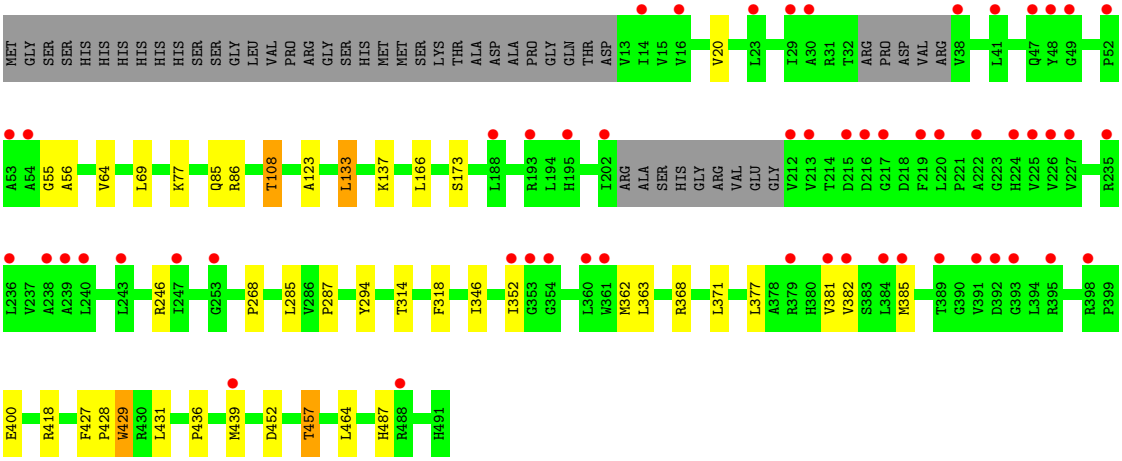
Chain G:



• Molecule 1: N-formimidoyl fortimicin A synthase

Chain H:





4 Data and refinement statistics (i)

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 29.38 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.39-2.12) 96.4 (29.38-2.12)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.12%)	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 , 27.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, I60

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	0.66	0/3737	0.78	0/5092
1	B	0.67	0/3743	0.77	0/5100
1	C	0.69	0/3670	0.81	0/4998
1	D	0.64	0/3622	0.78	0/4934
1	E	0.66	0/3737	0.78	0/5092
1	F	0.67	0/3743	0.78	0/5100
1	G	0.69	0/3670	0.81	0/4998
1	H	0.63	0/3604	0.77	0/4910
All	All	0.66	0/29526	0.79	0/40224

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

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	18	0
1	B	3660	0	3588	25	0
1	C	3590	0	3520	23	0
1	D	3542	0	3476	36	0
1	E	3654	0	3584	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3660	0	3588	20	0
1	G	3590	0	3520	24	0
1	H	3525	0	3457	36	0
2	A	53	0	31	2	0
2	B	53	0	31	2	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	2	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	198	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 (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:PRO:HA	1:D:439:MET:HE3	1.62	0.81
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:D:382:VAL:HA	1:D:385:MET:HE2	1.69	0.74
1:H:382:VAL:HA	1:H:385:MET:HE2	1.70	0.73
1:G:304:GLU:OE2	1:G:305:PRO:O	2.08	0.72
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:H:436:PRO:HA	1:H:439:MET:HE3	1.74	0.68
1:D:123:ALA:HB1	1:D:418:ARG:HD2	1.75	0.68
1:D:67:HIS:ND1	5:D:801:HOH:O	2.27	0.68
1:D:108:THR:HG21	1:D:287:PRO:O	1.95	0.67
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:H:436:PRO:HA	1:H:439:MET:HE2	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:G:363:LEU:HD11	1:G:377:LEU:HB3	1.80	0.64
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:B:439:MET:HE2	1:D:439:MET:HG2	1.81	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:429:TRP:CH2	1:D:439:MET:HE1	2.39	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:F:439:MET:HE2	1:H:439:MET:HG2	1.88	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:D:436:PRO:HA	1:D:439:MET:HE2	1.89	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: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
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:H:436:PRO:CA	1:H:439:MET:HE2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H:382:VAL:HA	1:H:385:MET:HE3	1.91	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:H:314:THR:CG2	1:H:318:PHE:CE2	2.98	0.47
1:D:382:VAL:CA	1:D:385:MET:HE2	2.41	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: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:HA	1:C:439:MET:HE1	1.97	0.47
1:F:363:LEU:HD11	1:F:377:LEU:HB3	1.97	0.47
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:H:381:VAL:O	1:H:385:MET:HE2	2.15	0.46
1:G:468:ILE:HD13	1:G:479:LEU:CD2	2.46	0.46
1:D:382:VAL:HA	1:D:385:MET:HE3	1.94	0.46
1:C:76:LYS:NZ	5:C:819:HOH:O	2.48	0.46
1:G:83:GLN:NE2	5:G:804:HOH:O	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:ILE:HD13	1:C:479:LEU:CD2	2.46	0.45
1:D:436:PRO:CA	1:D:439:MET:HE2	2.47	0.45
1:D:381:VAL:O	1:D:385:MET:HE2	2.16	0.45
2:B:701:FAD:H9	2:B:701:FAD:H1'2	1.75	0.45
1:H:429:TRP:CH2	1:H:439:MET:HE1	2.51	0.45
1:D:335:ARG:HD3	1:D:335:ARG:HA	1.52	0.45
1:D:20:VAL:HG11	1:D:371:LEU:HA	1.98	0.44
1:H:382:VAL:CA	1:H:385:MET:HE2	2.42	0.44
1:G:304:GLU:OE2	1:G:304:GLU:C	2.55	0.44
1:H:436:PRO:N	1:H:439:MET:HE2	2.32	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: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: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: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:HG2	1:G:439:MET:HE2	2.00	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:F:439:MET:CE	1:H:439:MET:HG2	2.49	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:297:ALA:HB1	2:A:701:FAD:HM73	2.02	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:297:ALA:HB1	2:B:701:FAD:HM73	2.03	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:D:436:PRO:N	1:D:439:MET:HE2	2.36	0.41
1:F:33:ARG:HD2	5:F:927:HOH:O	2.21	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:B:362:MET:HE2	1:B:362:MET:HB2	1.97	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
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%)	365 (97%)	11 (3%)	42	44
1	B	377/400 (94%)	367 (97%)	10 (3%)	44	47
1	C	372/400 (93%)	362 (97%)	10 (3%)	44	47
1	D	365/400 (91%)	352 (96%)	13 (4%)	35	35
1	E	376/400 (94%)	368 (98%)	8 (2%)	53	57
1	F	377/400 (94%)	366 (97%)	11 (3%)	42	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	372/400 (93%)	363 (98%)	9 (2%)	49 52
1	H	363/400 (91%)	354 (98%)	9 (2%)	47 50
All	All	2978/3200 (93%)	2897 (97%)	81 (3%)	44 47

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
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	429	TRP
1	A	452	ASP
1	A	457	THR
1	A	464	LEU
1	B	33	ARG
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	429	TRP
1	B	452	ASP
1	B	457	THR
1	C	33	ARG
1	C	77	LYS
1	C	85	GLN
1	C	203	ARG
1	C	335	ARG
1	C	386	ASP
1	C	429	TRP
1	C	431	LEU
1	C	452	ASP
1	C	457	THR
1	D	33	ARG
1	D	37	ARG
1	D	77	LYS

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Mol	Chain	Res	Type
1	D	85	GLN
1	D	108	THR
1	D	133	LEU
1	D	137	LYS
1	D	193	ARG
1	D	335	ARG
1	D	362	MET
1	D	429	TRP
1	D	452	ASP
1	D	457	THR
1	E	77	LYS
1	E	133	LEU
1	E	189	GLN
1	E	203	ARG
1	E	362	MET
1	E	429	TRP
1	E	452	ASP
1	E	457	THR
1	F	33	ARG
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	429	TRP
1	F	452	ASP
1	F	457	THR
1	G	33	ARG
1	G	77	LYS
1	G	85	GLN
1	G	203	ARG
1	G	386	ASP
1	G	429	TRP
1	G	431	LEU
1	G	452	ASP
1	G	457	THR
1	H	77	LYS
1	H	85	GLN
1	H	108	THR
1	H	133	LEU

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Mol	Chain	Res	Type
1	H	137	LYS
1	H	362	MET
1	H	429	TRP
1	H	452	ASP
1	H	457	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	HIS
1	D	487	HIS
1	E	487	HIS
1	G	83	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	$\#\|Z\|>2$
4	I60	E	703	-	31,34,34	1.15	2 (6%)	36,48,48	1.25	3 (8%)
2	FAD	D	701	-	53,58,58	0.61	0	68,89,89	0.77	1 (1%)
4	I60	C	703	-	31,34,34	0.76	1 (3%)	36,48,48	1.17	3 (8%)
4	I60	F	703	-	31,34,34	0.89	1 (3%)	36,48,48	1.07	2 (5%)
3	GLY	A	702	-	4,4,4	0.95	0	3,4,4	0.74	0
3	GLY	H	702	-	4,4,4	0.95	0	3,4,4	2.21	2 (66%)
4	I60	G	703	-	31,34,34	0.79	1 (3%)	36,48,48	1.06	2 (5%)
3	GLY	B	702	-	4,4,4	1.14	0	3,4,4	0.95	0
2	FAD	H	701	-	53,58,58	0.60	0	68,89,89	0.75	1 (1%)
3	GLY	D	702	-	4,4,4	0.99	0	3,4,4	2.37	2 (66%)
2	FAD	A	701	-	53,58,58	0.71	1 (1%)	68,89,89	0.86	3 (4%)
4	I60	H	703	-	31,34,34	0.71	1 (3%)	36,48,48	0.91	3 (8%)
2	FAD	B	701	-	53,58,58	0.75	1 (1%)	68,89,89	0.85	3 (4%)
4	I60	A	703	-	31,34,34	1.03	2 (6%)	36,48,48	1.16	3 (8%)
3	GLY	F	702	-	4,4,4	1.02	0	3,4,4	1.25	0
2	FAD	F	701	-	53,58,58	0.73	0	68,89,89	0.81	2 (2%)
4	I60	D	703	-	31,34,34	0.92	1 (3%)	36,48,48	0.96	2 (5%)
2	FAD	C	701	-	53,58,58	0.62	0	68,89,89	0.78	0
3	GLY	E	702	-	4,4,4	0.98	0	3,4,4	1.23	0
3	GLY	G	702	-	4,4,4	1.15	1 (25%)	3,4,4	1.89	1 (33%)
2	FAD	E	701	-	53,58,58	0.79	1 (1%)	68,89,89	0.88	4 (5%)
3	GLY	C	702	-	4,4,4	1.20	1 (25%)	3,4,4	1.87	1 (33%)
4	I60	B	703	-	31,34,34	0.84	1 (3%)	36,48,48	1.05	4 (11%)
2	FAD	G	701	-	53,58,58	0.64	0	68,89,89	0.84	0

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
4	I60	E	703	-	-	1/16/63/63	0/3/3/3
2	FAD	D	701	-	-	6/30/50/50	0/6/6/6
4	I60	C	703	-	-	4/16/63/63	0/3/3/3
4	I60	F	703	-	-	1/16/63/63	0/3/3/3
3	GLY	A	702	-	-	0/2/2/2	-
3	GLY	H	702	-	-	0/2/2/2	-
4	I60	G	703	-	-	4/16/63/63	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	B	702	-	-	0/2/2/2	-
2	FAD	H	701	-	-	6/30/50/50	0/6/6/6
3	GLY	D	702	-	-	0/2/2/2	-
2	FAD	A	701	-	-	1/30/50/50	0/6/6/6
4	I60	H	703	-	-	2/16/63/63	0/3/3/3
2	FAD	B	701	-	-	2/30/50/50	0/6/6/6
4	I60	A	703	-	-	1/16/63/63	0/3/3/3
3	GLY	F	702	-	-	0/2/2/2	-
2	FAD	F	701	-	-	3/30/50/50	0/6/6/6
4	I60	D	703	-	-	4/16/63/63	0/3/3/3
2	FAD	C	701	-	-	12/30/50/50	0/6/6/6
3	GLY	E	702	-	-	0/2/2/2	-
3	GLY	G	702	-	-	1/2/2/2	-
2	FAD	E	701	-	-	1/30/50/50	0/6/6/6
3	GLY	C	702	-	-	0/2/2/2	-
4	I60	B	703	-	-	1/16/63/63	0/3/3/3
2	FAD	G	701	-	-	13/30/50/50	0/6/6/6

All (15) 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
4	F	703	I60	C11-C5	-3.67	1.50	1.53
4	B	703	I60	C11-C5	-3.41	1.51	1.53
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'	-2.83	1.48	1.52
2	A	701	FAD	C1'-C2'	-2.49	1.49	1.52
4	C	703	I60	C11-C5	-2.48	1.51	1.53
3	C	702	GLY	OXT-C	-2.31	1.23	1.30
2	B	701	FAD	C1'-C2'	-2.29	1.49	1.52
4	E	703	I60	C15-C16	2.25	1.54	1.52
4	A	703	I60	C15-C16	2.20	1.54	1.52
3	G	702	GLY	OXT-C	-2.19	1.23	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	703	I60	C17-N7-C12	-5.59	107.20	112.56
4	A	703	I60	C17-N7-C12	-4.85	107.92	112.56
4	G	703	I60	C17-N7-C12	-3.80	108.92	112.56
4	F	703	I60	C17-N7-C12	-3.63	109.08	112.56
4	C	703	I60	C11-C5-N2	3.35	115.94	111.08
4	C	703	I60	C13-C14-N6	-3.31	114.11	118.19
4	B	703	I60	C17-N7-C12	-3.17	109.52	112.56
3	D	702	GLY	OXT-C-O	-3.00	115.81	123.30
4	D	703	I60	C13-C14-N6	-2.96	114.54	118.19
4	B	703	I60	C16-C15-N6	2.94	112.87	109.83
4	C	703	I60	C17-N7-C12	-2.75	109.92	112.56
3	D	702	GLY	OXT-C-CA	2.73	124.30	113.45
3	H	702	GLY	OXT-C-CA	2.69	124.16	113.45
4	D	703	I60	C17-N7-C12	-2.67	110.00	112.56
2	B	701	FAD	O2A-PA-O1A	2.65	125.36	112.24
3	C	702	GLY	OXT-C-O	-2.65	116.70	123.30
3	G	702	GLY	OXT-C-O	-2.65	116.71	123.30
3	H	702	GLY	OXT-C-O	-2.60	116.81	123.30
4	E	703	I60	C16-C15-N6	2.57	112.49	109.83
4	F	703	I60	C16-C15-N6	2.44	112.36	109.83
2	A	701	FAD	C4'-C3'-C2'	2.42	118.39	113.36
2	F	701	FAD	C4'-C3'-C2'	2.41	118.37	113.36
4	A	703	I60	N7-C12-N5	-2.35	106.79	109.20
2	A	701	FAD	C5A-C6A-N6A	2.34	123.92	120.35
2	E	701	FAD	C4'-C3'-C2'	2.34	118.23	113.36
2	A	701	FAD	O2A-PA-O1A	2.32	123.72	112.24
2	B	701	FAD	C4'-C3'-C2'	2.32	118.18	113.36
4	H	703	I60	C17-N7-C12	-2.31	110.35	112.56
4	E	703	I60	N7-C12-N5	-2.24	106.89	109.20
2	E	701	FAD	C5A-C6A-N6A	2.23	123.75	120.35
2	F	701	FAD	O2A-PA-O1A	2.21	123.18	112.24
2	E	701	FAD	O2A-PA-O1A	2.19	123.09	112.24
2	H	701	FAD	C5A-C6A-N6A	2.18	123.67	120.35
4	G	703	I60	C11-C5-N2	2.18	114.25	111.08
2	D	701	FAD	C5A-C6A-N6A	2.16	123.64	120.35
4	B	703	I60	N7-C12-N5	-2.14	107.00	109.20
4	A	703	I60	C16-C15-N6	2.11	112.02	109.83
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
4	H	703	I60	N7-C12-N5	-2.09	107.05	109.20
2	B	701	FAD	C4-N3-C2	-2.03	121.88	125.64
2	E	701	FAD	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (63) 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
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	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	D	701	FAD	O4B-C4B-C5B-O5B
2	H	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	C3'-C4'-C5'-O5'
2	D	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
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	C	701	FAD	C5'-O5'-P-O3P
2	G	701	FAD	C5'-O5'-P-O3P
2	H	701	FAD	C5B-O5B-PA-O3P
2	A	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	C5'-O5'-P-O1P
2	G	701	FAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
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
2	E	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	C2'-C1'-N10-C10
3	G	702	GLY	OXT-C-CA-N
2	D	701	FAD	C5B-O5B-PA-O3P
2	C	701	FAD	C5'-O5'-P-O1P
2	D	701	FAD	C5B-O5B-PA-O1A
2	G	701	FAD	C5B-O5B-PA-O1A
2	H	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C3B-C4B-C5B-O5B
2	C	701	FAD	C3B-C4B-C5B-O5B
2	F	701	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

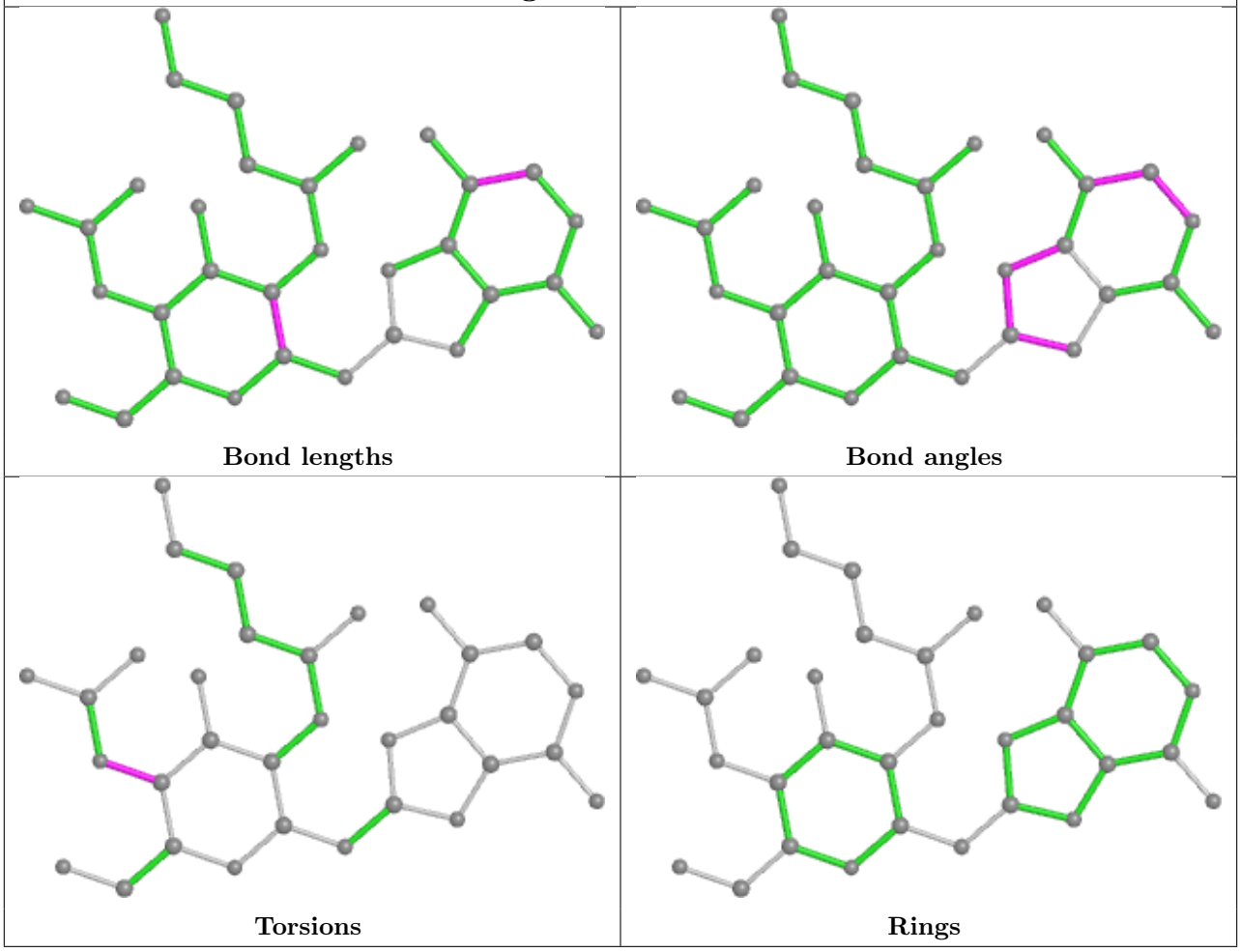
8 monomers are involved in 11 short contacts:

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

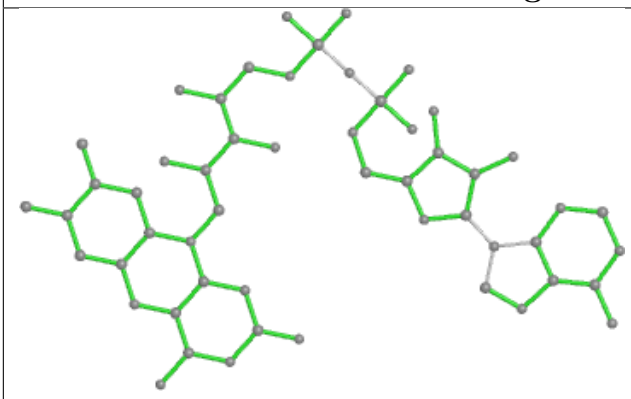
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 I60 E 703



Ligand FAD D 701



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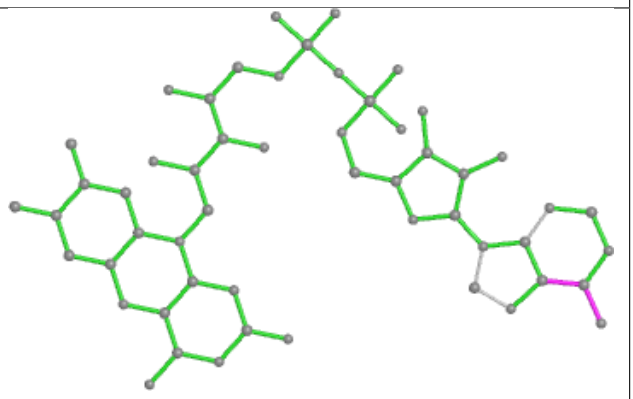

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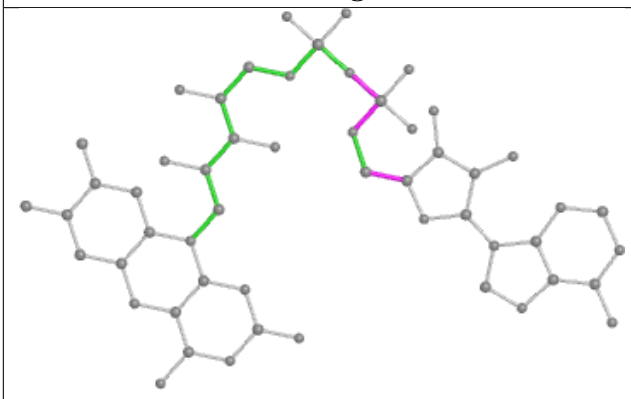

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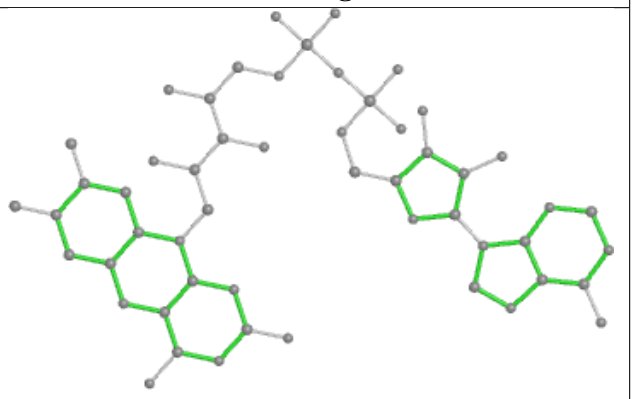
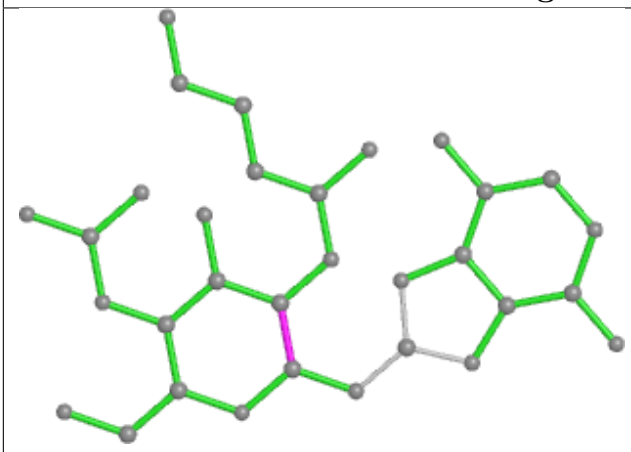


Rings

Ligand I60 C 703



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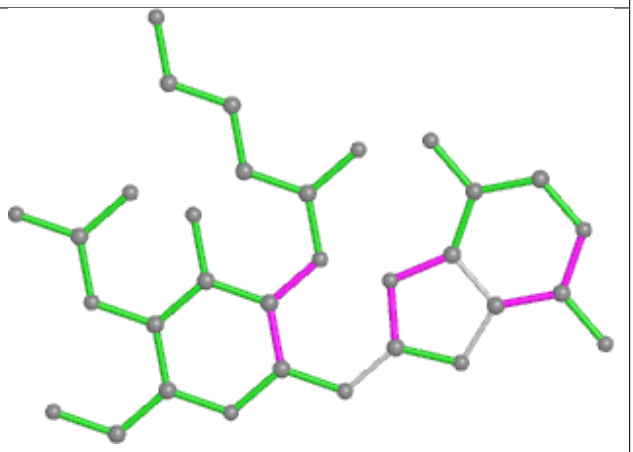

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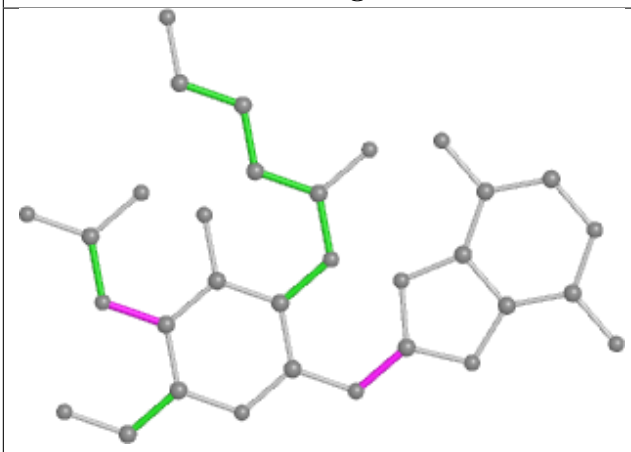

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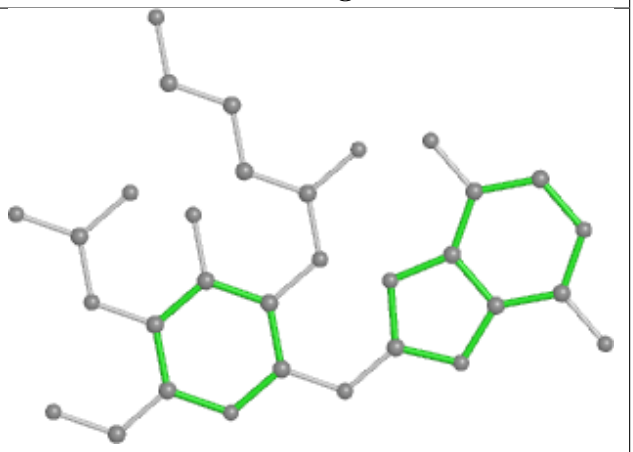

Rings

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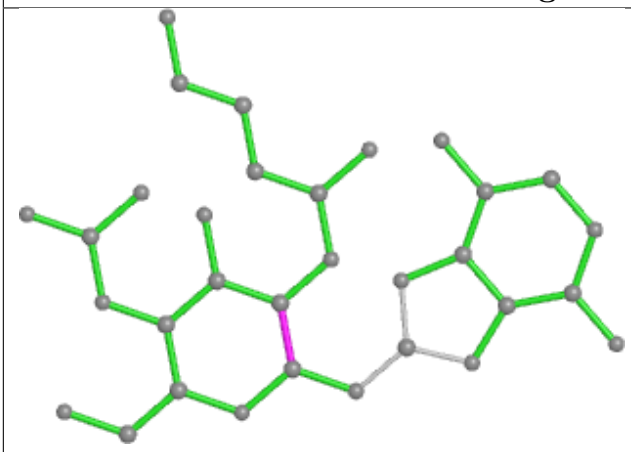

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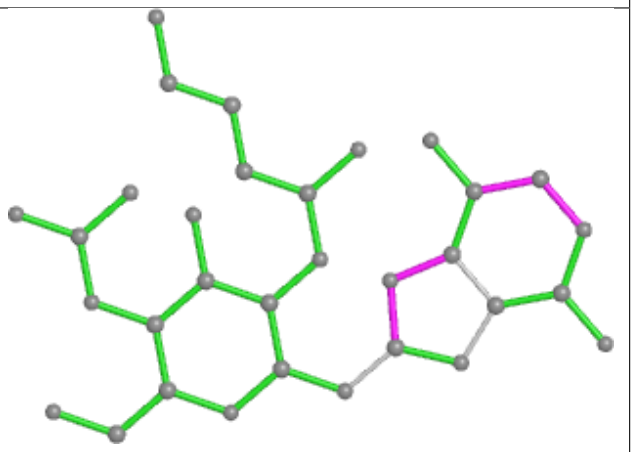

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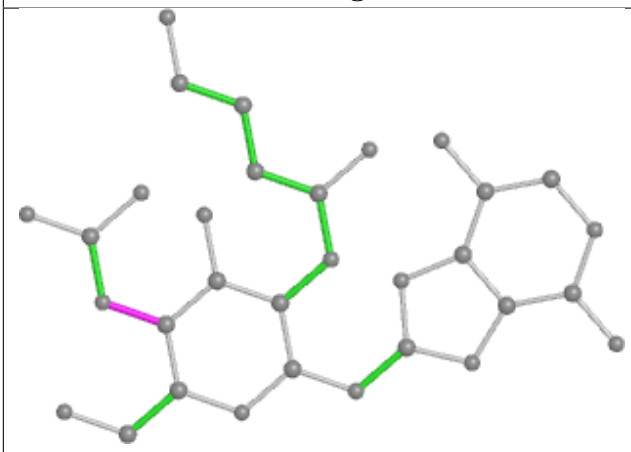

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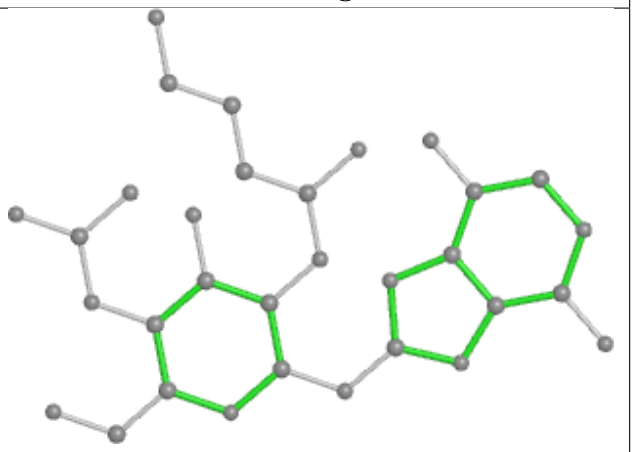
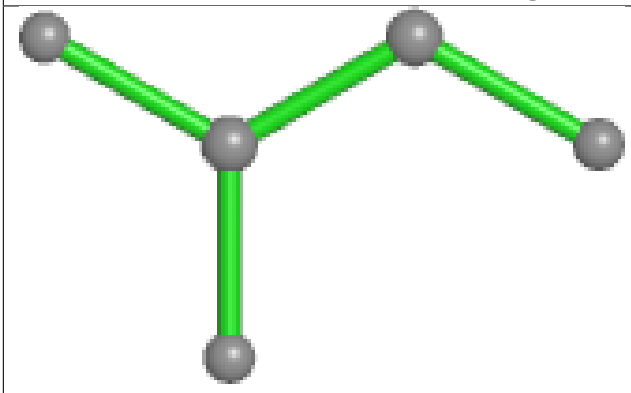


Rings

Ligand GLY A 702



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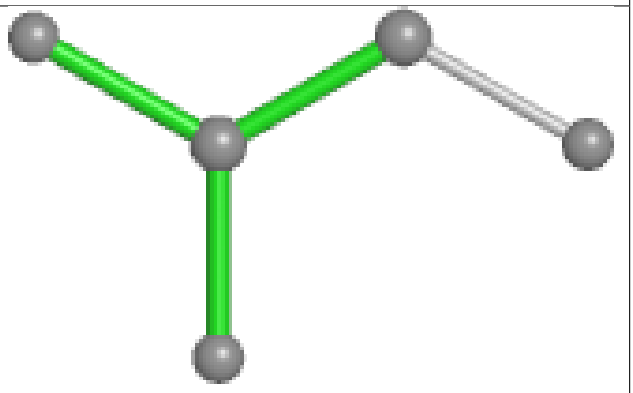

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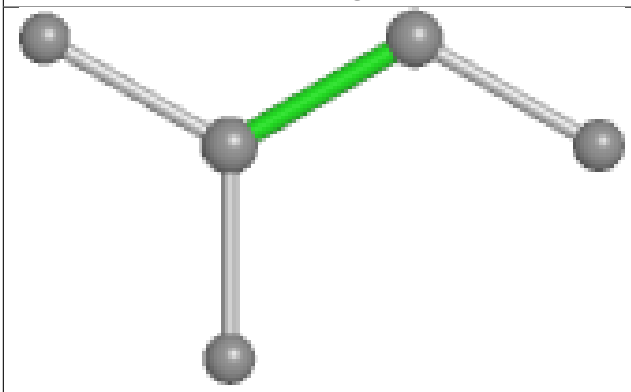

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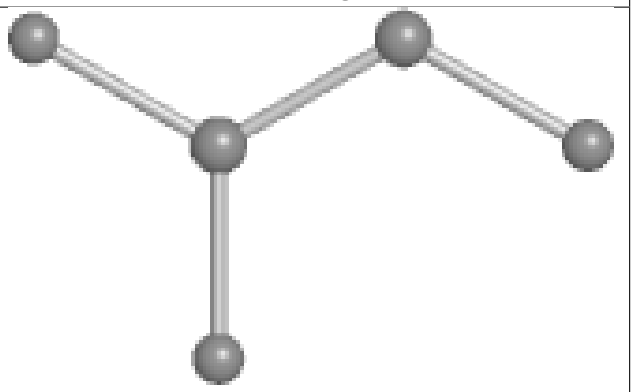
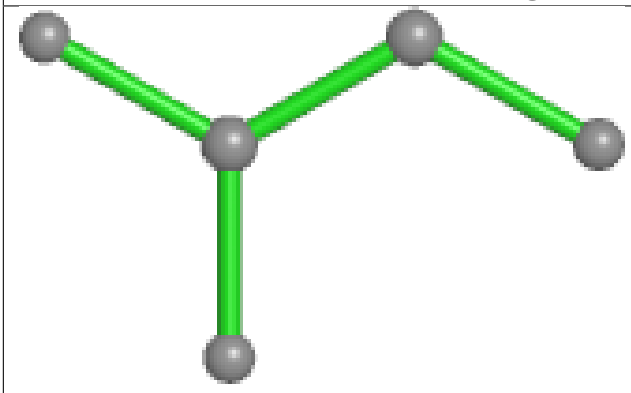


Rings

Ligand GLY H 702



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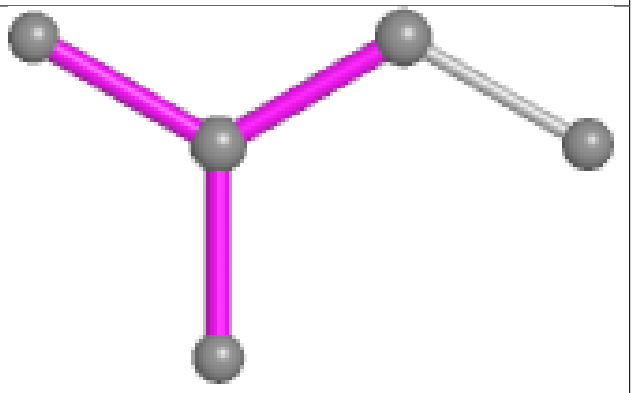

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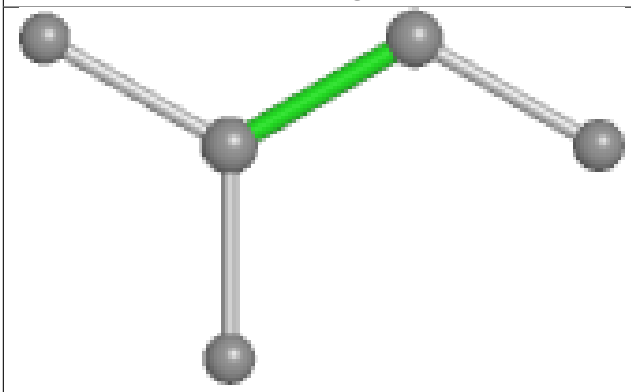

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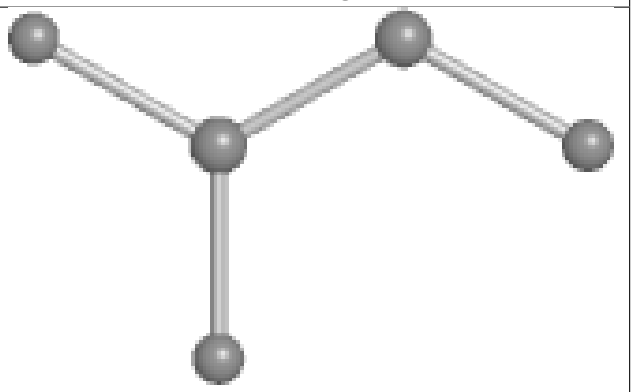
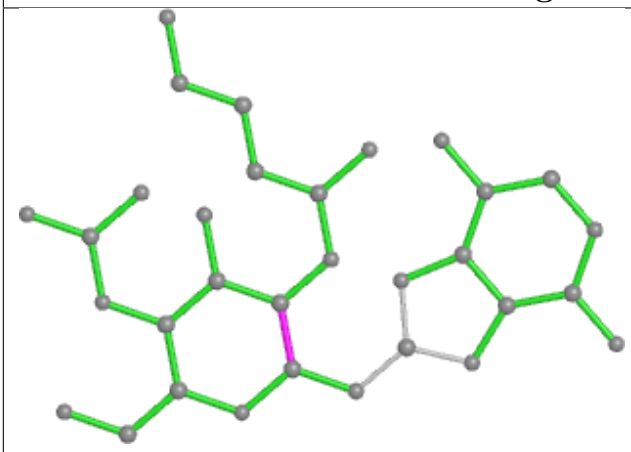


Rings

Ligand I60 G 703



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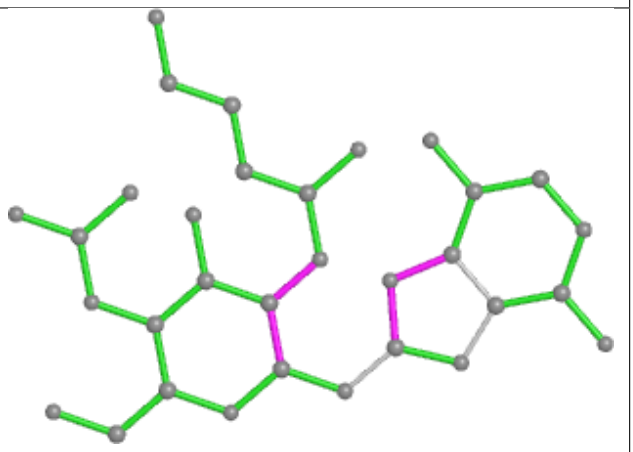

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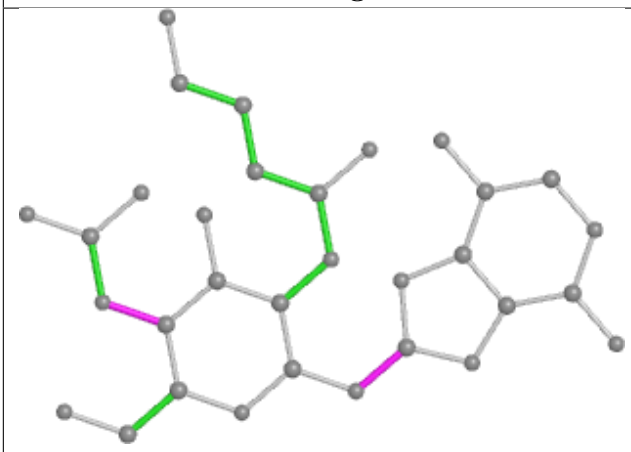

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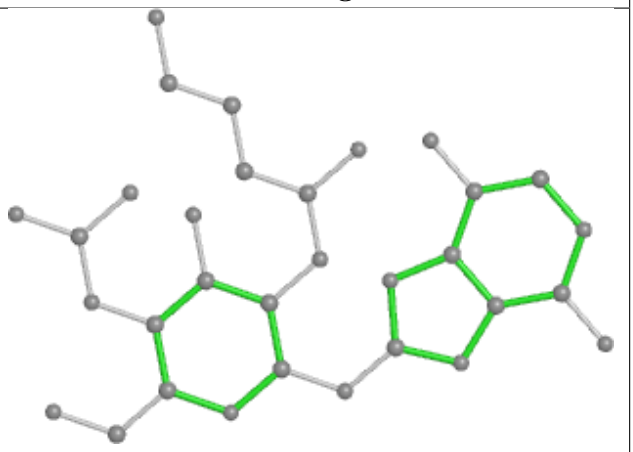
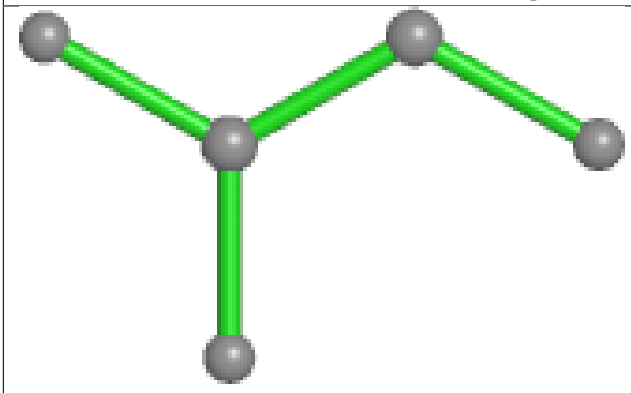


Rings

Ligand GLY B 702



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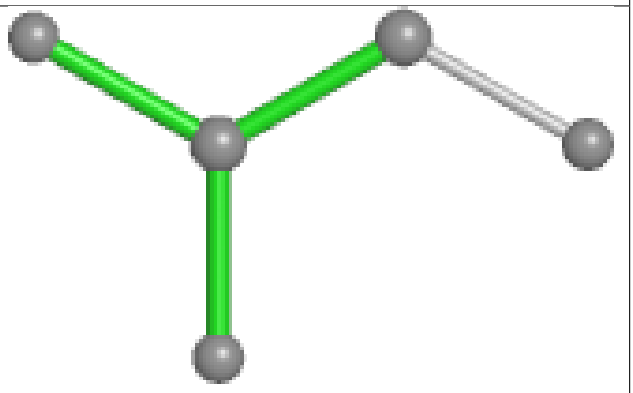

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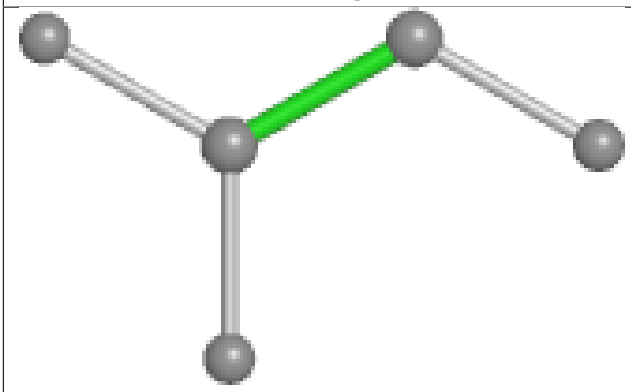

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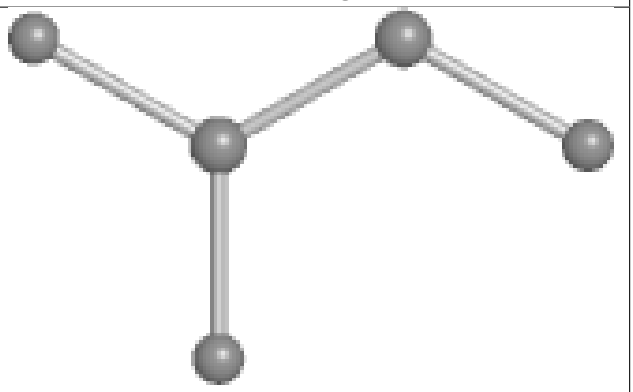
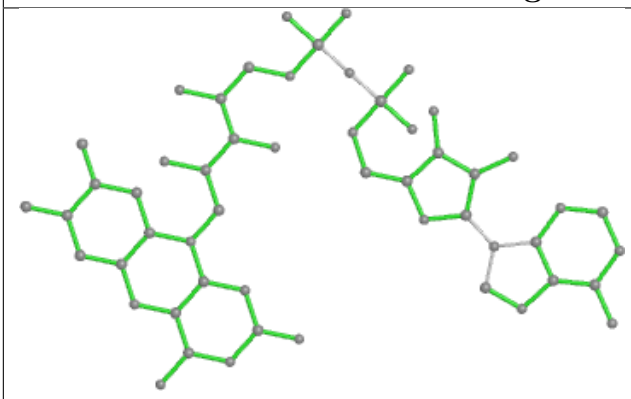


Rings

Ligand FAD H 701



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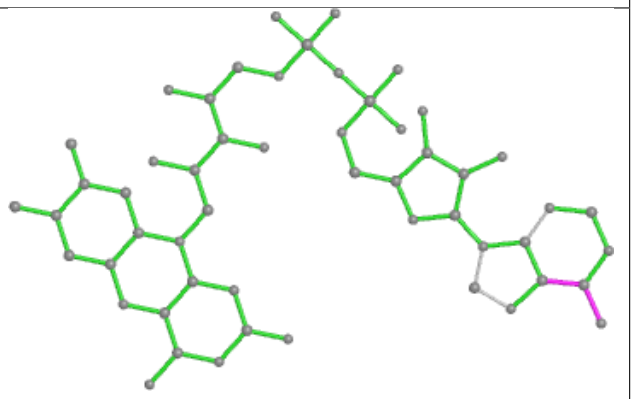

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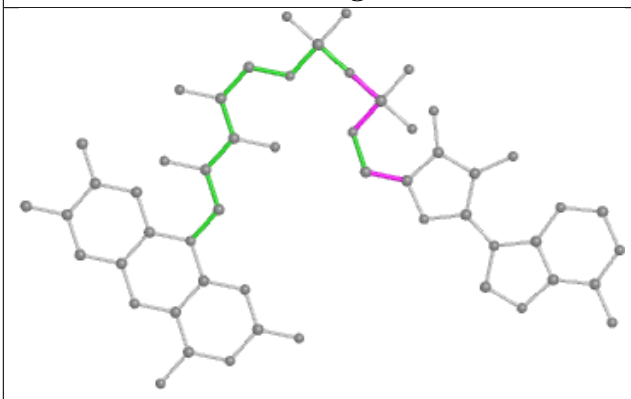

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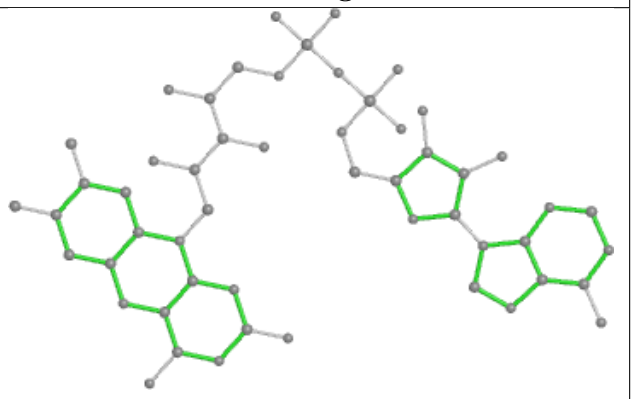
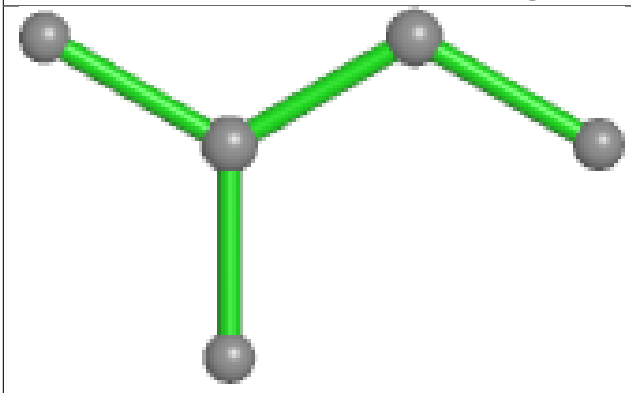


Rings

Ligand GLY D 702



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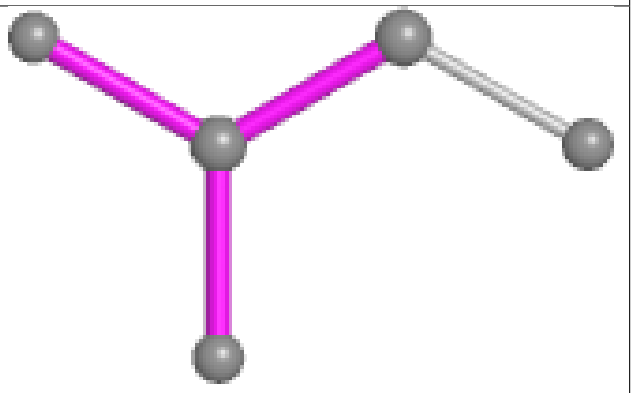

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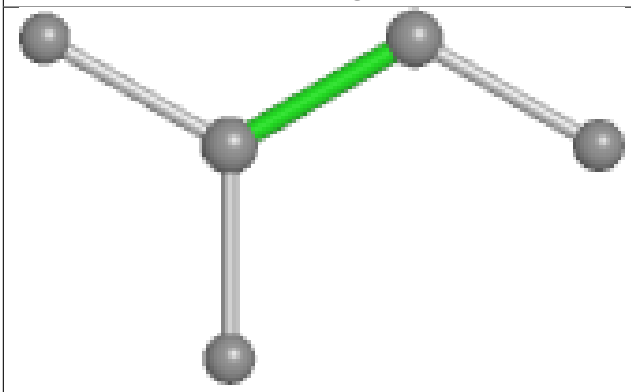

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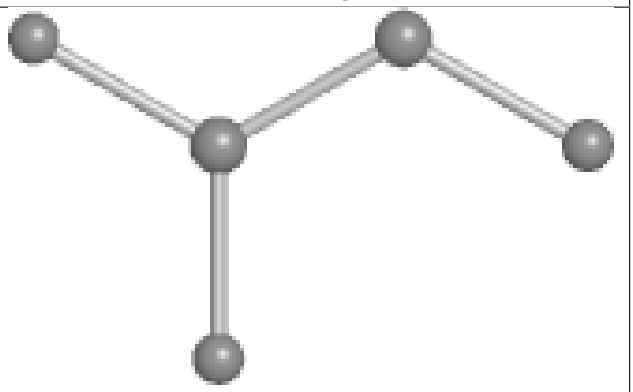

Rings

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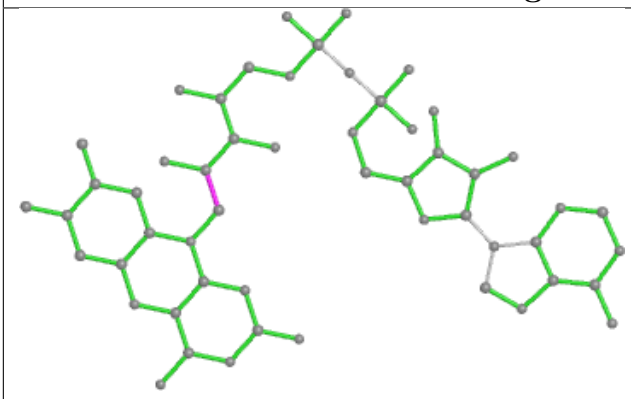

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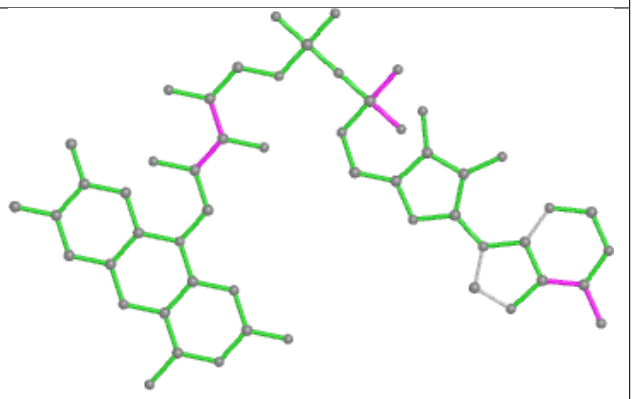

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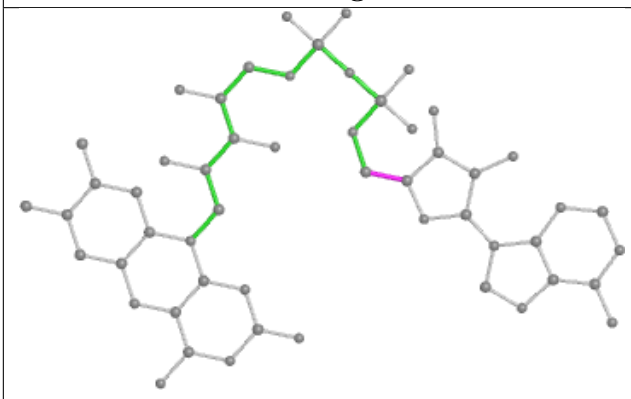

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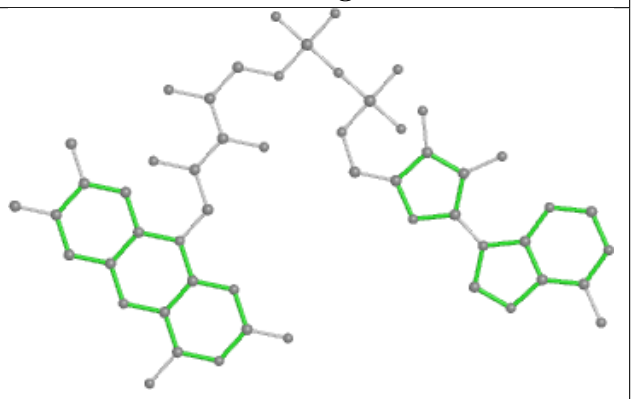
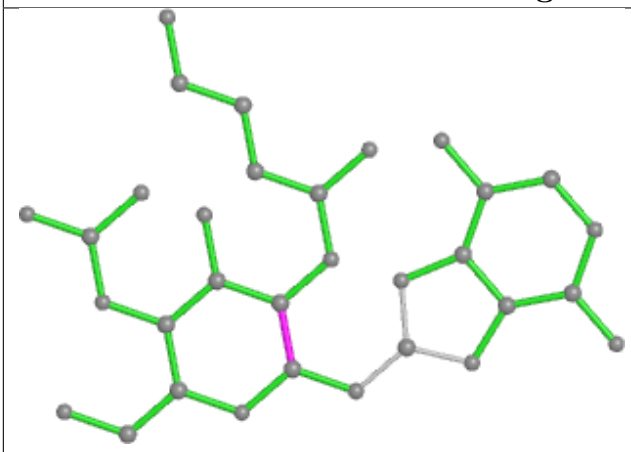


Rings

Ligand I60 H 703



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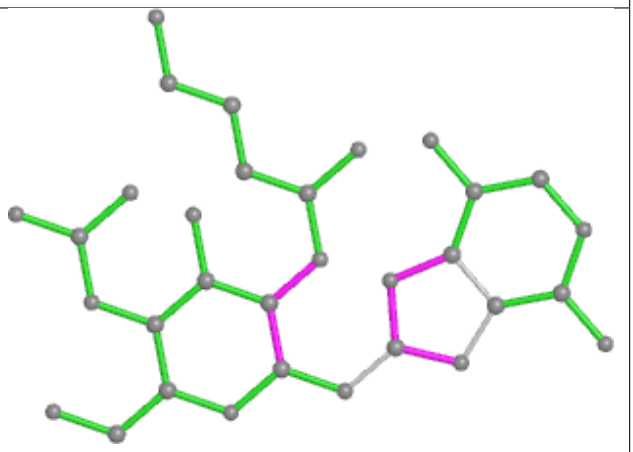

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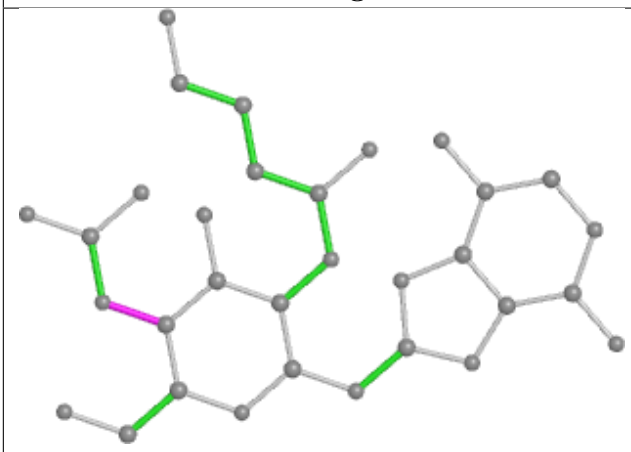

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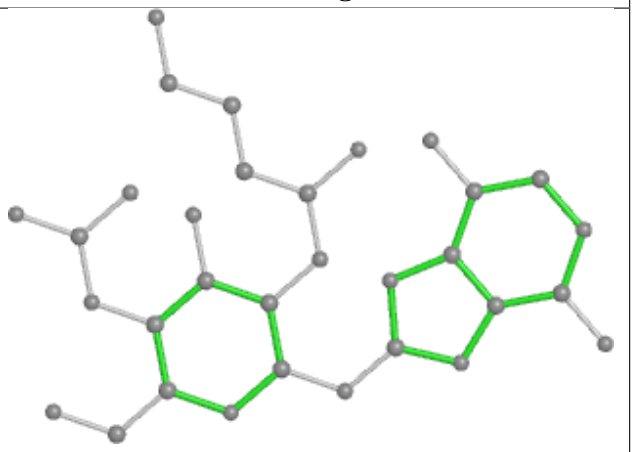
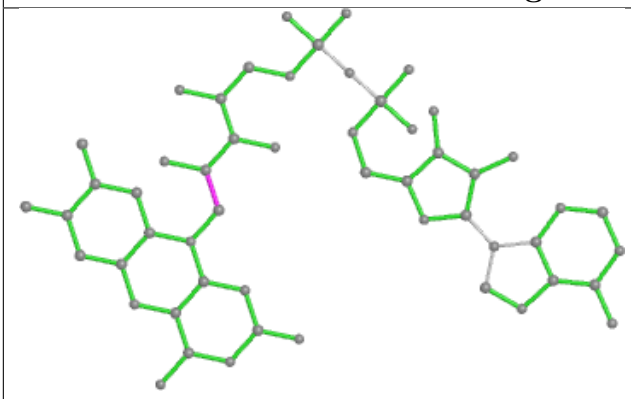


Rings

Ligand FAD B 701



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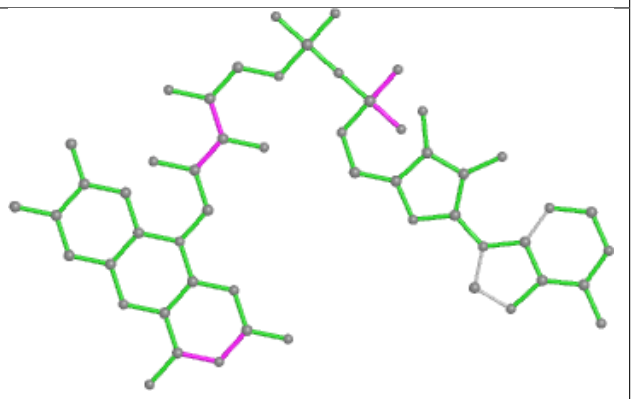
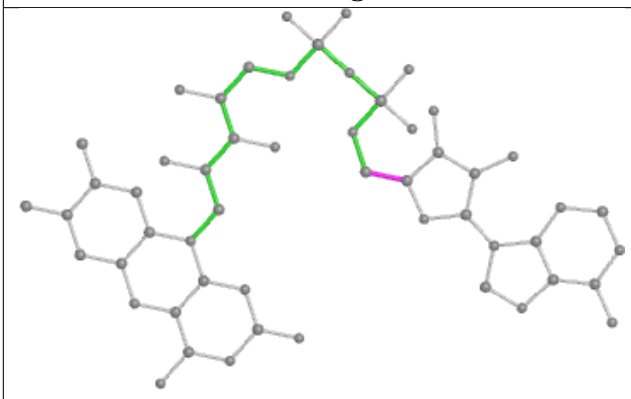


Bond angles



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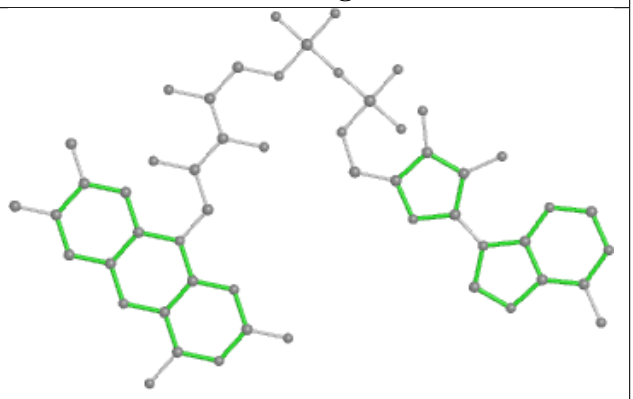
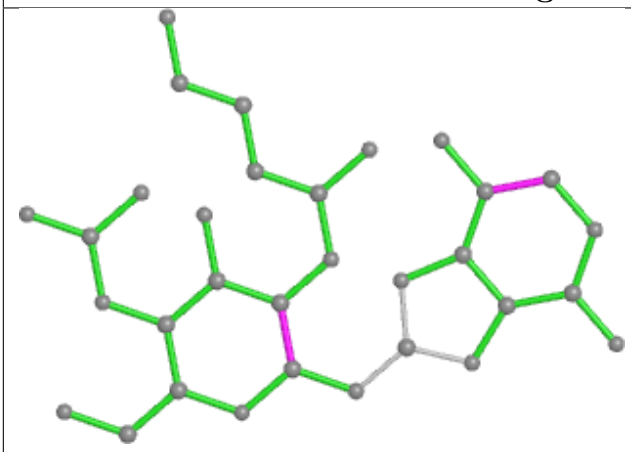
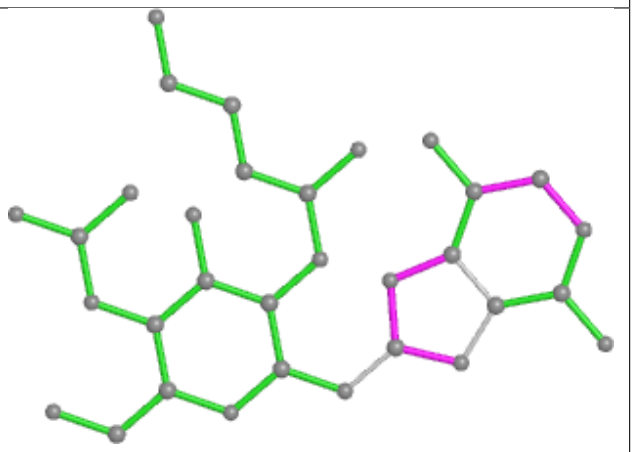


Rings

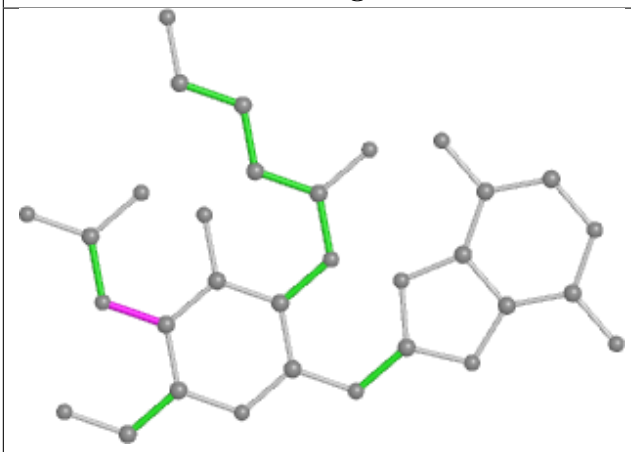
Ligand I60 A 703



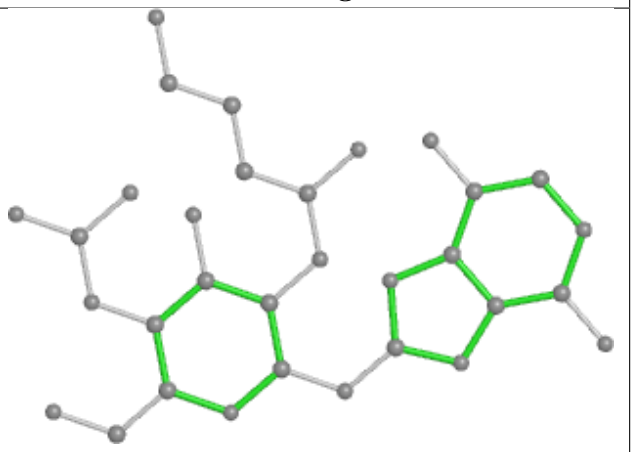
Bond lengths



Bond angles

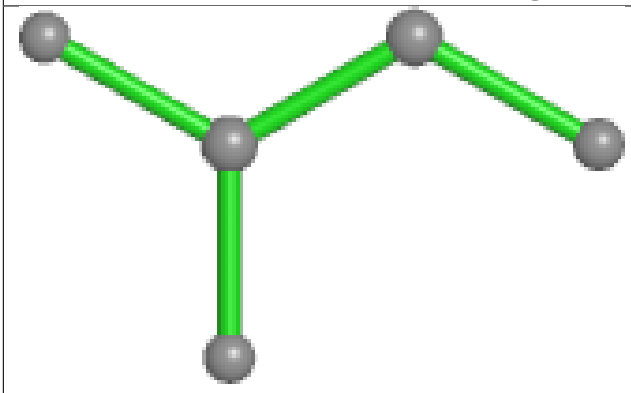


Torsions

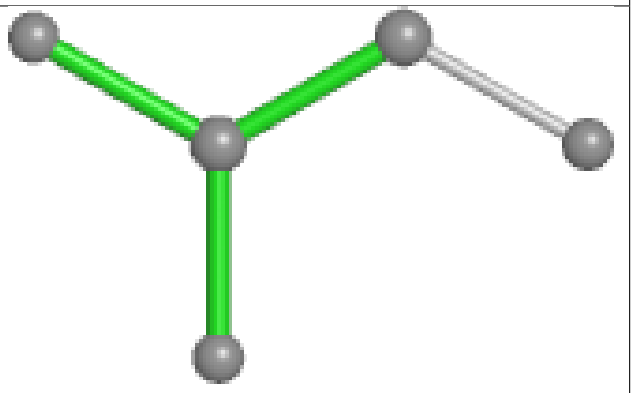


Rings

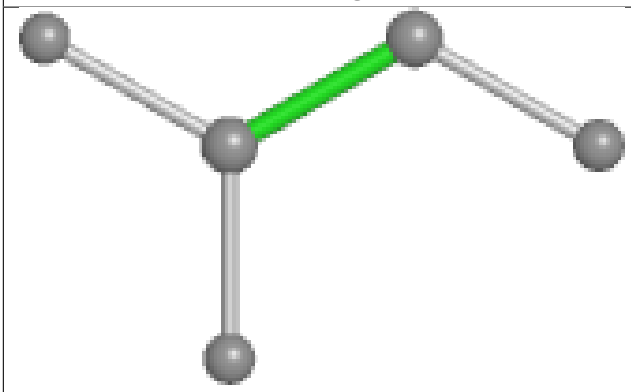
Ligand GLY F 702



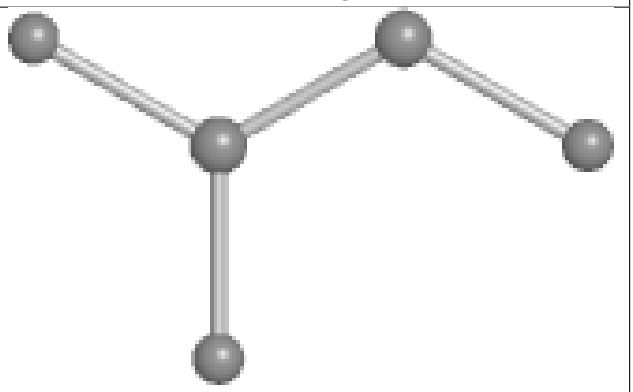
Bond lengths



Bond angles

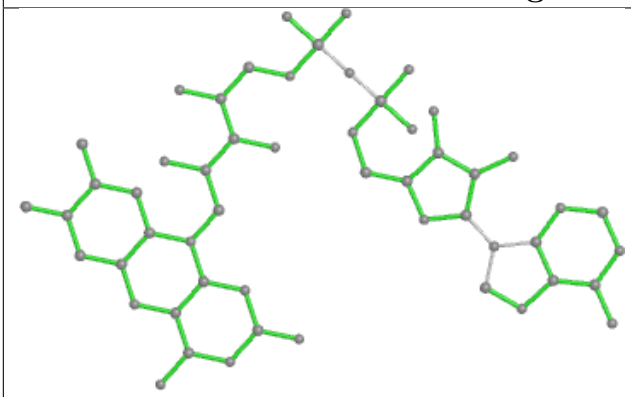


Torsions

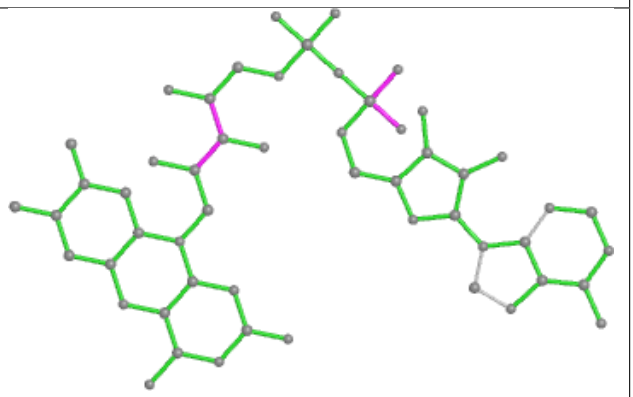


Rings

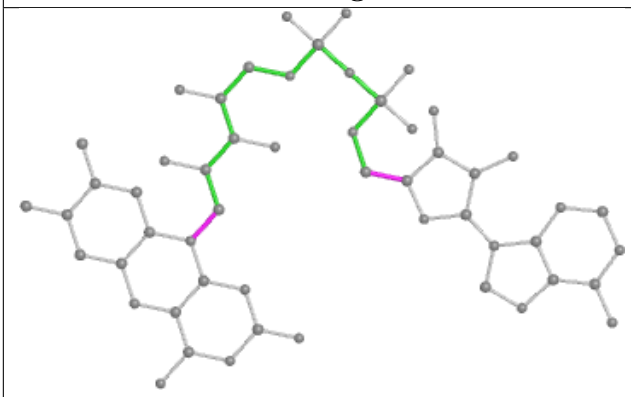
Ligand FAD F 701



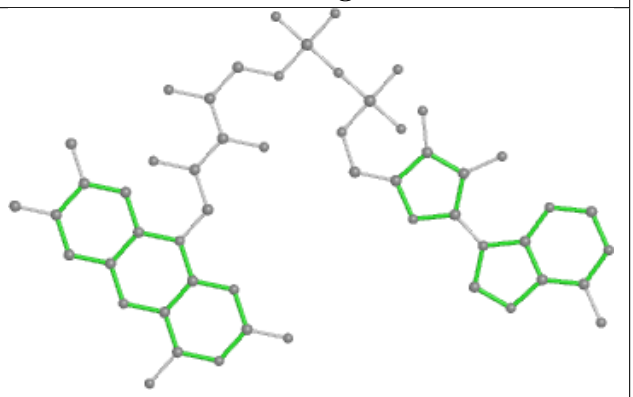
Bond lengths



Bond angles

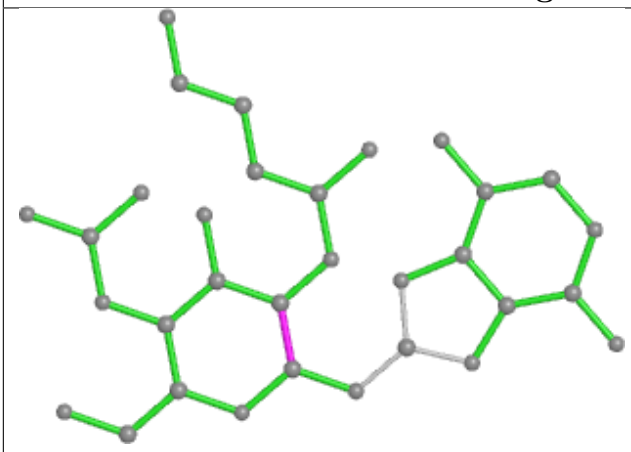


Torsions

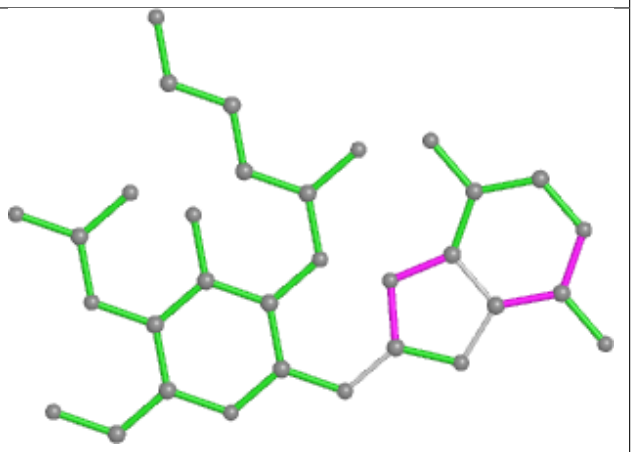


Rings

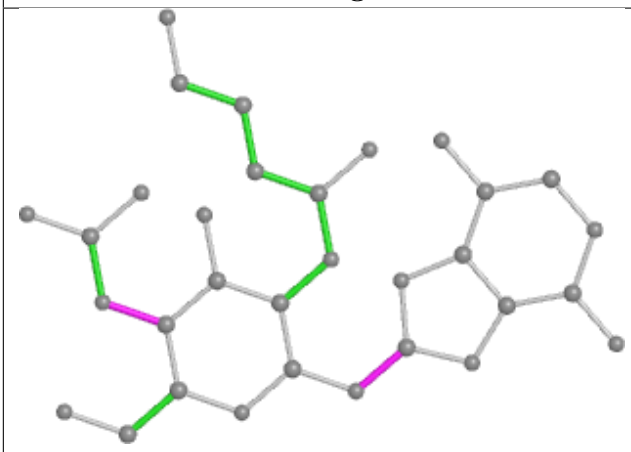
Ligand I60 D 703



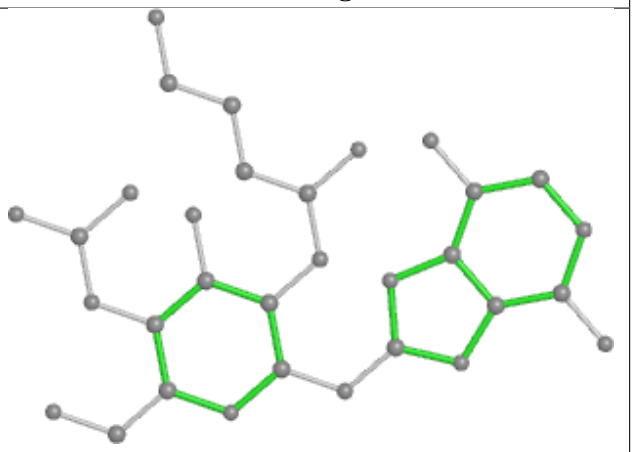
Bond lengths



Bond angles

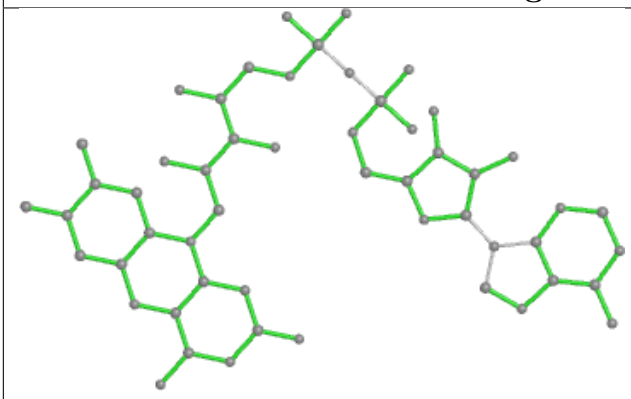


Torsions

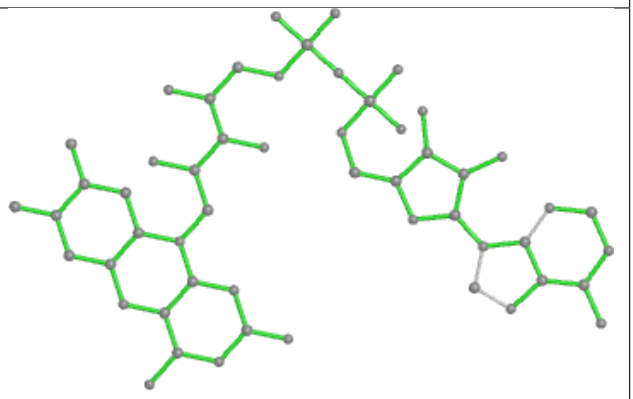


Rings

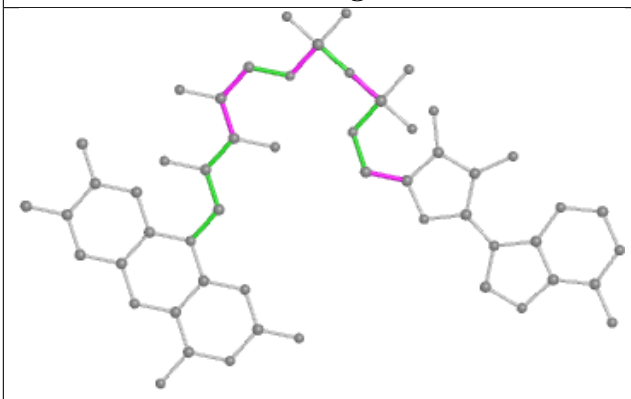
Ligand FAD C 701



Bond lengths



Bond angles



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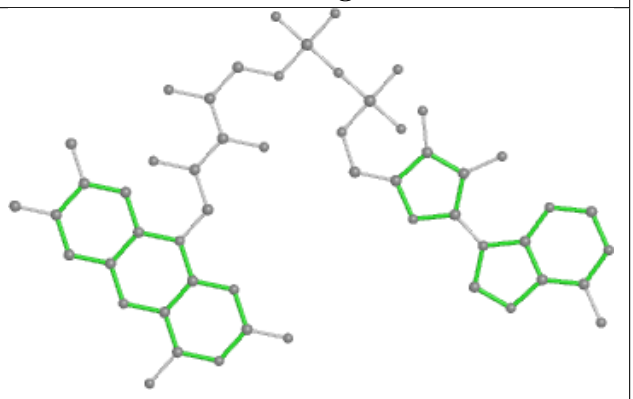
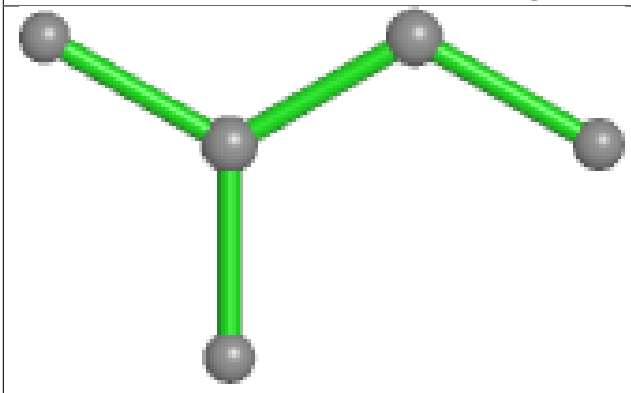
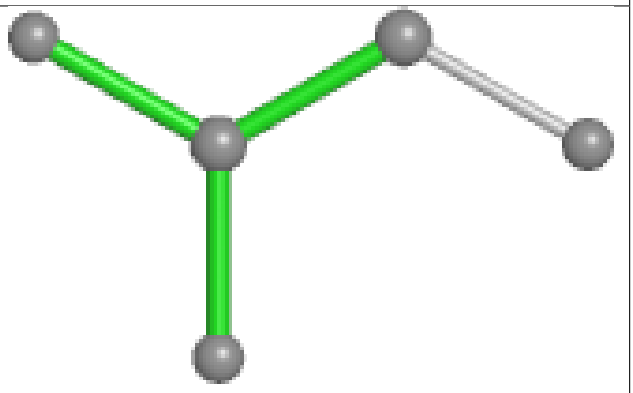


Rings

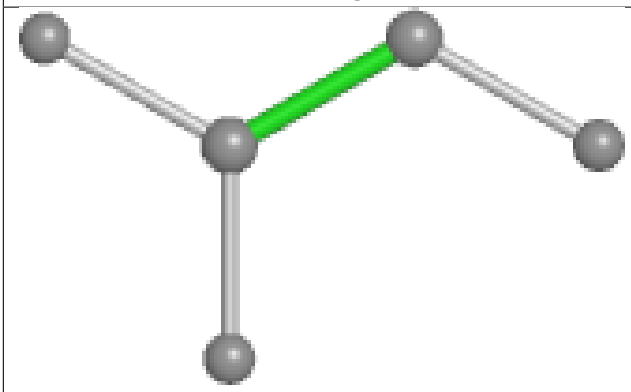
Ligand GLY E 702



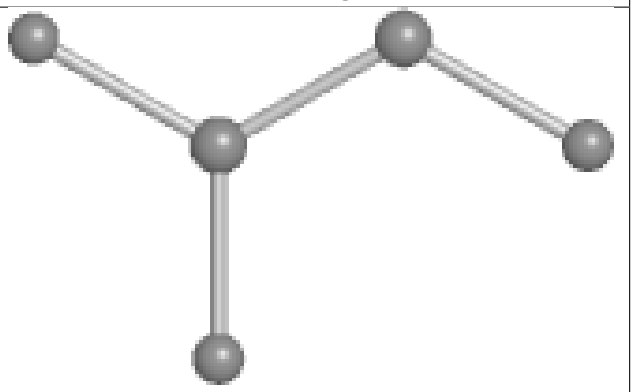
Bond lengths



Bond angles

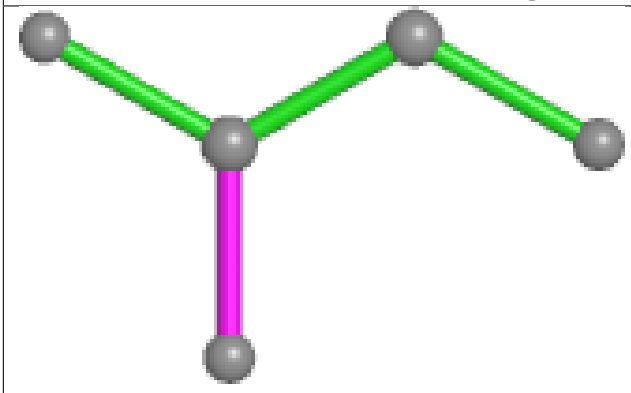


Torsions

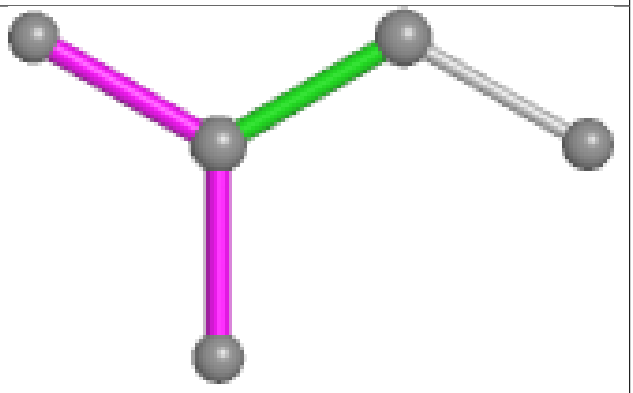


Rings

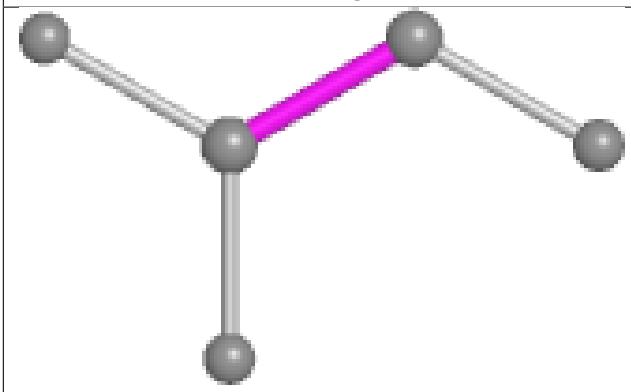
Ligand GLY G 702



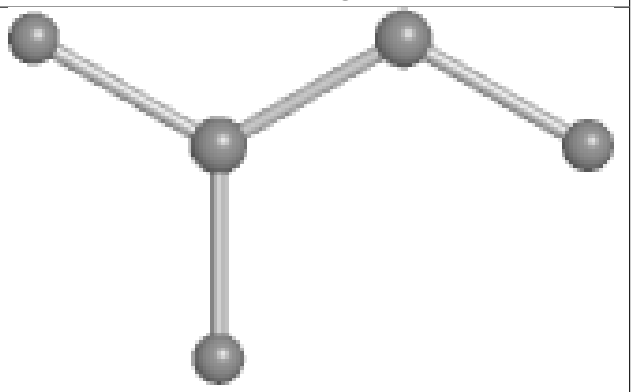
Bond lengths



Bond angles

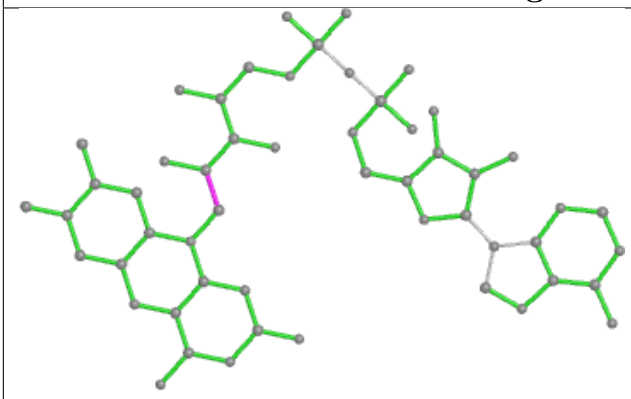


Torsions

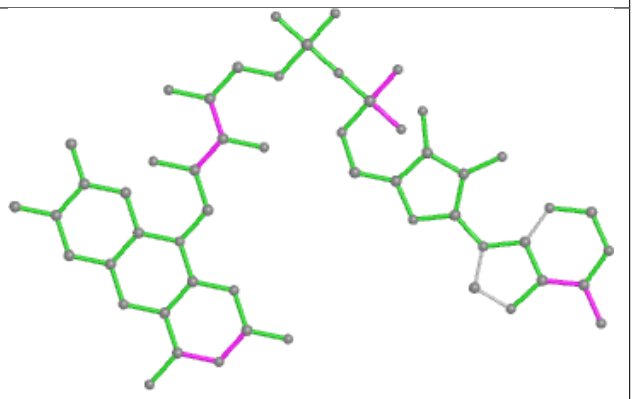


Rings

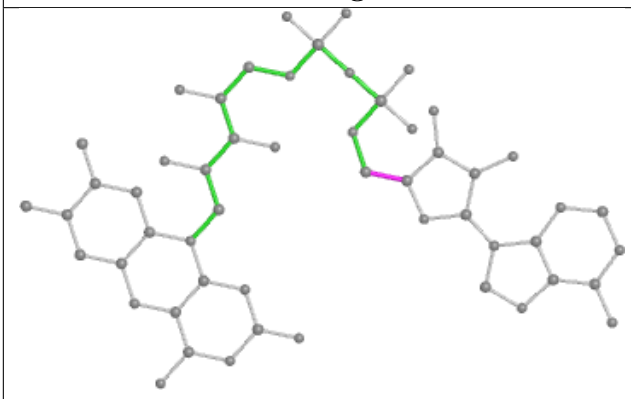
Ligand FAD E 701



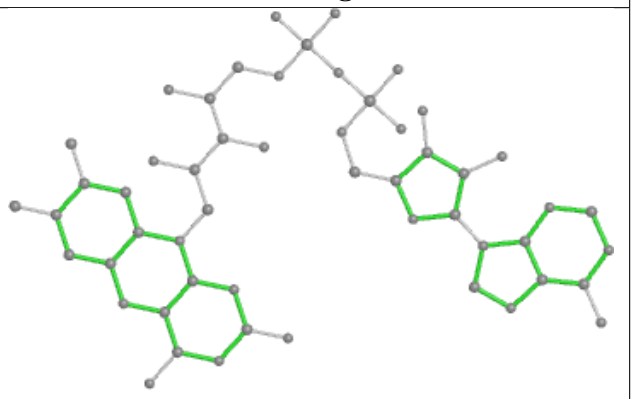
Bond lengths



Bond angles

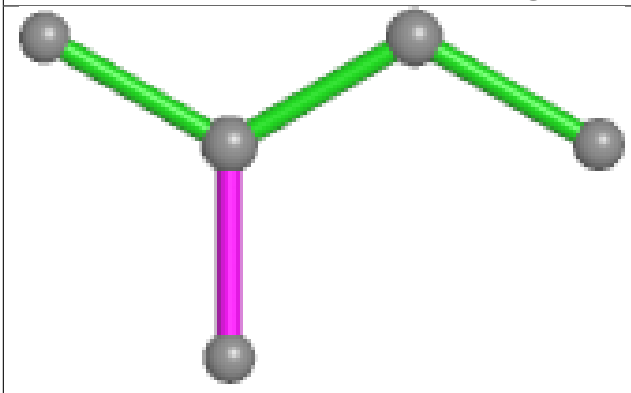


Torsions

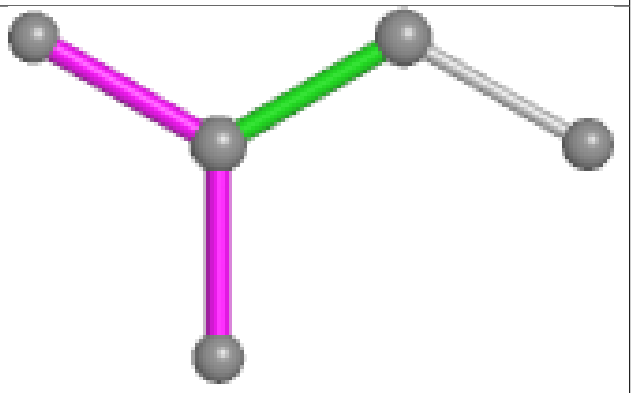


Rings

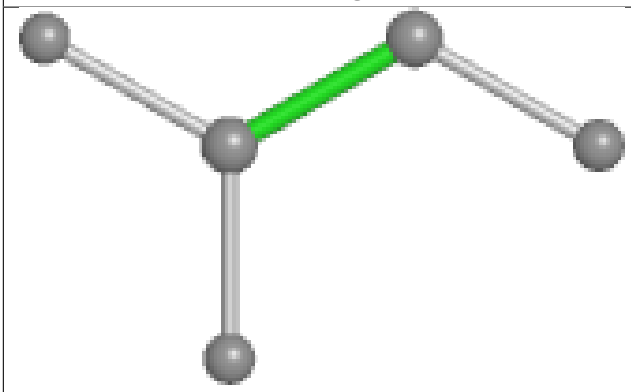
Ligand GLY C 702



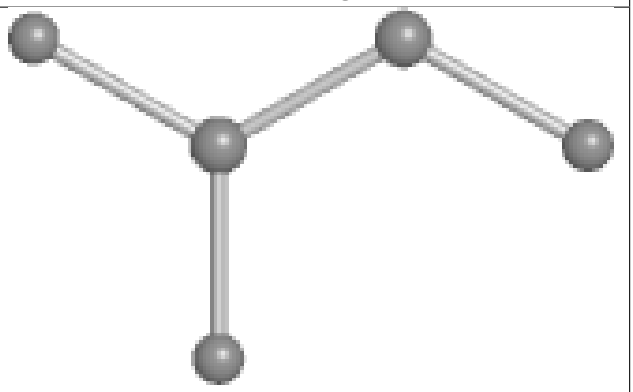
Bond lengths



Bond angles

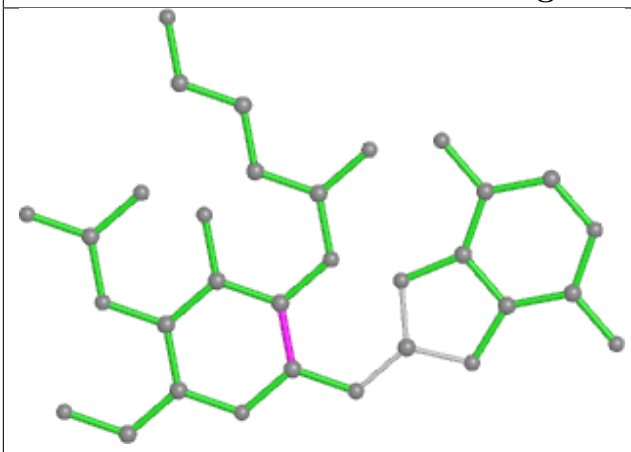


Torsions

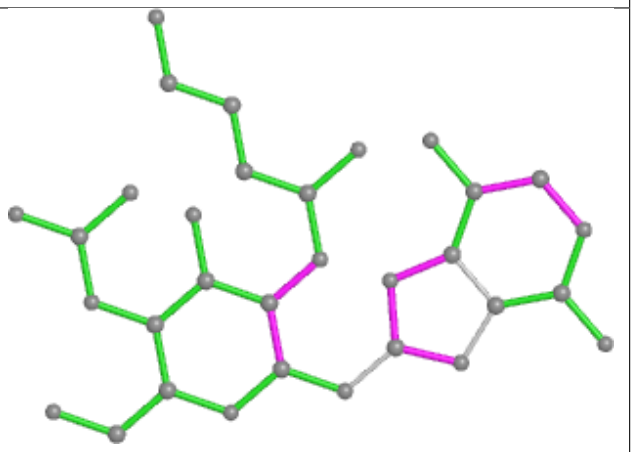


Rings

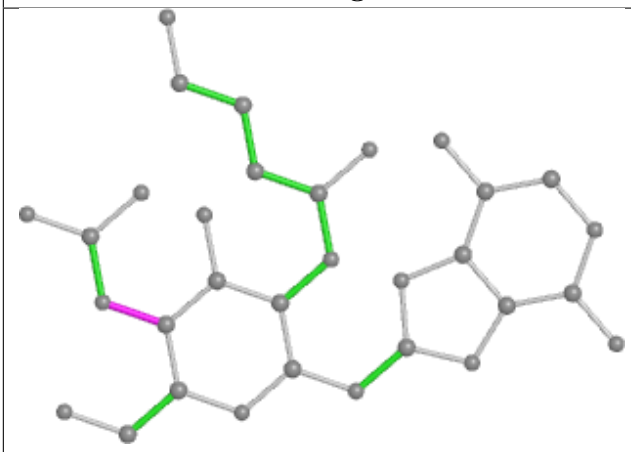
Ligand I60 B 703



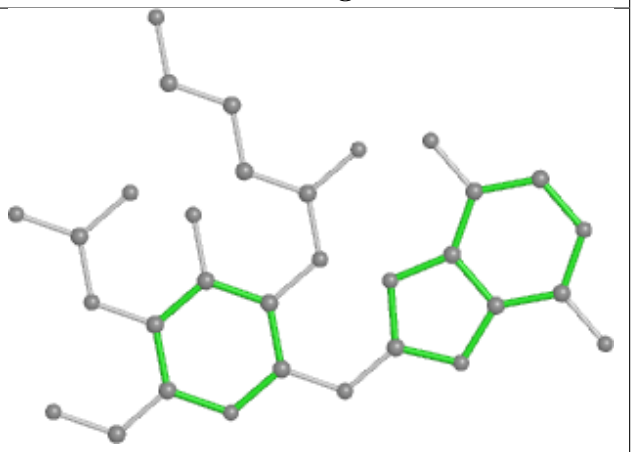
Bond lengths



Bond angles

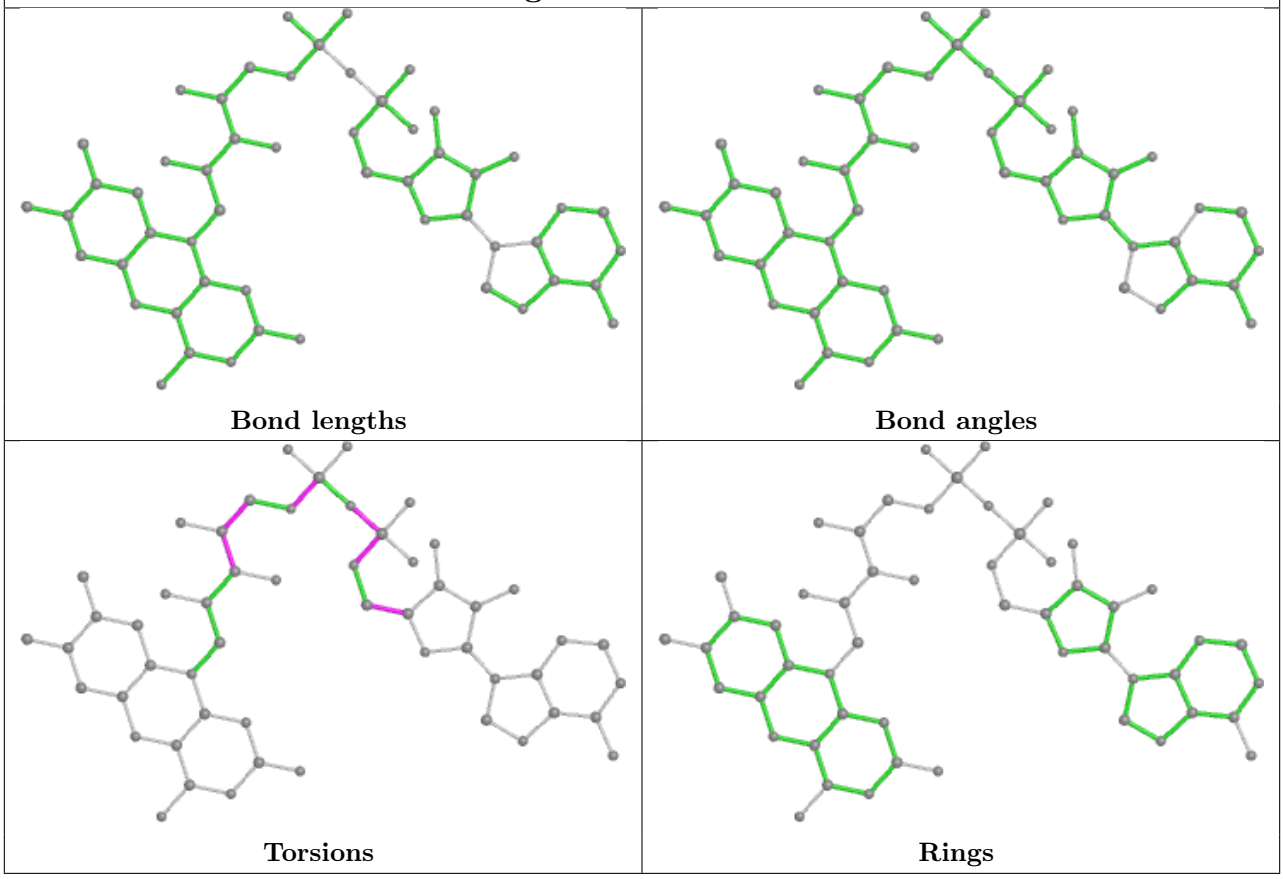


Torsions



Rings

Ligand FAD G 701



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^{th} 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%)	0.05	2 (0%) 92 93	12, 25, 47, 77	0
1	B	482/512 (94%)	0.05	2 (0%) 92 93	12, 24, 45, 73	0
1	C	472/512 (92%)	0.31	13 (2%) 53 59	12, 27, 58, 82	0
1	D	466/512 (91%)	0.73	54 (11%) 4 6	15, 41, 84, 104	0
1	E	482/512 (94%)	0.09	3 (0%) 89 91	11, 25, 46, 76	0
1	F	482/512 (94%)	0.07	4 (0%) 86 88	12, 25, 46, 72	0
1	G	472/512 (92%)	0.37	25 (5%) 26 31	12, 27, 58, 85	0
1	H	465/512 (90%)	0.74	55 (11%) 4 5	15, 41, 83, 96	0
All	All	3803/4096 (92%)	0.30	158 (4%) 36 42	11, 28, 68, 104	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	LEU	7.4
1	G	253	GLY	7.1
1	D	202	ILE	6.7
1	H	202	ILE	5.9
1	H	236	LEU	5.6
1	H	243	LEU	5.3
1	D	361	TRP	5.3
1	D	222	ALA	5.1
1	H	219	PHE	5.1
1	H	239	ALA	5.0
1	C	44	PRO	5.0
1	H	238	ALA	4.8
1	D	223	GLY	4.7
1	D	352	ILE	4.5
1	H	220	LEU	4.3
1	G	343	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	361	TRP	4.2
1	D	226	VAL	4.0
1	D	34	PRO	4.0
1	B	35	ASP	3.9
1	H	227	VAL	3.9
1	D	33	ARG	3.8
1	D	212	VAL	3.8
1	H	217	GLY	3.8
1	H	225	VAL	3.8
1	D	199	ALA	3.8
1	H	222	ALA	3.8
1	D	224	HIS	3.8
1	D	32	THR	3.7
1	D	387	GLY	3.7
1	G	242	GLY	3.7
1	C	238	ALA	3.6
1	H	29	ILE	3.6
1	H	213	VAL	3.6
1	H	193	ARG	3.6
1	H	360	LEU	3.5
1	G	367	TYR	3.5
1	D	491	HIS	3.5
1	D	360	LEU	3.5
1	D	237	VAL	3.4
1	G	342	ARG	3.4
1	D	35	ASP	3.4
1	H	353	GLY	3.4
1	H	384	LEU	3.3
1	D	219	PHE	3.3
1	H	54	ALA	3.3
1	H	240	LEU	3.3
1	H	48	TYR	3.3
1	D	190	ALA	3.3
1	G	216	ASP	3.3
1	D	39	THR	3.2
1	D	193	ARG	3.2
1	H	393	GLY	3.2
1	H	16	VAL	3.2
1	D	392	ASP	3.2
1	H	212	VAL	3.2
1	D	243	LEU	3.2
1	D	14	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	14	ILE	3.1
1	H	38	VAL	3.0
1	C	236	LEU	3.0
1	D	194	LEU	3.0
1	G	363	LEU	3.0
1	G	491	HIS	3.0
1	E	11	THR	2.9
1	G	235	ARG	2.9
1	D	356	SER	2.9
1	G	206	HIS	2.9
1	H	391	VAL	2.8
1	H	235	ARG	2.8
1	H	216	ASP	2.8
1	D	384	LEU	2.8
1	D	225	VAL	2.8
1	G	254	VAL	2.8
1	H	215	ASP	2.8
1	D	192	GLY	2.8
1	H	53	ALA	2.7
1	D	90	GLU	2.7
1	C	232	ARG	2.7
1	D	376	LEU	2.7
1	G	55	GLY	2.7
1	H	352	ILE	2.7
1	H	188	LEU	2.7
1	H	253	GLY	2.7
1	H	30	ALA	2.7
1	H	379	ARG	2.7
1	D	394	LEU	2.7
1	E	395	ARG	2.6
1	C	251	TYR	2.6
1	H	224	HIS	2.6
1	H	389	THR	2.6
1	G	369	ASP	2.6
1	C	244	ALA	2.6
1	D	187	PHE	2.6
1	G	243	LEU	2.6
1	H	23	LEU	2.5
1	D	221	PRO	2.5
1	D	54	ALA	2.5
1	G	204	ALA	2.5
1	H	395	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	398	ARG	2.5
1	G	366	THR	2.5
1	D	191	GLY	2.5
1	D	50	ALA	2.5
1	D	197	VAL	2.4
1	C	341	SER	2.4
1	G	303	LEU	2.4
1	G	11	THR	2.4
1	D	382	VAL	2.4
1	B	392	ASP	2.4
1	H	488	ARG	2.4
1	D	38	VAL	2.3
1	H	47	GLN	2.3
1	H	226	VAL	2.3
1	G	232	ARG	2.3
1	H	195	HIS	2.3
1	C	218	ASP	2.3
1	F	392	ASP	2.3
1	G	236	LEU	2.3
1	H	354	GLY	2.3
1	D	20	VAL	2.3
1	H	392	ASP	2.3
1	H	247	ILE	2.3
1	H	439	MET	2.2
1	H	381	VAL	2.2
1	C	282	GLY	2.2
1	A	11	THR	2.2
1	D	183	LEU	2.2
1	D	240	LEU	2.2
1	D	227	VAL	2.2
1	A	99	GLY	2.2
1	F	363	LEU	2.2
1	G	41	LEU	2.2
1	D	48	TYR	2.2
1	F	36	VAL	2.2
1	C	10	GLN	2.2
1	C	235	ARG	2.2
1	H	385	MET	2.2
1	G	21	LEU	2.2
1	G	197	VAL	2.2
1	H	52	PRO	2.1
1	D	490	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	379	ARG	2.1
1	H	49	GLY	2.1
1	D	51	THR	2.1
1	C	208	ARG	2.1
1	G	215	ASP	2.0
1	H	41	LEU	2.0
1	C	253	GLY	2.0
1	E	223	GLY	2.0
1	F	398	ARG	2.0
1	D	236	LEU	2.0
1	D	353	GLY	2.0
1	G	43	LYS	2.0
1	D	182	ALA	2.0
1	D	366	THR	2.0
1	D	488	ARG	2.0
1	H	382	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	G	701	53/53	0.40	0.39	67,91,115,120	0
2	FAD	C	701	53/53	0.41	0.40	66,93,119,124	0
3	GLY	D	702	5/5	0.80	0.20	47,52,53,54	0
2	FAD	D	701	53/53	0.81	0.18	52,62,82,84	0
3	GLY	G	702	5/5	0.82	0.35	53,65,70,71	0
4	I60	C	703	32/32	0.84	0.19	23,40,80,90	0
2	FAD	H	701	53/53	0.85	0.19	52,62,83,85	0

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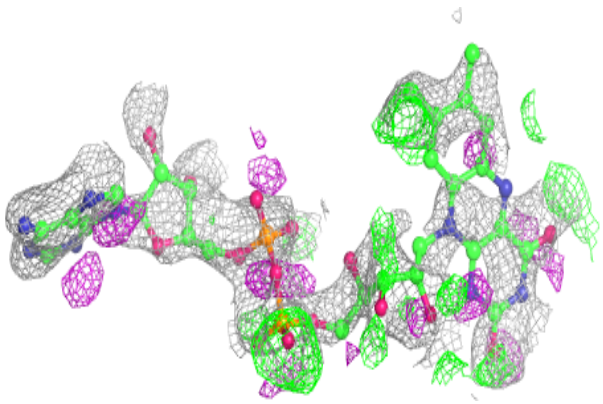
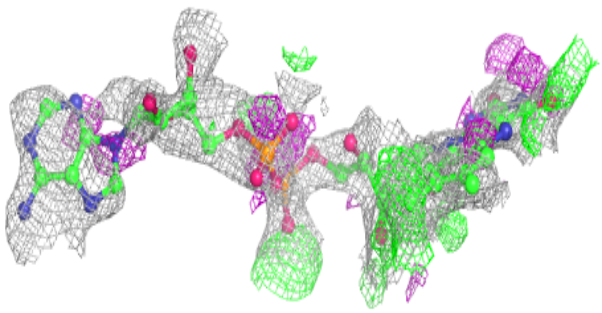
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLY	C	702	5/5	0.87	0.36	58,70,75,76	0
4	I60	E	703	32/32	0.87	0.17	19,33,41,44	0
4	I60	G	703	32/32	0.87	0.15	25,40,74,75	0
3	GLY	H	702	5/5	0.88	0.13	43,49,52,53	0
4	I60	F	703	32/32	0.88	0.15	21,41,51,54	0
4	I60	D	703	32/32	0.88	0.17	25,49,81,82	0
4	I60	H	703	32/32	0.89	0.17	28,46,70,70	0
4	I60	A	703	32/32	0.90	0.14	20,34,45,49	0
4	I60	B	703	32/32	0.90	0.19	23,42,51,56	0
2	FAD	F	701	53/53	0.94	0.11	16,18,20,22	0
3	GLY	F	702	5/5	0.94	0.17	21,25,27,27	0
2	FAD	A	701	53/53	0.95	0.11	18,20,23,25	0
2	FAD	E	701	53/53	0.95	0.11	18,22,24,26	0
3	GLY	E	702	5/5	0.96	0.14	23,25,33,33	0
3	GLY	B	702	5/5	0.97	0.12	21,24,26,27	0
2	FAD	B	701	53/53	0.97	0.10	17,18,20,21	0
3	GLY	A	702	5/5	0.97	0.09	22,24,31,31	0

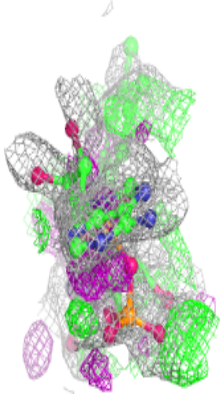
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

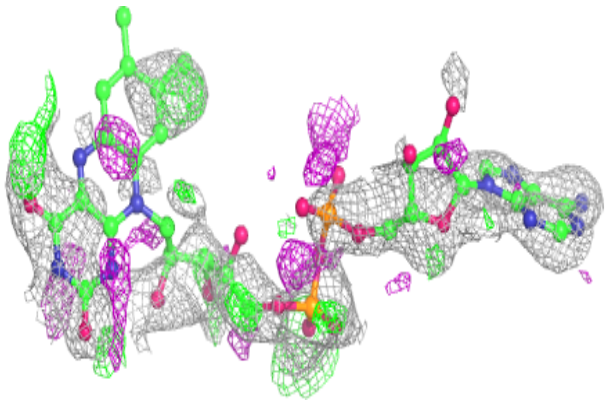


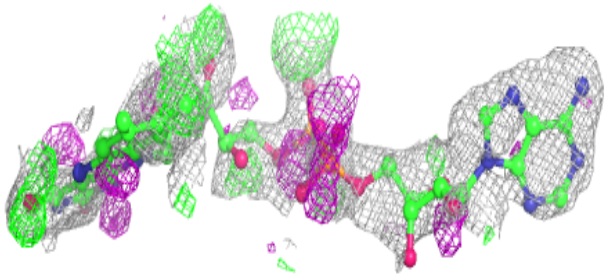


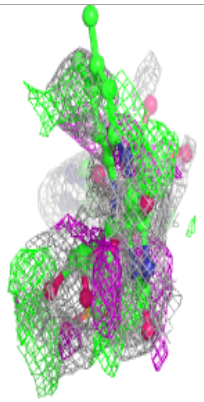


Electron density around FAD C 701:

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

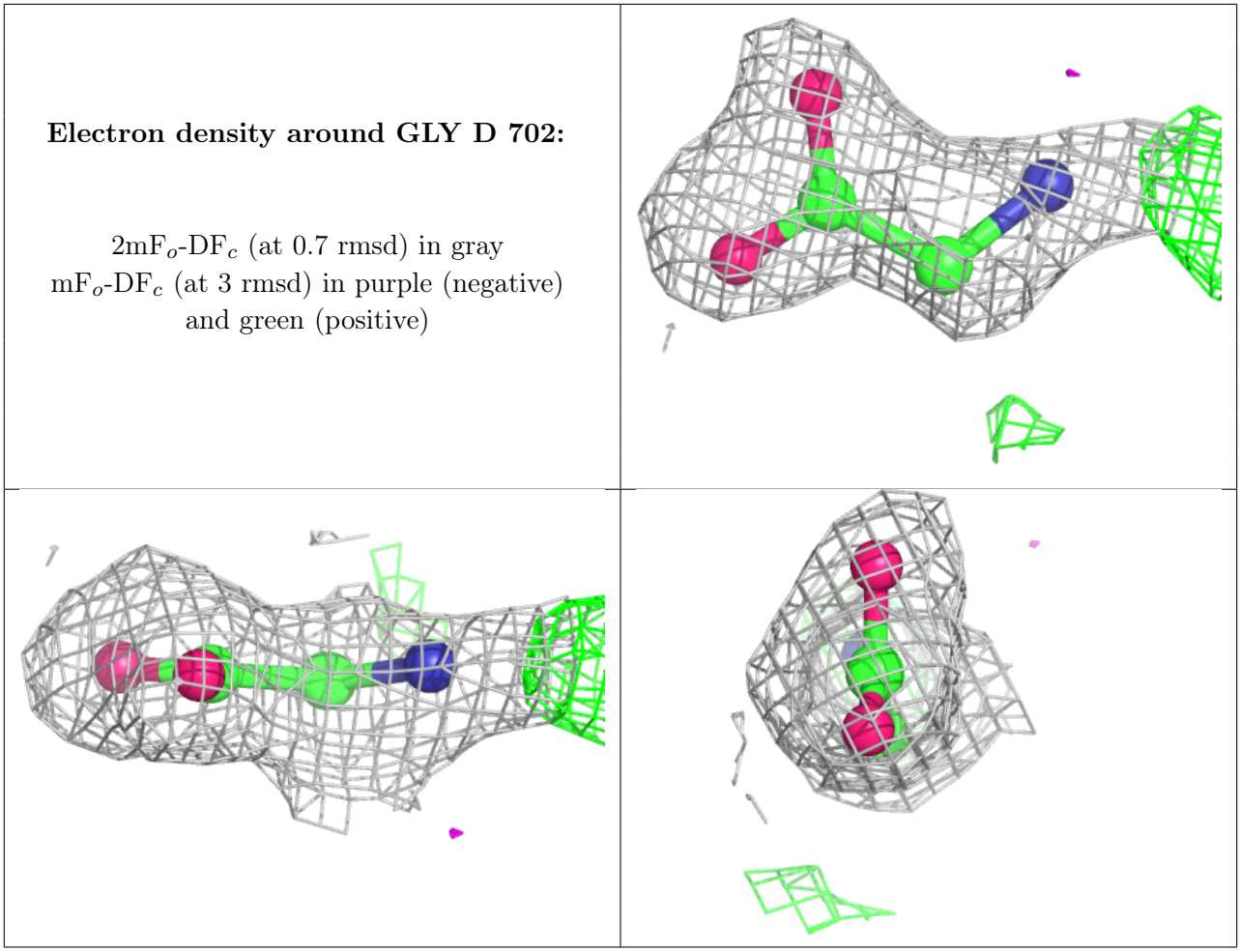






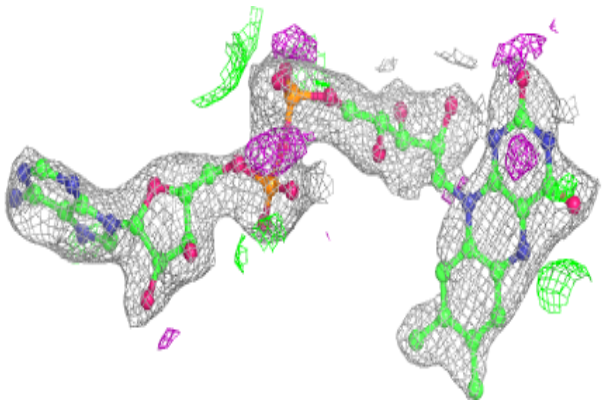
Electron density around GLY D 702:

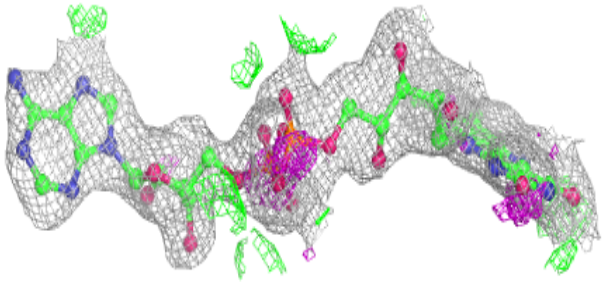
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

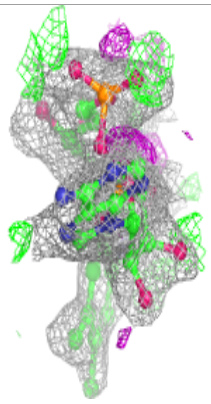


Electron density around FAD D 701:

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

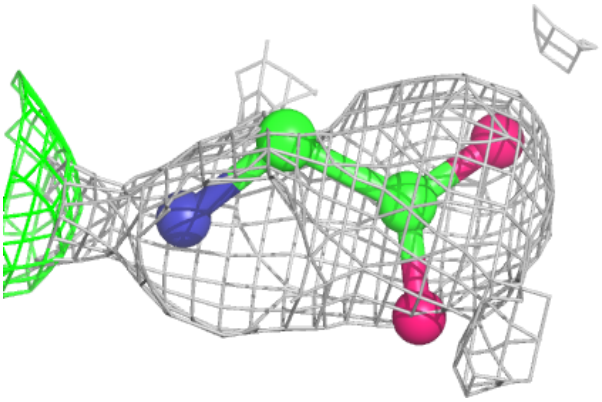


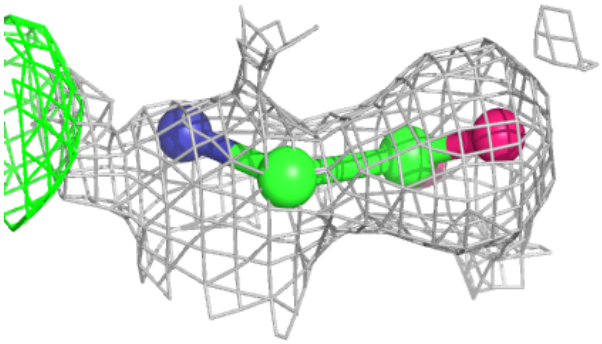


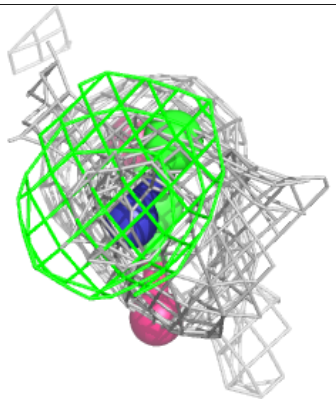


Electron density around GLY G 702:

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

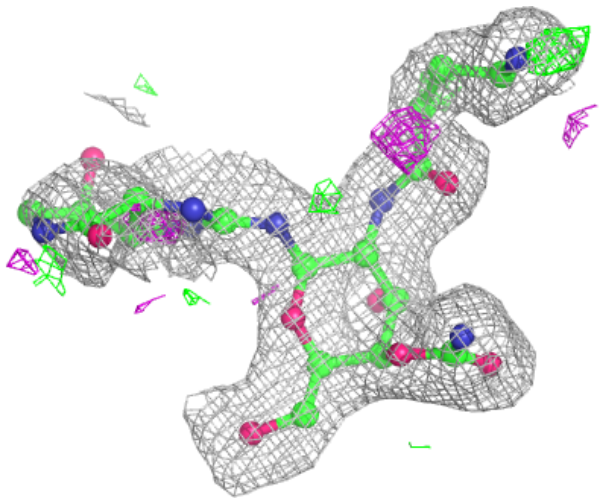


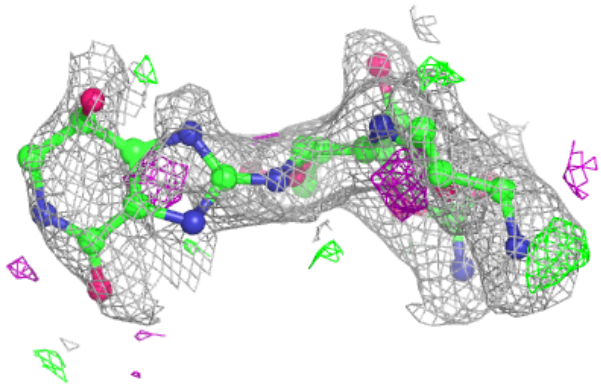


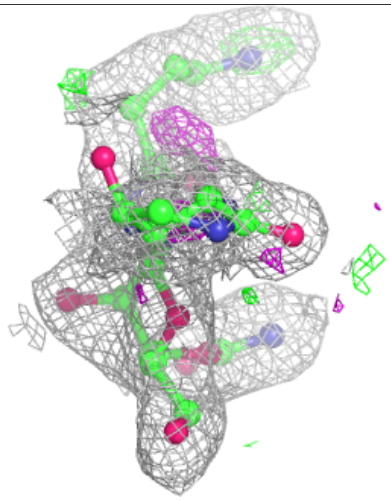


Electron density around I60 C 703:

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

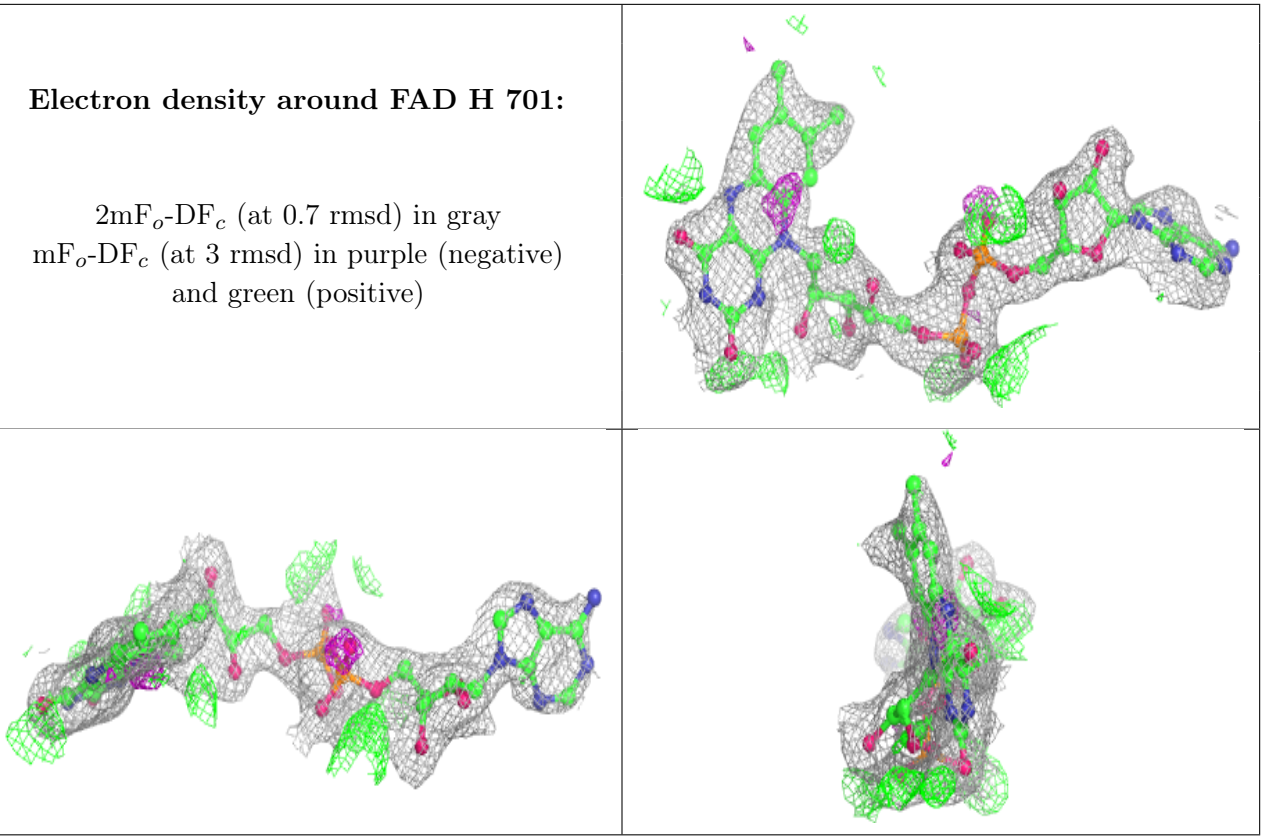






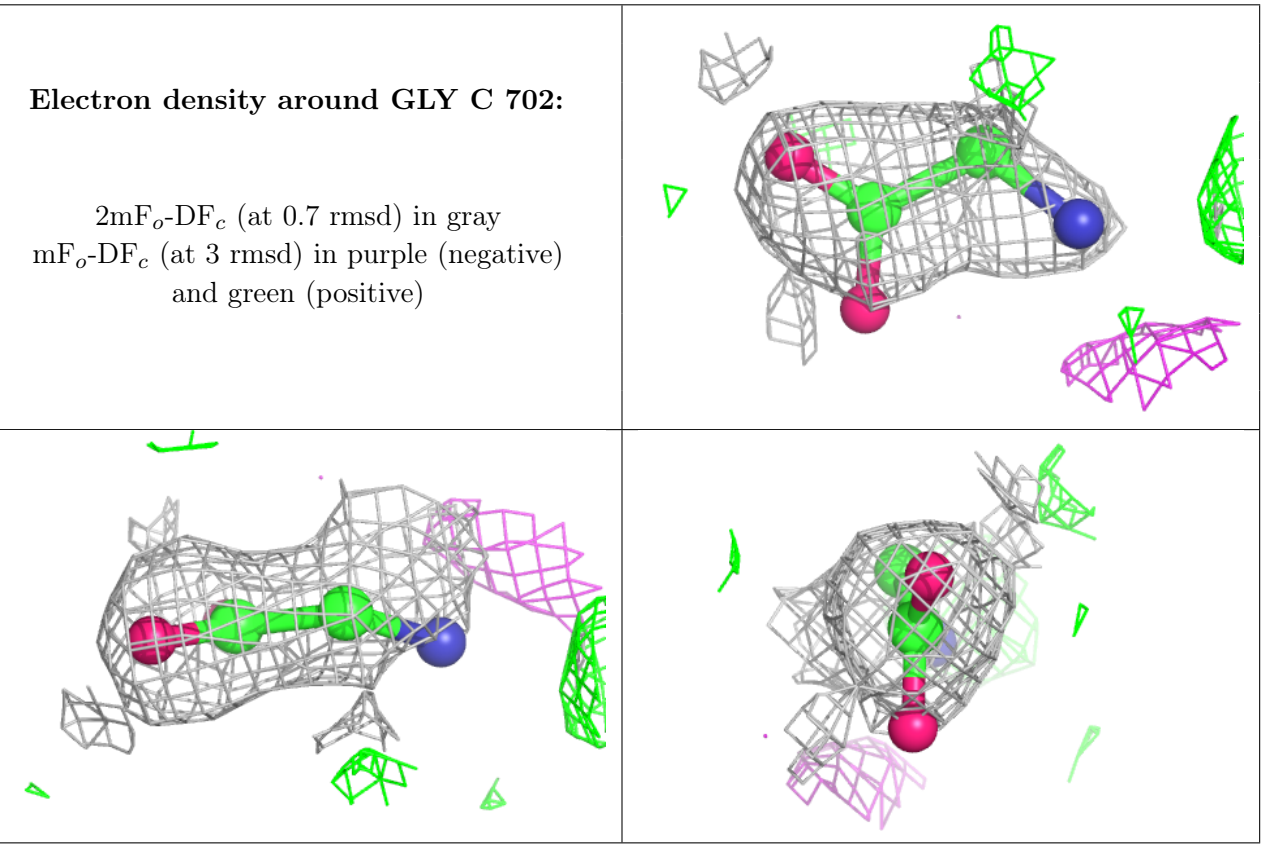
Electron density around FAD H 701:

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



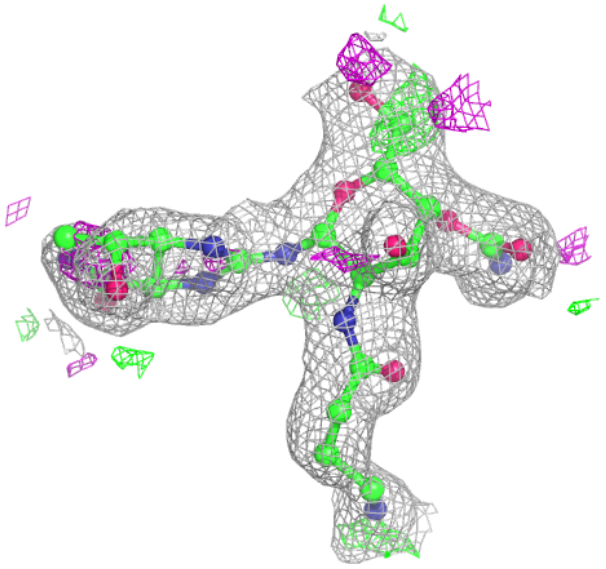
Electron density around GLY C 702:

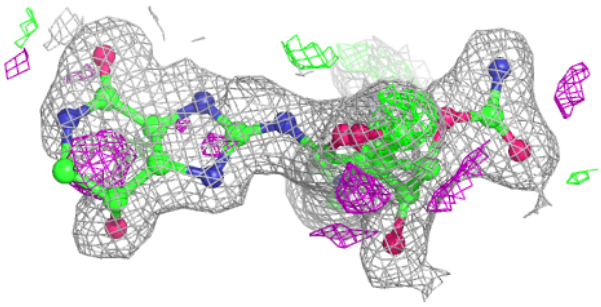
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

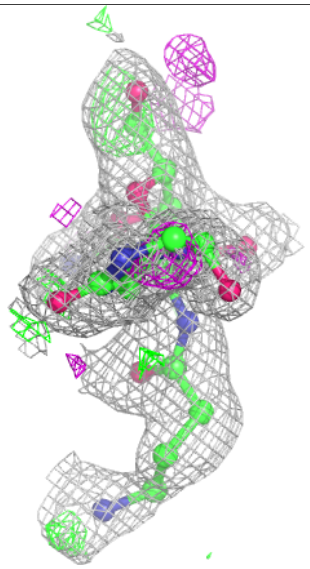


Electron density around I60 E 703:

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

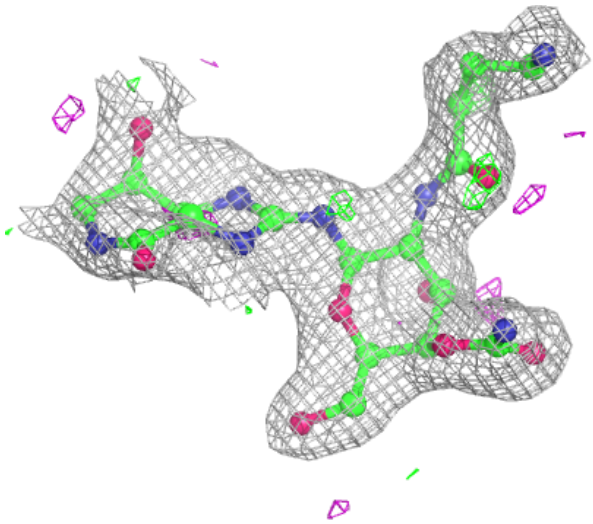


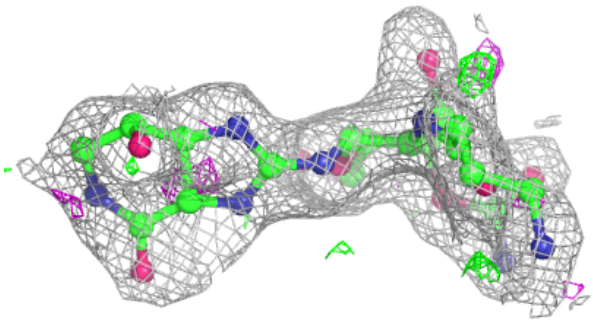


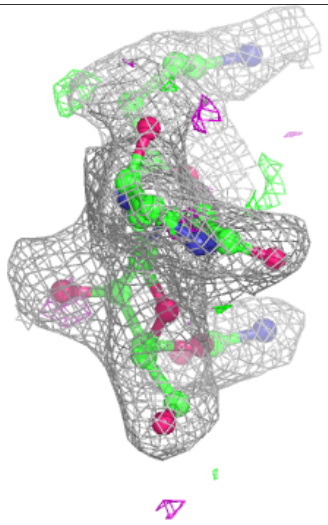


Electron density around I60 G 703:

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

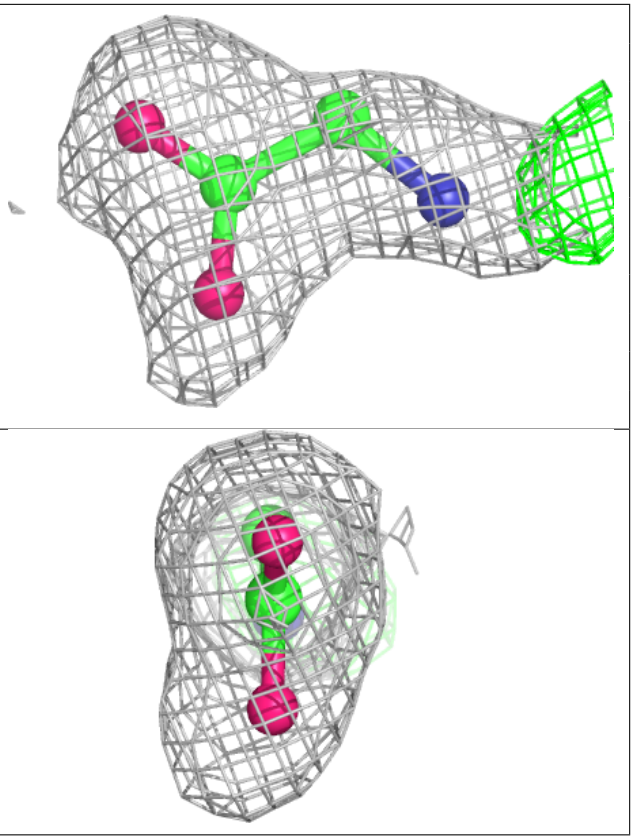






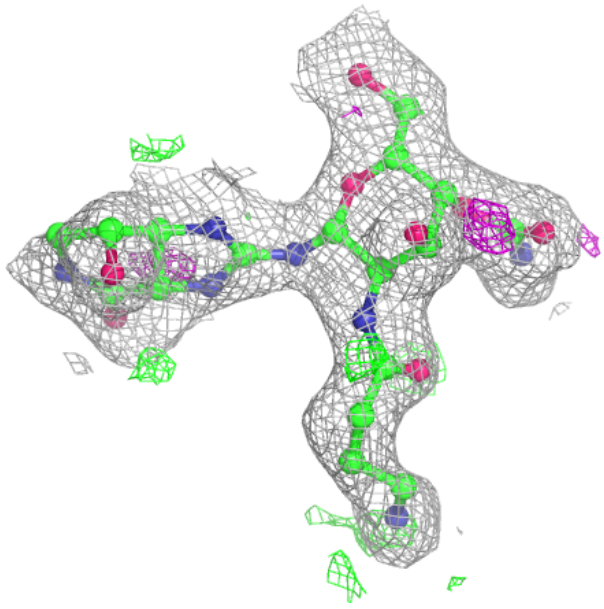
Electron density around GLY H 702:

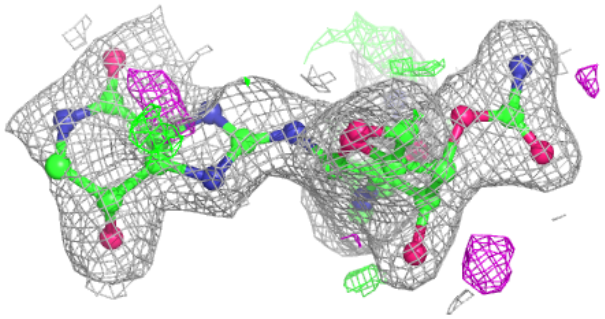
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

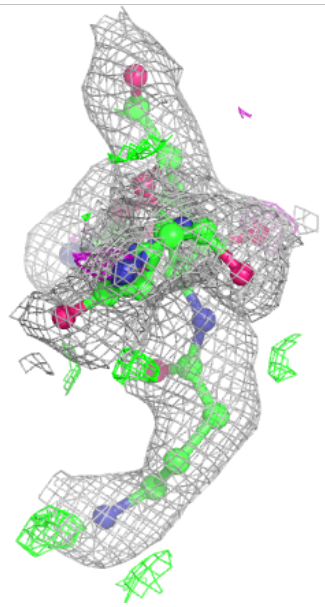


Electron density around I60 F 703:

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

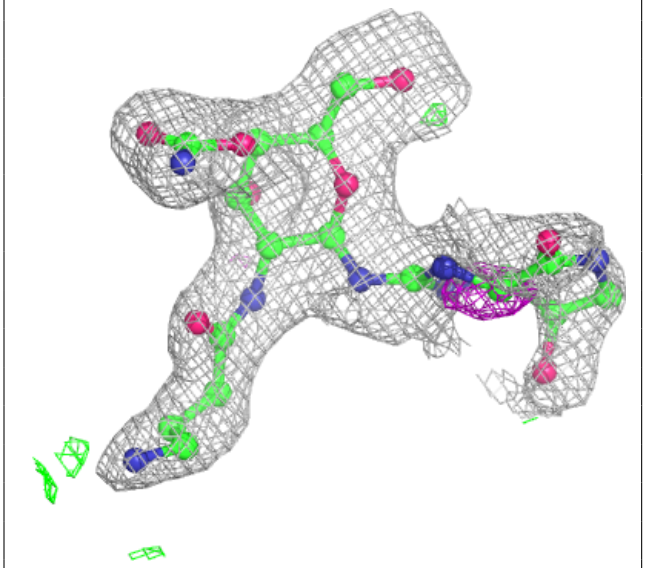


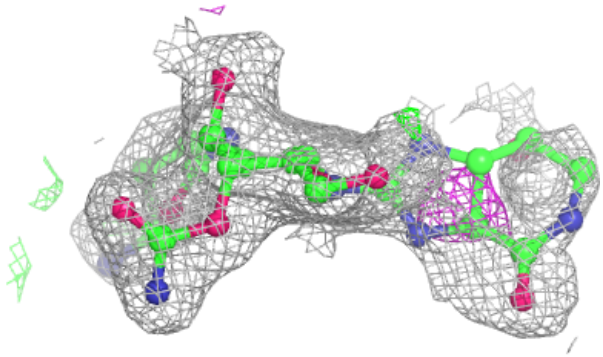


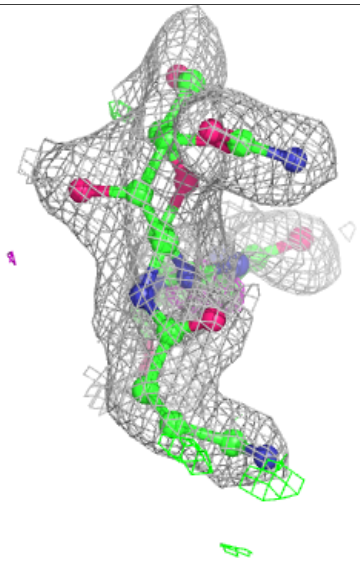


Electron density around I60 D 703:

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

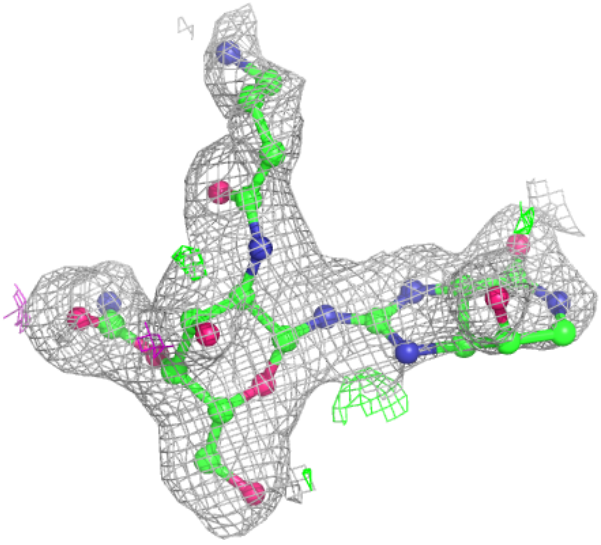


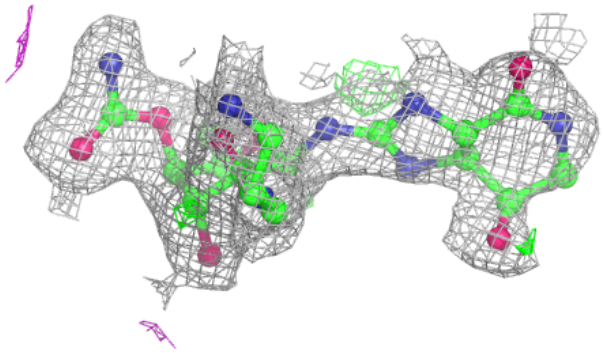


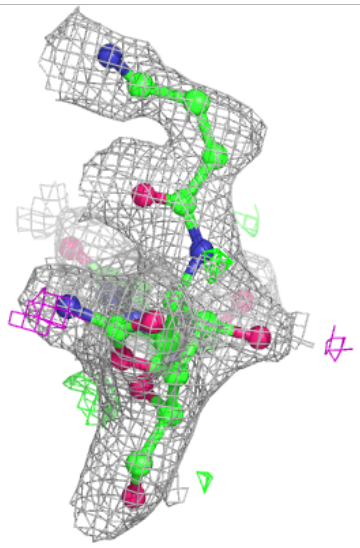


Electron density around I60 H 703:

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

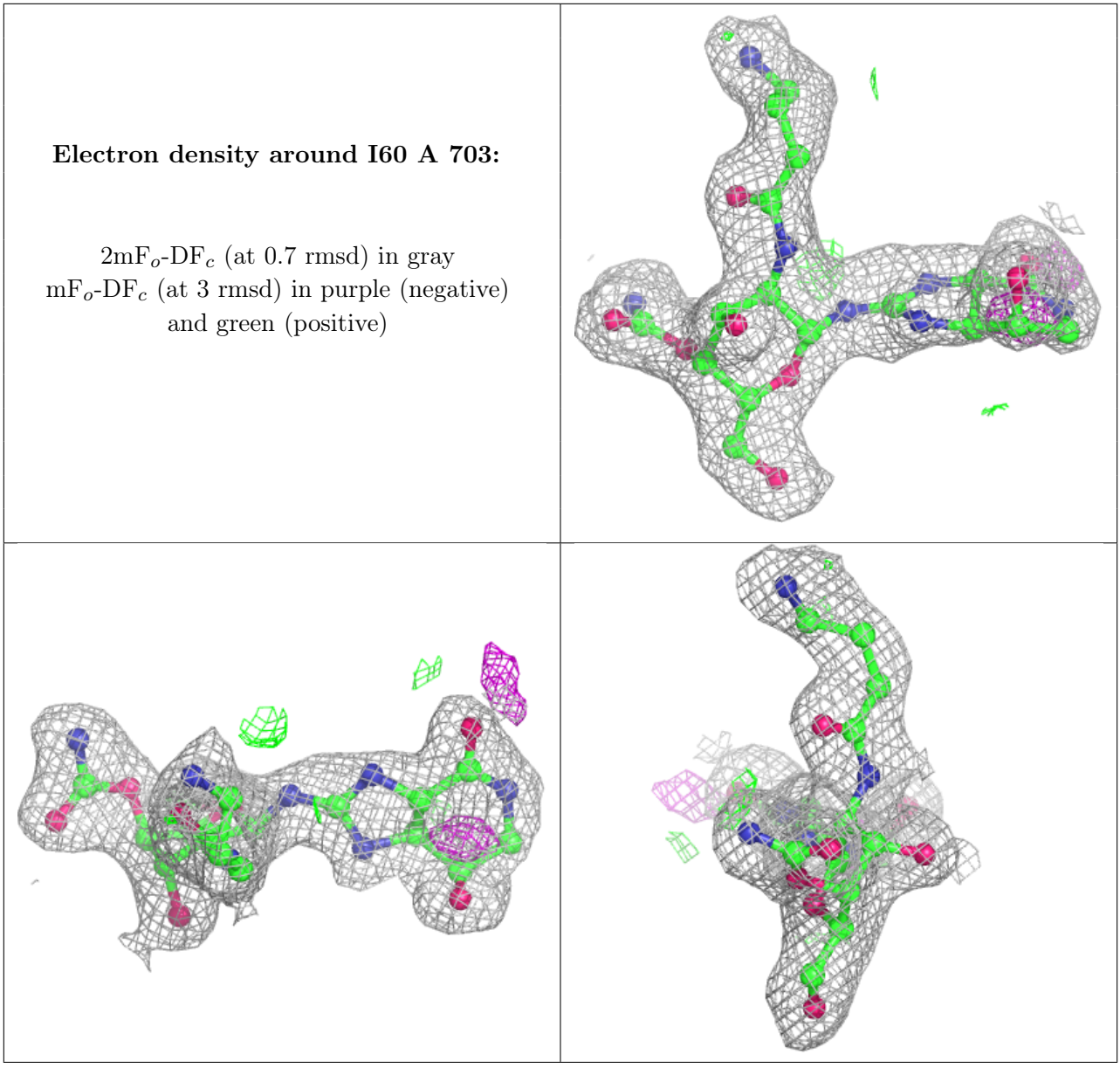






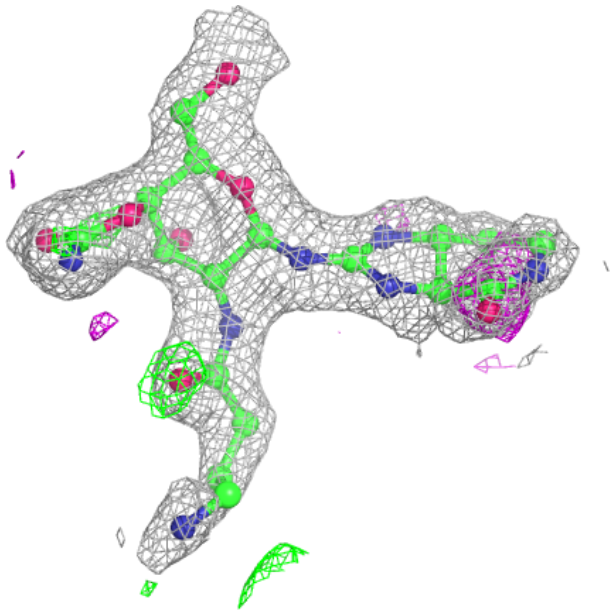
Electron density around I60 A 703:

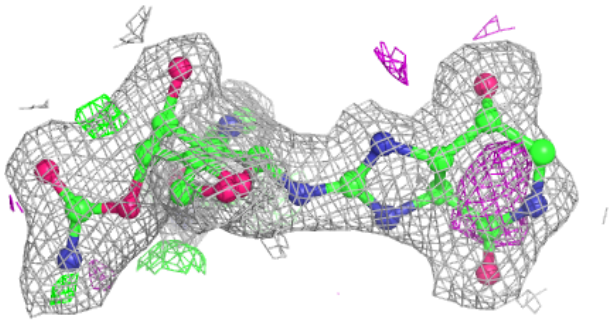
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

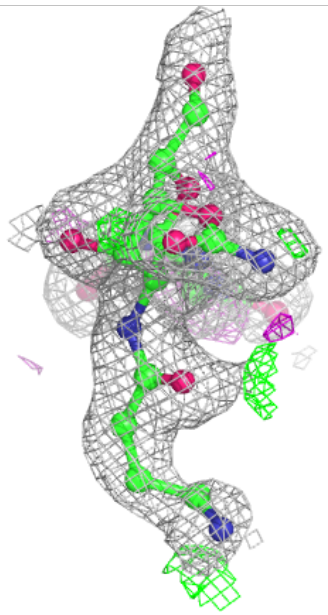


Electron density around I60 B 703:

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







Electron density around FAD F 701:

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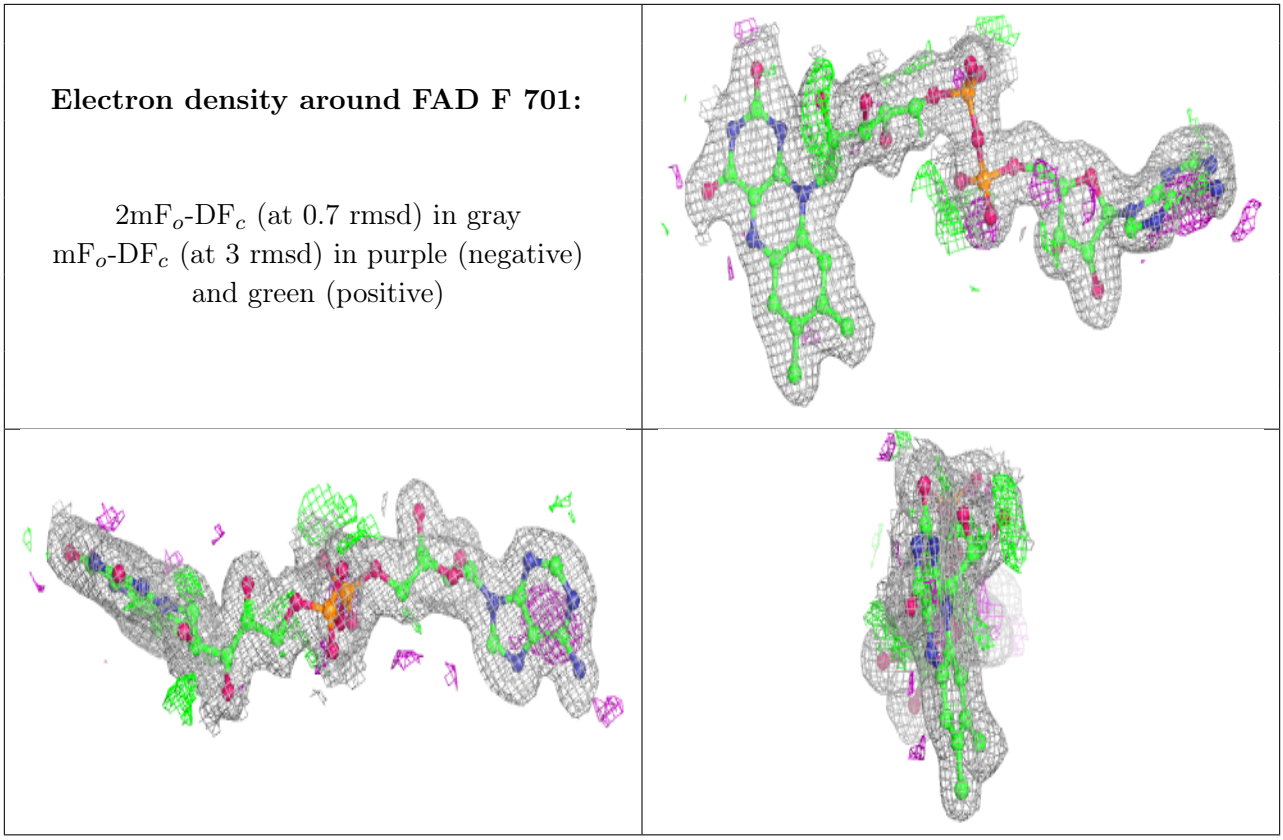
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GLY F 702:

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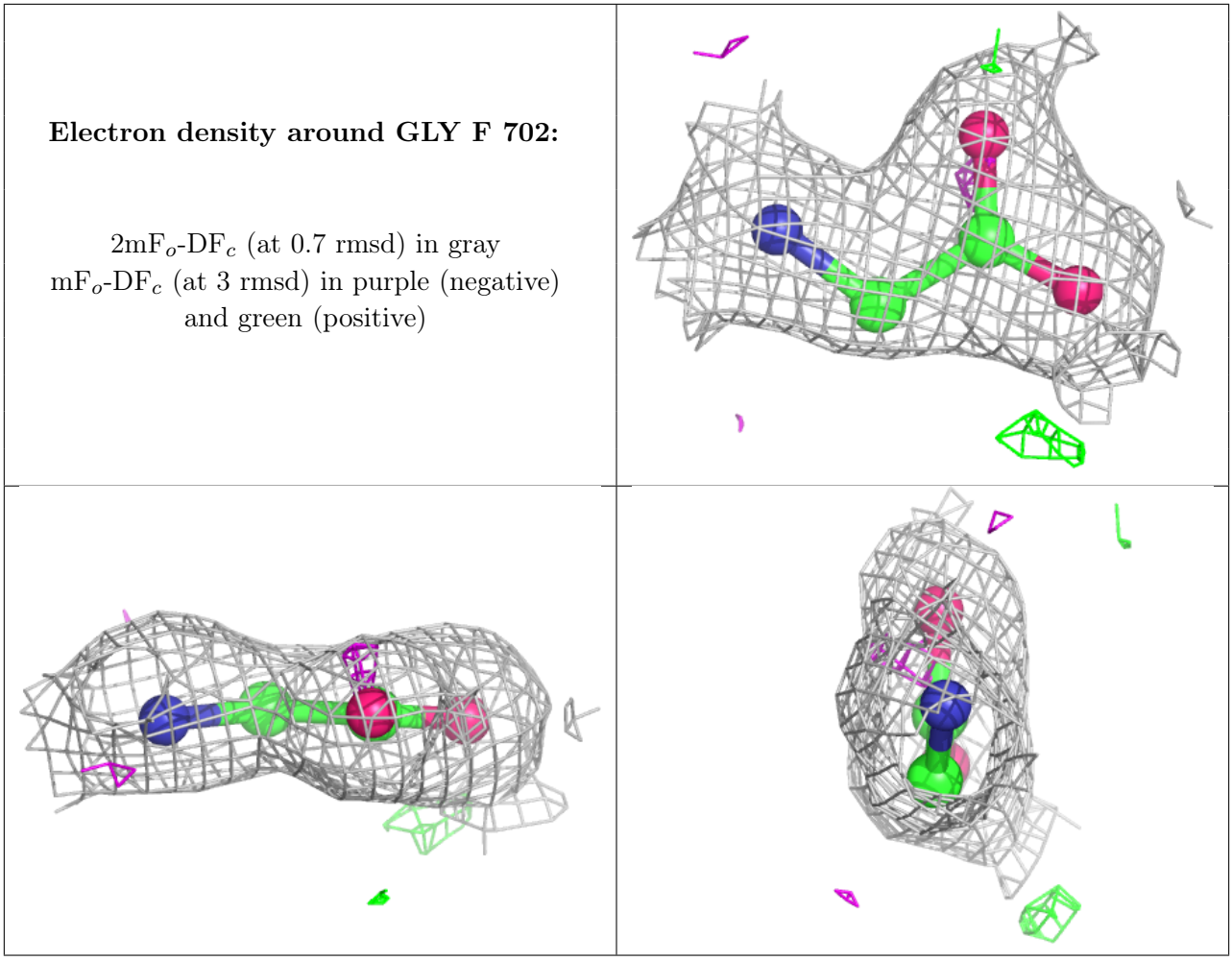
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD A 701:

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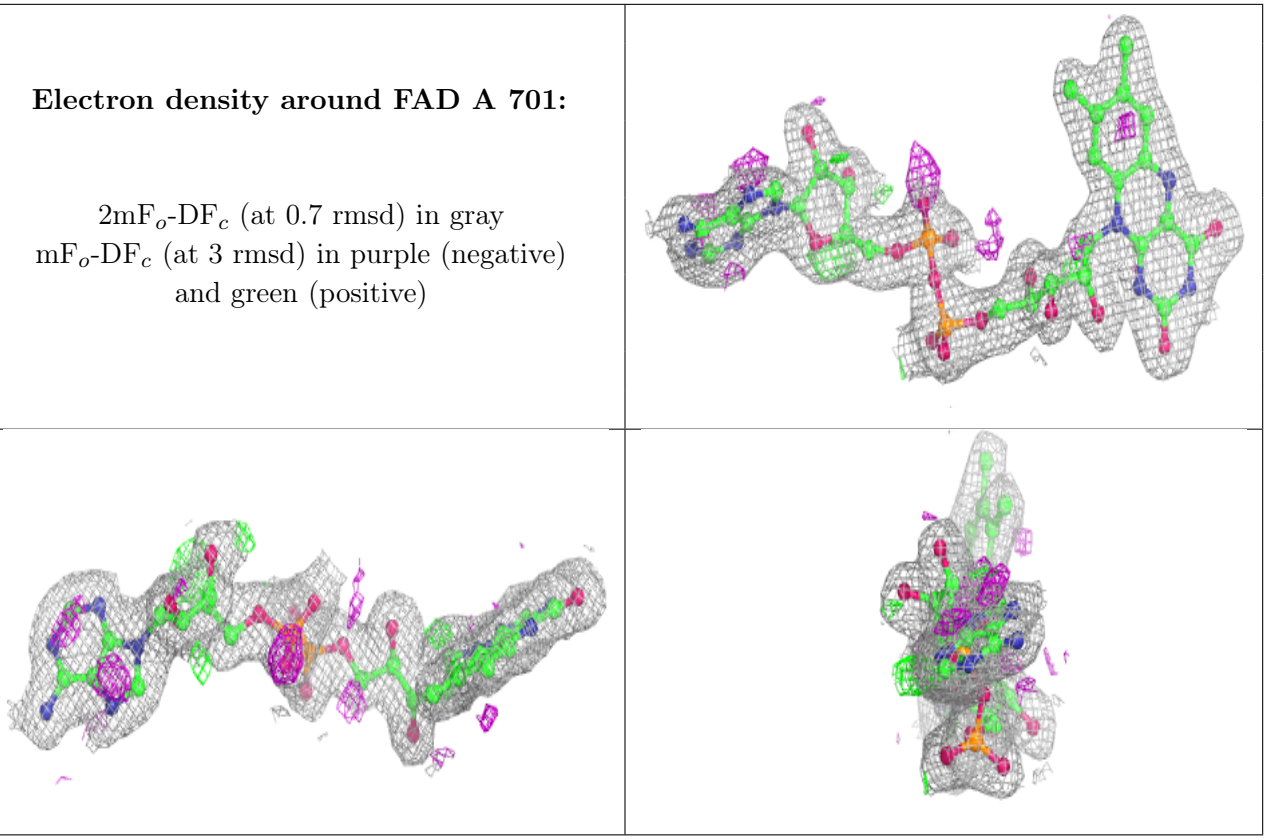
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD E 701:

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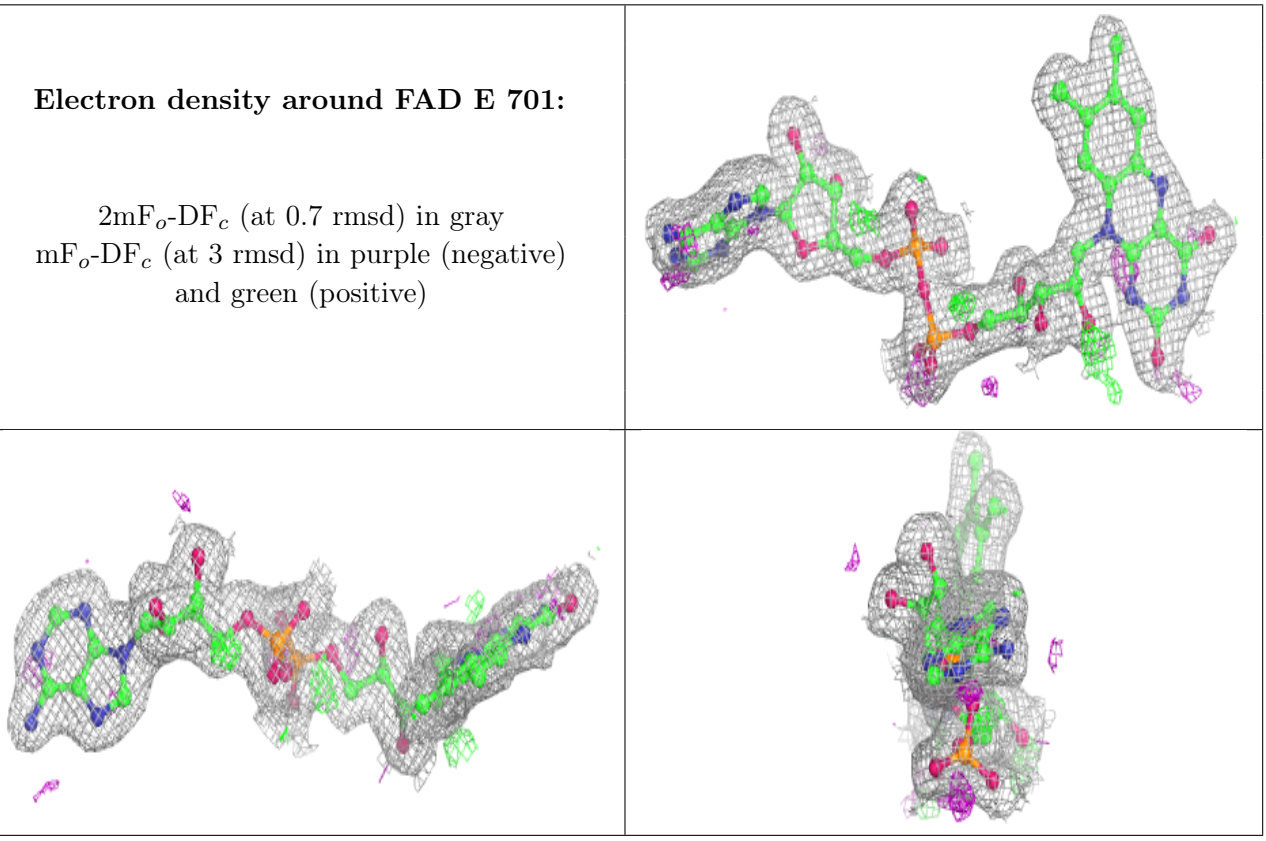
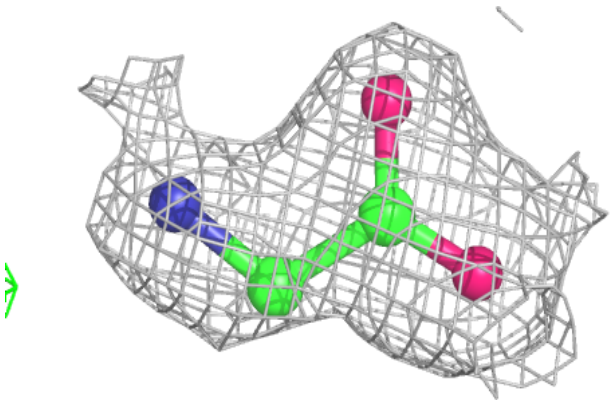
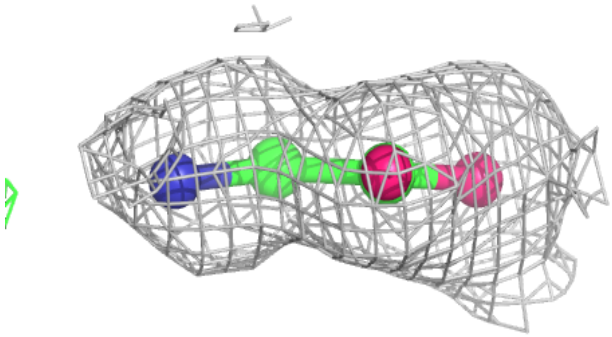
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

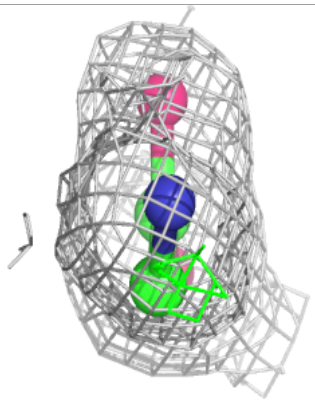


Electron density around GLY E 702:

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

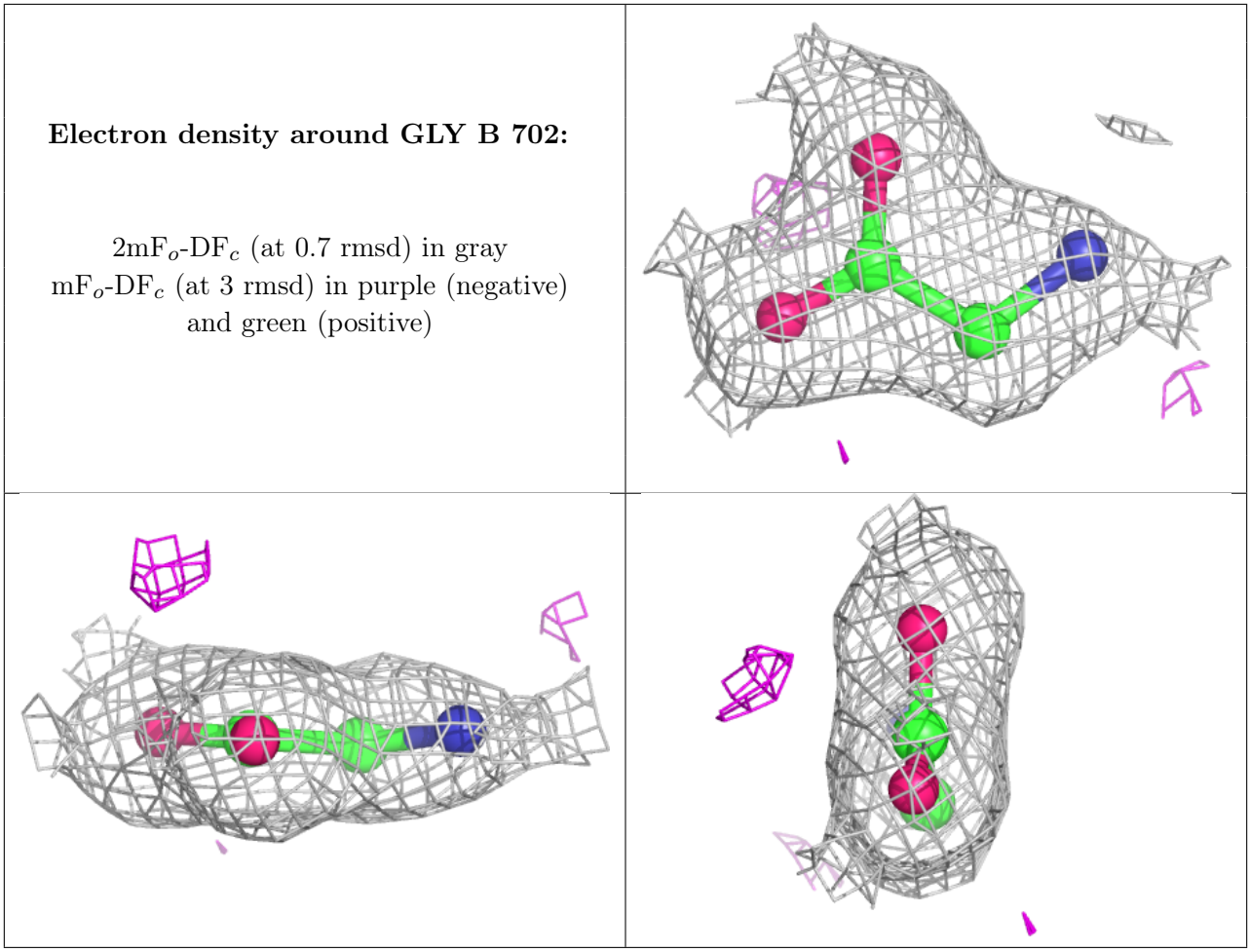






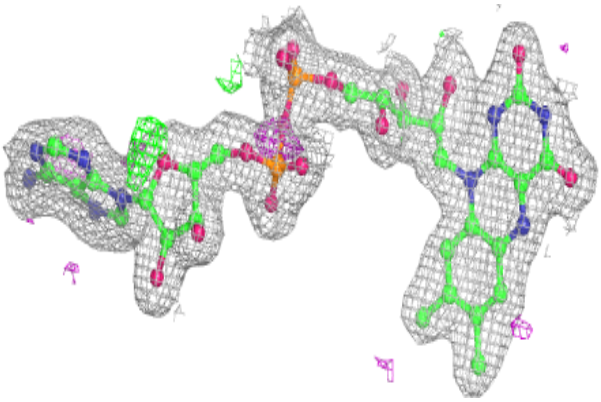
Electron density around GLY B 702:

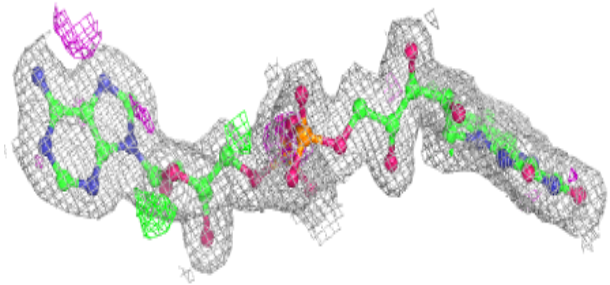
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

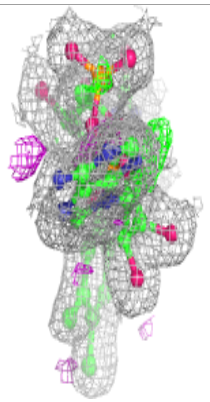


Electron density around FAD B 701:

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

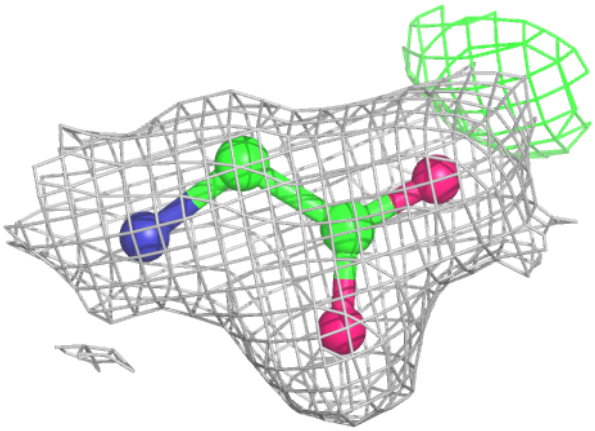


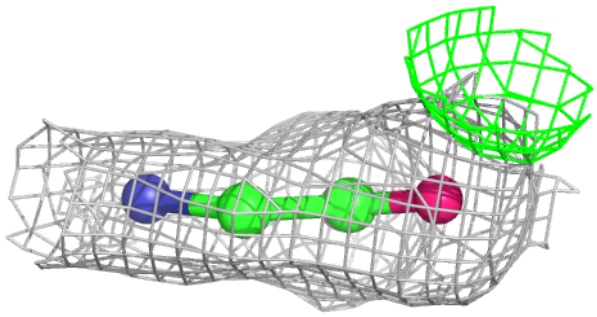


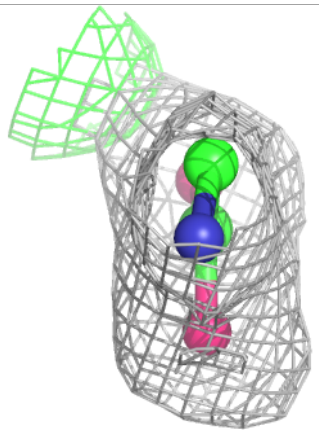


Electron density around GLY A 702:

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







6.5 Other polymers (i)

There are no such residues in this entry.