



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:49 PM UTC

PDB ID : 8GRI / pdb_00008gri
Title : Orf1-E312A-glycine-glycylthricin
Authors : Wang, Y.L.; Li, T.L.
Deposited on : 2022-09-01
Resolution : 2.37 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

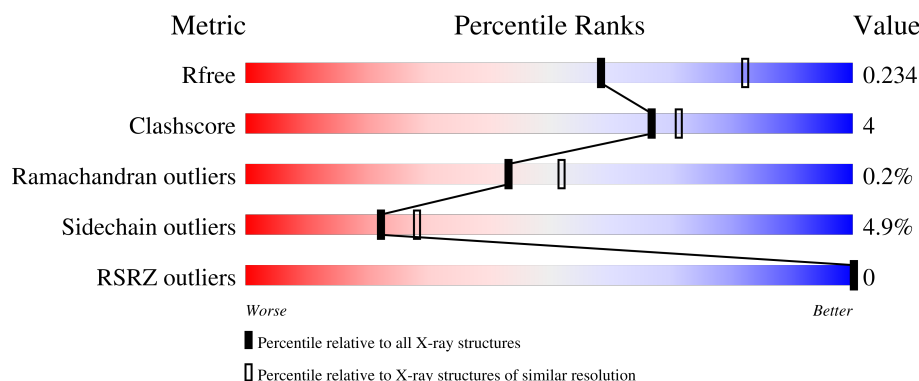
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	512	 85% 8% • 6%
1	B	512	 84% 9% • 6%
1	F	512	 85% 8% • 6%
2	C	512	 84% 9% • 6%
2	D	512	 84% 8% • 7%

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Mol	Chain	Length	Quality of chain
2	E	512	85% 8% • 6%
2	G	512	84% 9% • 6%
2	H	512	82% 8% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30454 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	481	Total	C	N	O	S	0	1	0
			3653	2291	660	689	13			
1	B	481	Total	C	N	O	S	0	1	0
			3653	2291	660	689	13			
1	F	482	Total	C	N	O	S	0	1	0
			3662	2296	662	691	13			

There are 66 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
A	-7	LEU	-	expression tag	UNP A0A125SZC1
A	-6	VAL	-	expression tag	UNP A0A125SZC1
A	-5	PRO	-	expression tag	UNP A0A125SZC1
A	-4	ARG	-	expression tag	UNP A0A125SZC1
A	-3	GLY	-	expression tag	UNP A0A125SZC1
A	-2	SER	-	expression tag	UNP A0A125SZC1
A	-1	HIS	-	expression tag	UNP A0A125SZC1
A	0	MET	-	expression tag	UNP A0A125SZC1
A	312	ALA	GLU	engineered mutation	UNP A0A125SZC1
B	-20	MET	-	initiating methionine	UNP A0A125SZC1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP A0A125SZC1
B	-18	SER	-	expression tag	UNP A0A125SZC1
B	-17	SER	-	expression tag	UNP A0A125SZC1
B	-16	HIS	-	expression tag	UNP A0A125SZC1
B	-15	HIS	-	expression tag	UNP A0A125SZC1
B	-14	HIS	-	expression tag	UNP A0A125SZC1
B	-13	HIS	-	expression tag	UNP A0A125SZC1
B	-12	HIS	-	expression tag	UNP A0A125SZC1
B	-11	HIS	-	expression tag	UNP A0A125SZC1
B	-10	SER	-	expression tag	UNP A0A125SZC1
B	-9	SER	-	expression tag	UNP A0A125SZC1
B	-8	GLY	-	expression tag	UNP A0A125SZC1
B	-7	LEU	-	expression tag	UNP A0A125SZC1
B	-6	VAL	-	expression tag	UNP A0A125SZC1
B	-5	PRO	-	expression tag	UNP A0A125SZC1
B	-4	ARG	-	expression tag	UNP A0A125SZC1
B	-3	GLY	-	expression tag	UNP A0A125SZC1
B	-2	SER	-	expression tag	UNP A0A125SZC1
B	-1	HIS	-	expression tag	UNP A0A125SZC1
B	0	MET	-	expression tag	UNP A0A125SZC1
B	312	ALA	GLU	engineered mutation	UNP A0A125SZC1
F	-20	MET	-	initiating methionine	UNP A0A125SZC1
F	-19	GLY	-	expression tag	UNP A0A125SZC1
F	-18	SER	-	expression tag	UNP A0A125SZC1
F	-17	SER	-	expression tag	UNP A0A125SZC1
F	-16	HIS	-	expression tag	UNP A0A125SZC1
F	-15	HIS	-	expression tag	UNP A0A125SZC1
F	-14	HIS	-	expression tag	UNP A0A125SZC1
F	-13	HIS	-	expression tag	UNP A0A125SZC1
F	-12	HIS	-	expression tag	UNP A0A125SZC1
F	-11	HIS	-	expression tag	UNP A0A125SZC1
F	-10	SER	-	expression tag	UNP A0A125SZC1
F	-9	SER	-	expression tag	UNP A0A125SZC1
F	-8	GLY	-	expression tag	UNP A0A125SZC1
F	-7	LEU	-	expression tag	UNP A0A125SZC1
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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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	312	ALA	GLU	engineered mutation	UNP A0A125SZC1

- Molecule 2 is a protein called N-formimidoyl fortimicin A synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	480	Total	C	N	O	S	0	1	0
			3640	2285	658	684	13			
2	D	477	Total	C	N	O	S	0	1	0
			3611	2269	652	677	13			
2	E	481	Total	C	N	O	S	0	1	0
			3641	2286	656	686	13			
2	G	481	Total	C	N	O	S	0	1	0
			3647	2289	659	686	13			
2	H	469	Total	C	N	O	S	0	1	0
			3557	2236	642	666	13			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
C	-7	LEU	-	expression tag	UNP A0A125SZC1
C	-6	VAL	-	expression tag	UNP A0A125SZC1
C	-5	PRO	-	expression tag	UNP A0A125SZC1
C	-4	ARG	-	expression tag	UNP A0A125SZC1
C	-3	GLY	-	expression tag	UNP A0A125SZC1
C	-2	SER	-	expression tag	UNP A0A125SZC1
C	-1	HIS	-	expression tag	UNP A0A125SZC1
C	0	MET	-	expression tag	UNP A0A125SZC1
C	312	ALA	GLU	engineered mutation	UNP A0A125SZC1
D	-20	MET	-	initiating methionine	UNP A0A125SZC1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	GLY	-	expression tag	UNP A0A125SZC1
D	-18	SER	-	expression tag	UNP A0A125SZC1
D	-17	SER	-	expression tag	UNP A0A125SZC1
D	-16	HIS	-	expression tag	UNP A0A125SZC1
D	-15	HIS	-	expression tag	UNP A0A125SZC1
D	-14	HIS	-	expression tag	UNP A0A125SZC1
D	-13	HIS	-	expression tag	UNP A0A125SZC1
D	-12	HIS	-	expression tag	UNP A0A125SZC1
D	-11	HIS	-	expression tag	UNP A0A125SZC1
D	-10	SER	-	expression tag	UNP A0A125SZC1
D	-9	SER	-	expression tag	UNP A0A125SZC1
D	-8	GLY	-	expression tag	UNP A0A125SZC1
D	-7	LEU	-	expression tag	UNP A0A125SZC1
D	-6	VAL	-	expression tag	UNP A0A125SZC1
D	-5	PRO	-	expression tag	UNP A0A125SZC1
D	-4	ARG	-	expression tag	UNP A0A125SZC1
D	-3	GLY	-	expression tag	UNP A0A125SZC1
D	-2	SER	-	expression tag	UNP A0A125SZC1
D	-1	HIS	-	expression tag	UNP A0A125SZC1
D	0	MET	-	expression tag	UNP A0A125SZC1
D	312	ALA	GLU	engineered mutation	UNP A0A125SZC1
E	-20	MET	-	initiating methionine	UNP A0A125SZC1
E	-19	GLY	-	expression tag	UNP A0A125SZC1
E	-18	SER	-	expression tag	UNP A0A125SZC1
E	-17	SER	-	expression tag	UNP A0A125SZC1
E	-16	HIS	-	expression tag	UNP A0A125SZC1
E	-15	HIS	-	expression tag	UNP A0A125SZC1
E	-14	HIS	-	expression tag	UNP A0A125SZC1
E	-13	HIS	-	expression tag	UNP A0A125SZC1
E	-12	HIS	-	expression tag	UNP A0A125SZC1
E	-11	HIS	-	expression tag	UNP A0A125SZC1
E	-10	SER	-	expression tag	UNP A0A125SZC1
E	-9	SER	-	expression tag	UNP A0A125SZC1
E	-8	GLY	-	expression tag	UNP A0A125SZC1
E	-7	LEU	-	expression tag	UNP A0A125SZC1
E	-6	VAL	-	expression tag	UNP A0A125SZC1
E	-5	PRO	-	expression tag	UNP A0A125SZC1
E	-4	ARG	-	expression tag	UNP A0A125SZC1
E	-3	GLY	-	expression tag	UNP A0A125SZC1
E	-2	SER	-	expression tag	UNP A0A125SZC1
E	-1	HIS	-	expression tag	UNP A0A125SZC1
E	0	MET	-	expression tag	UNP A0A125SZC1

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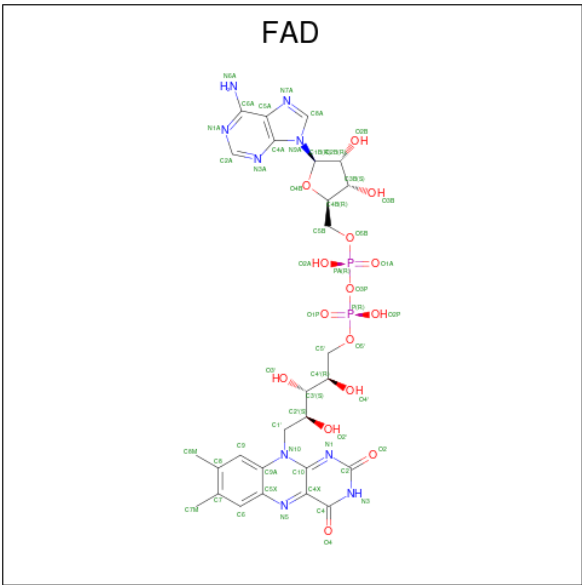
Chain	Residue	Modelled	Actual	Comment	Reference
E	312	ALA	GLU	engineered mutation	UNP A0A125SZC1
G	-20	MET	-	initiating methionine	UNP A0A125SZC1
G	-19	GLY	-	expression tag	UNP A0A125SZC1
G	-18	SER	-	expression tag	UNP A0A125SZC1
G	-17	SER	-	expression tag	UNP A0A125SZC1
G	-16	HIS	-	expression tag	UNP A0A125SZC1
G	-15	HIS	-	expression tag	UNP A0A125SZC1
G	-14	HIS	-	expression tag	UNP A0A125SZC1
G	-13	HIS	-	expression tag	UNP A0A125SZC1
G	-12	HIS	-	expression tag	UNP A0A125SZC1
G	-11	HIS	-	expression tag	UNP A0A125SZC1
G	-10	SER	-	expression tag	UNP A0A125SZC1
G	-9	SER	-	expression tag	UNP A0A125SZC1
G	-8	GLY	-	expression tag	UNP A0A125SZC1
G	-7	LEU	-	expression tag	UNP A0A125SZC1
G	-6	VAL	-	expression tag	UNP A0A125SZC1
G	-5	PRO	-	expression tag	UNP A0A125SZC1
G	-4	ARG	-	expression tag	UNP A0A125SZC1
G	-3	GLY	-	expression tag	UNP A0A125SZC1
G	-2	SER	-	expression tag	UNP A0A125SZC1
G	-1	HIS	-	expression tag	UNP A0A125SZC1
G	0	MET	-	expression tag	UNP A0A125SZC1
G	312	ALA	GLU	engineered mutation	UNP A0A125SZC1
H	-20	MET	-	initiating methionine	UNP A0A125SZC1
H	-19	GLY	-	expression tag	UNP A0A125SZC1
H	-18	SER	-	expression tag	UNP A0A125SZC1
H	-17	SER	-	expression tag	UNP A0A125SZC1
H	-16	HIS	-	expression tag	UNP A0A125SZC1
H	-15	HIS	-	expression tag	UNP A0A125SZC1
H	-14	HIS	-	expression tag	UNP A0A125SZC1
H	-13	HIS	-	expression tag	UNP A0A125SZC1
H	-12	HIS	-	expression tag	UNP A0A125SZC1
H	-11	HIS	-	expression tag	UNP A0A125SZC1
H	-10	SER	-	expression tag	UNP A0A125SZC1
H	-9	SER	-	expression tag	UNP A0A125SZC1
H	-8	GLY	-	expression tag	UNP A0A125SZC1
H	-7	LEU	-	expression tag	UNP A0A125SZC1
H	-6	VAL	-	expression tag	UNP A0A125SZC1
H	-5	PRO	-	expression tag	UNP A0A125SZC1
H	-4	ARG	-	expression tag	UNP A0A125SZC1
H	-3	GLY	-	expression tag	UNP A0A125SZC1
H	-2	SER	-	expression tag	UNP A0A125SZC1

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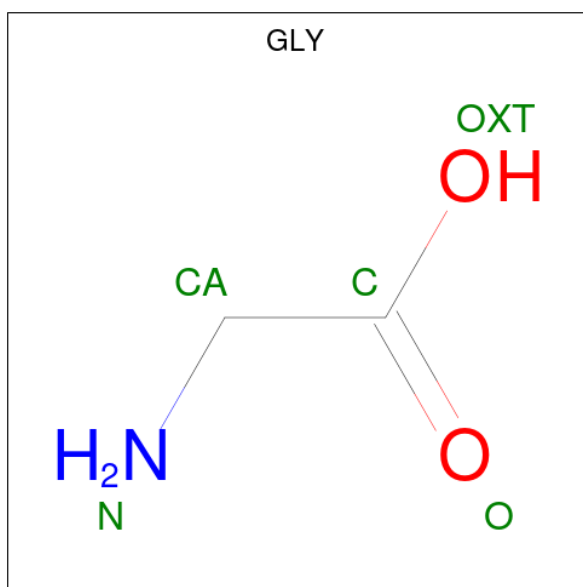
Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	HIS	-	expression tag	UNP A0A125SZC1
H	0	MET	-	expression tag	UNP A0A125SZC1
H	312	ALA	GLU	engineered mutation	UNP A0A125SZC1

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



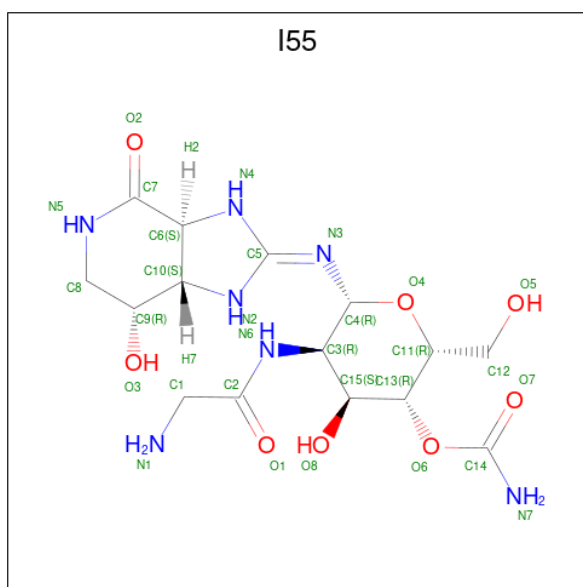
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	G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

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is [(2 {R},3 {R},4 {S},5 {R},6 {R})-6-[({E})-(3 {a} {S},7 {R},7 {a} {S})-7-oxidanyl-4-oxidanylidene-3,3 {a},5,6,7,7 {a}-hexahydro-1 {H}-imidazo[4,5-c]pyridin-2-ylidene]amino]-5-(2-azanylethanoylamino)-2-(hydroxymethyl)-4-oxidanyl-oxan-3-yl] carbamate (CCD ID: I55) (formula: C₁₅H₂₅N₇O₈) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	95	Total	O	0	0
			95	95		
6	B	108	Total	O	0	0
			108	108		
6	C	98	Total	O	0	0
			98	98		
6	D	43	Total	O	0	0
			43	43		

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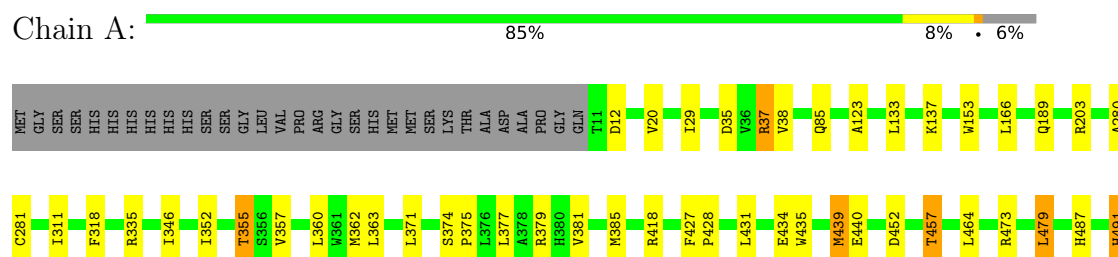
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	96	Total 96	O 96	0	0
6	F	96	Total 96	O 96	0	0
6	G	104	Total 104	O 104	0	0
6	H	46	Total 46	O 46	0	0

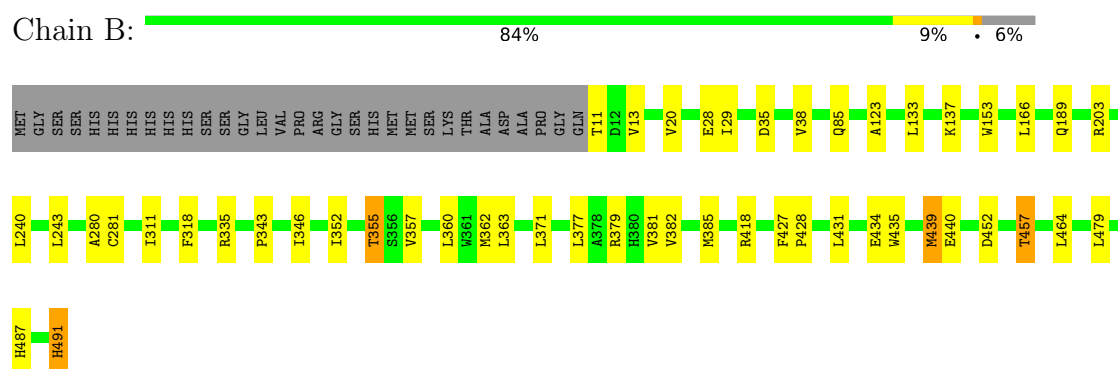
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

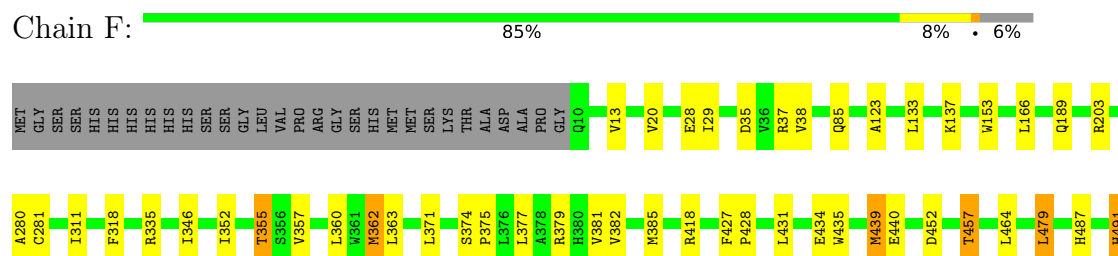
- Molecule 1: N-formimidoyl fortimicin A synthase



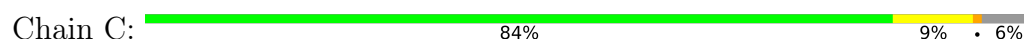
- Molecule 1: N-formimidoyl fortimicin A synthase

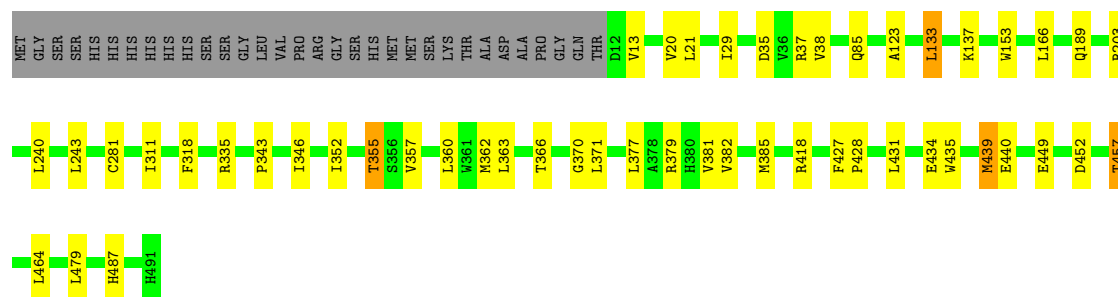


- Molecule 1: N-formimidoyl fortimicin A synthase



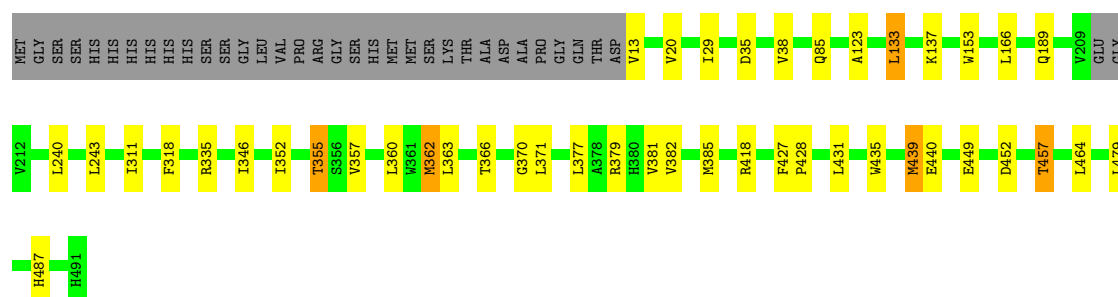
- Molecule 2: N-formimidoyl fortimicin A synthase





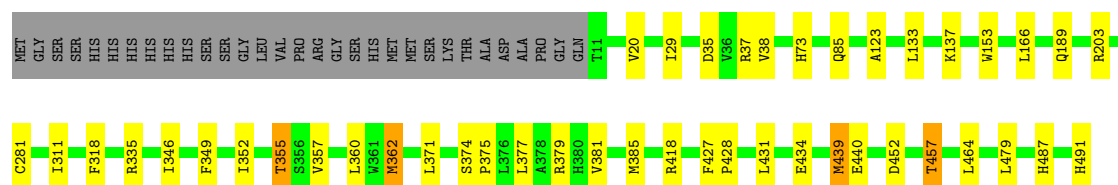
• Molecule 2: N-formimidoyl fortimicin A synthase

Chain D: 84% 8% 7%



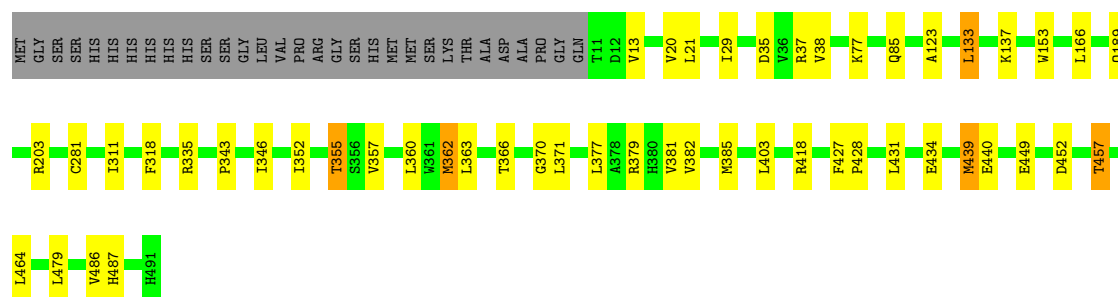
• Molecule 2: N-formimidoyl fortimicin A synthase

Chain E: 85% 8% 6%



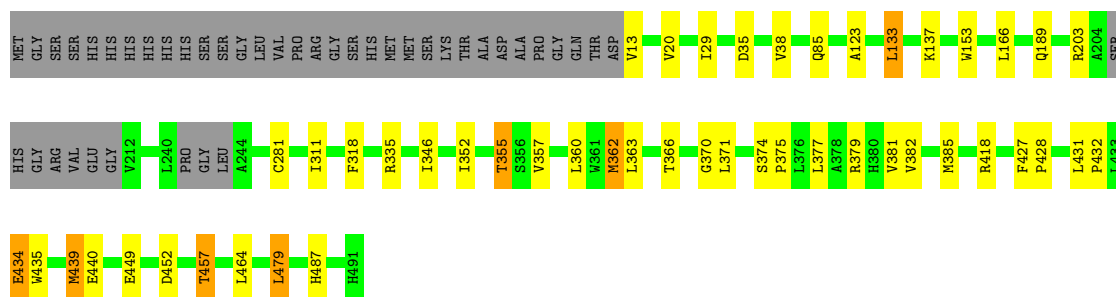
• Molecule 2: N-formimidoyl fortimicin A synthase

Chain G: 84% 9% 6%



• Molecule 2: N-formimidoyl fortimicin A synthase

Chain H: 82% 8% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.29Å 108.08Å 133.46Å 89.80° 89.98° 96.34°	Depositor
Resolution (Å)	29.67 – 2.37 29.67 – 2.37	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.67-2.37) 94.6 (29.67-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.233 0.210 , 0.234	Depositor DCC
R_{free} test set	10823 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.459 for -h,-k,l 0.012 for k,h,-l 0.011 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30454	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	0/3717	1.37	0/5064
1	B	1.01	0/3717	1.37	0/5064
1	F	1.00	0/3726	1.36	0/5076
2	C	1.01	0/3723	1.37	0/5073
2	D	0.99	0/3693	1.37	0/5032
2	E	1.01	0/3724	1.38	0/5076
2	G	1.01	0/3730	1.37	1/5083 (0.0%)
2	H	0.99	0/3636	1.36	0/4952
All	All	1.00	0/29666	1.37	1/40420 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	F	0	2
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	434	GLU	CB-CG-CD	5.01	121.13	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	ALA	Peptide,Mainchain
1	B	280	ALA	Peptide,Mainchain
1	F	280	ALA	Peptide,Mainchain

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	3653	0	3569	30	0
1	B	3653	0	3569	32	0
1	F	3662	0	3577	32	0
2	C	3640	0	3572	31	0
2	D	3611	0	3540	32	0
2	E	3641	0	3568	28	0
2	G	3647	0	3579	30	0
2	H	3557	0	3494	32	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
3	E	53	0	31	0	0
3	F	53	0	31	2	0
3	G	53	0	31	0	0
3	H	53	0	31	1	0
4	A	5	0	2	0	0
4	B	5	0	2	0	0
4	C	5	0	2	0	0
4	D	5	0	2	0	0
4	E	5	0	2	0	0
4	F	5	0	2	0	0
4	G	5	0	2	0	0
4	H	5	0	2	0	0
5	A	30	0	0	0	0
5	B	30	0	0	0	0
5	C	30	0	0	0	0
5	D	30	0	0	0	0
5	E	30	0	0	0	0
5	F	30	0	0	0	0
5	G	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	30	0	0	0	0
6	A	95	0	0	2	0
6	B	108	0	0	1	0
6	C	98	0	0	1	0
6	D	43	0	0	0	0
6	E	96	0	0	0	0
6	F	96	0	0	0	0
6	G	104	0	0	1	0
6	H	46	0	0	0	0
All	All	30454	0	28732	218	0

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

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:MET:HE3	2:C:439:MET:CE	2.06	0.84
2:E:439:MET:HE3	2:G:439:MET:CE	2.08	0.84
1:A:439:MET:CE	2:C:439:MET:HE3	2.09	0.83
2:E:439:MET:CE	2:G:439:MET:HE3	2.09	0.82
1:B:439:MET:HE3	2:D:439:MET:CE	2.10	0.81
1:B:439:MET:CE	2:D:439:MET:HE3	2.10	0.81
1:F:439:MET:CE	2:H:439:MET:HE3	2.12	0.80
1:F:439:MET:HE3	2:H:439:MET:CE	2.13	0.77
1:A:439:MET:HE3	2:C:439:MET:HE2	1.73	0.71
2:E:439:MET:HE3	2:G:439:MET:HE2	1.75	0.67
2:E:439:MET:CE	2:G:439:MET:CE	2.72	0.66
1:B:439:MET:HE3	2:D:439:MET:HE3	1.75	0.66
1:A:29:ILE:HD11	1:A:385:MET:HE1	1.78	0.66
1:A:439:MET:CE	2:C:439:MET:CE	2.71	0.65
1:A:439:MET:HE2	2:C:439:MET:HE3	1.77	0.65
2:E:439:MET:HE2	2:G:439:MET:HE3	1.78	0.64
1:B:355:THR:HG22	1:B:357:VAL:H	1.63	0.63
2:C:123:ALA:HB1	2:C:418:ARG:HD2	1.80	0.63
1:F:355:THR:HG22	1:F:357:VAL:H	1.63	0.63
1:A:355:THR:HG22	1:A:357:VAL:H	1.63	0.63
1:F:439:MET:HE2	2:H:439:MET:HE3	1.79	0.63
1:B:439:MET:HE3	2:D:439:MET:HE2	1.81	0.63
2:E:355:THR:HG22	2:E:357:VAL:H	1.64	0.63
2:H:355:THR:HG22	2:H:357:VAL:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:355:THR:HG22	2:G:357:VAL:H	1.65	0.62
2:D:355:THR:HG22	2:D:357:VAL:H	1.64	0.62
1:B:439:MET:HE2	2:D:439:MET:HE3	1.80	0.62
2:G:123:ALA:HB1	2:G:418:ARG:HD2	1.82	0.61
2:C:355:THR:HG22	2:C:357:VAL:H	1.64	0.61
2:E:311:ILE:HG23	1:F:318:PHE:HB3	1.83	0.61
2:E:29:ILE:HD11	2:E:385:MET:HE1	1.84	0.60
1:B:352:ILE:HD13	1:B:377:LEU:HD22	1.85	0.59
1:F:352:ILE:HD13	1:F:377:LEU:HD22	1.84	0.59
2:H:352:ILE:HD13	2:H:377:LEU:HD22	1.85	0.59
1:F:439:MET:HE3	2:H:439:MET:HE2	1.83	0.59
2:G:352:ILE:HD13	2:G:377:LEU:HD22	1.84	0.58
2:D:352:ILE:HD13	2:D:377:LEU:HD22	1.85	0.58
2:C:352:ILE:HD13	2:C:377:LEU:HD22	1.85	0.57
1:F:487:HIS:NE2	1:F:491:HIS:CD2	2.73	0.57
1:B:487:HIS:NE2	1:B:491:HIS:CD2	2.73	0.56
1:A:12:ASP:OD1	1:A:37:ARG:HB3	2.05	0.56
2:C:363:LEU:HD11	2:C:377:LEU:HB3	1.88	0.56
2:H:432:PRO:HB2	2:H:434:GLU:OE1	2.06	0.56
2:D:29:ILE:HD11	2:D:385:MET:HE1	1.88	0.55
1:F:29:ILE:HD11	1:F:385:MET:HE1	1.89	0.55
1:A:311:ILE:HG23	1:B:318:PHE:HB3	1.89	0.54
2:G:363:LEU:HD11	2:G:377:LEU:HB3	1.88	0.54
2:H:29:ILE:HD11	2:H:385:MET:HE1	1.88	0.54
1:B:29:ILE:HD11	1:B:385:MET:HE1	1.90	0.54
2:E:346:ILE:HG13	2:E:464:LEU:CD2	2.38	0.54
2:G:29:ILE:HD11	2:G:385:MET:HE1	1.90	0.54
2:G:346:ILE:HG13	2:G:464:LEU:CD2	2.39	0.54
1:A:355:THR:HB	1:A:360:LEU:O	2.09	0.53
1:A:346:ILE:HG13	1:A:464:LEU:CD2	2.38	0.53
1:B:123:ALA:HB1	1:B:418:ARG:HD2	1.90	0.53
1:B:355:THR:HB	1:B:360:LEU:O	2.09	0.53
2:H:355:THR:HB	2:H:360:LEU:O	2.09	0.53
2:C:29:ILE:HD11	2:C:385:MET:HE1	1.90	0.53
2:D:123:ALA:HB1	2:D:418:ARG:HD2	1.91	0.53
2:E:487:HIS:NE2	2:E:491:HIS:CD2	2.77	0.53
2:E:355:THR:HB	2:E:360:LEU:O	2.09	0.53
1:F:346:ILE:HG13	1:F:464:LEU:CD2	2.39	0.53
2:H:346:ILE:HG13	2:H:464:LEU:CD2	2.40	0.52
1:B:346:ILE:HG13	1:B:464:LEU:CD2	2.39	0.52
2:D:355:THR:HB	2:D:360:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:ILE:HG13	2:D:464:LEU:CD2	2.40	0.52
2:E:318:PHE:HB3	1:F:311:ILE:HG23	1.92	0.52
2:C:346:ILE:HG13	2:C:464:LEU:CD2	2.39	0.52
1:F:123:ALA:HB1	1:F:418:ARG:HD2	1.92	0.52
1:F:355:THR:HB	1:F:360:LEU:O	2.09	0.51
2:G:355:THR:HB	2:G:360:LEU:O	2.10	0.51
2:H:123:ALA:HB1	2:H:418:ARG:HD2	1.92	0.51
2:C:355:THR:HB	2:C:360:LEU:O	2.10	0.51
1:A:352:ILE:HD13	1:A:377:LEU:HD22	1.92	0.51
2:H:355:THR:HG21	2:H:360:LEU:HD23	1.94	0.50
2:C:13:VAL:HG11	2:C:29:ILE:HD13	1.94	0.50
1:F:355:THR:HG21	1:F:360:LEU:HD23	1.94	0.50
2:G:355:THR:HG21	2:G:360:LEU:HD23	1.93	0.50
1:B:355:THR:HG21	1:B:360:LEU:HD23	1.94	0.50
3:A:701:FAD:N1	3:A:701:FAD:O2'	2.41	0.50
2:C:355:THR:HG21	2:C:360:LEU:HD23	1.93	0.50
2:G:382:VAL:HA	2:G:385:MET:HE3	1.93	0.49
1:A:355:THR:HG21	1:A:360:LEU:HD23	1.94	0.49
2:E:123:ALA:HB1	2:E:418:ARG:HD2	1.95	0.49
2:G:13:VAL:HG11	2:G:29:ILE:HD13	1.95	0.49
2:G:381:VAL:HG12	2:G:385:MET:HE2	1.95	0.49
2:C:382:VAL:HA	2:C:385:MET:HE3	1.94	0.49
2:C:20:VAL:HG11	2:C:371:LEU:HA	1.95	0.49
2:C:381:VAL:HG12	2:C:385:MET:HE2	1.95	0.48
2:D:355:THR:HG21	2:D:360:LEU:HD23	1.95	0.48
2:G:20:VAL:HG11	2:G:371:LEU:HA	1.96	0.48
2:E:311:ILE:CG2	1:F:318:PHE:HB3	2.43	0.48
2:E:355:THR:HG21	2:E:360:LEU:HD23	1.96	0.48
2:E:73:HIS:HB3	2:E:349:PHE:CZ	2.48	0.47
1:A:318:PHE:HB3	1:B:311:ILE:HG23	1.96	0.47
2:G:457:THR:HG21	2:G:487:HIS:CD2	2.50	0.47
2:H:457:THR:HG21	2:H:487:HIS:CD2	2.50	0.47
2:D:362:MET:HE2	2:D:362:MET:HB2	1.81	0.47
2:E:20:VAL:HG11	2:E:371:LEU:HA	1.96	0.47
2:E:352:ILE:HD13	2:E:377:LEU:HD22	1.97	0.47
2:E:427:PHE:N	2:E:428:PRO:HA	2.30	0.47
1:B:20:VAL:HG11	1:B:371:LEU:HA	1.97	0.47
3:B:701:FAD:H9	3:B:701:FAD:H1'2	1.73	0.46
2:D:457:THR:HG21	2:D:487:HIS:CD2	2.50	0.46
1:F:20:VAL:HG11	1:F:371:LEU:HA	1.95	0.46
1:F:457:THR:HG21	1:F:487:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:427:PHE:N	2:H:428:PRO:HA	2.30	0.46
1:B:439:MET:CE	2:D:439:MET:CE	2.76	0.46
1:A:427:PHE:N	1:A:428:PRO:HA	2.31	0.46
1:B:457:THR:HG21	1:B:487:HIS:CD2	2.51	0.46
2:D:381:VAL:HG12	2:D:385:MET:HE2	1.96	0.46
2:H:381:VAL:HG12	2:H:385:MET:HE2	1.96	0.46
2:H:382:VAL:HA	2:H:385:MET:HE3	1.98	0.46
2:D:363:LEU:HD11	2:D:377:LEU:HB3	1.97	0.46
1:F:427:PHE:N	1:F:428:PRO:HA	2.30	0.46
1:A:487:HIS:NE2	1:A:491:HIS:ND1	2.63	0.46
2:C:457:THR:HG21	2:C:487:HIS:CD2	2.50	0.46
1:F:381:VAL:HG12	1:F:385:MET:HE2	1.98	0.46
1:B:427:PHE:N	1:B:428:PRO:HA	2.30	0.46
1:A:457:THR:HG21	1:A:487:HIS:CD2	2.51	0.46
2:D:382:VAL:HA	2:D:385:MET:HE3	1.98	0.46
1:A:346:ILE:HG13	1:A:464:LEU:HD21	1.98	0.45
2:D:20:VAL:HG11	2:D:371:LEU:HA	1.97	0.45
2:D:427:PHE:N	2:D:428:PRO:HA	2.30	0.45
2:G:427:PHE:N	2:G:428:PRO:HA	2.31	0.45
1:B:435:TRP:CE3	2:D:439:MET:HE2	2.51	0.45
2:H:20:VAL:HG11	2:H:371:LEU:HA	1.97	0.45
1:F:435:TRP:CE3	2:H:439:MET:HE2	2.52	0.45
1:B:363:LEU:HD11	1:B:377:LEU:HB3	1.98	0.45
2:D:431:LEU:N	2:D:431:LEU:HD23	2.32	0.45
1:A:123:ALA:HB1	1:A:418:ARG:HD2	1.99	0.45
1:B:381:VAL:HG12	1:B:385:MET:HE2	1.99	0.44
3:B:701:FAD:N1	3:B:701:FAD:O2'	2.37	0.44
2:E:457:THR:HG21	2:E:487:HIS:CD2	2.51	0.44
2:C:343:PRO:HG2	6:C:817:HOH:O	2.17	0.44
2:D:123:ALA:HB1	2:D:418:ARG:CD	2.47	0.44
2:H:363:LEU:HD11	2:H:377:LEU:HB3	1.98	0.44
2:C:318:PHE:HB3	2:D:311:ILE:HG23	1.99	0.44
2:D:133:LEU:HD12	2:D:133:LEU:HA	1.89	0.44
1:F:363:LEU:HD11	1:F:377:LEU:HB3	1.98	0.44
2:H:123:ALA:HB1	2:H:418:ARG:CD	2.47	0.44
1:A:20:VAL:HG11	1:A:371:LEU:HA	1.99	0.44
3:F:701:FAD:H9	3:F:701:FAD:H1'2	1.75	0.44
2:E:431:LEU:N	2:E:431:LEU:HD23	2.33	0.44
1:A:479:LEU:HD22	6:A:807:HOH:O	2.17	0.44
2:H:431:LEU:N	2:H:431:LEU:HD23	2.32	0.43
3:F:701:FAD:N1	3:F:701:FAD:O2'	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:318:PHE:HB3	2:H:311:ILE:HG23	2.00	0.43
2:C:427:PHE:N	2:C:428:PRO:HA	2.31	0.43
1:A:431:LEU:HD23	1:A:431:LEU:N	2.33	0.43
1:B:28:GLU:HB3	1:B:382:VAL:HG21	2.00	0.43
3:A:701:FAD:H1'2	3:A:701:FAD:H9	1.72	0.43
1:B:439:MET:HE2	2:D:435:TRP:CE3	2.53	0.43
2:C:431:LEU:N	2:C:431:LEU:HD23	2.34	0.43
2:E:381:VAL:HG12	2:E:385:MET:HE2	2.01	0.43
2:G:346:ILE:HG13	2:G:464:LEU:HD21	2.01	0.43
1:F:133:LEU:HD12	1:F:133:LEU:HA	1.88	0.43
1:F:439:MET:HE2	2:H:435:TRP:CE3	2.54	0.43
2:E:346:ILE:HG13	2:E:464:LEU:HD21	2.00	0.42
1:F:28:GLU:HB3	1:F:382:VAL:HG21	2.00	0.42
1:B:346:ILE:HG13	1:B:464:LEU:HD21	2.01	0.42
1:B:431:LEU:N	1:B:431:LEU:HD23	2.34	0.42
1:B:13:VAL:HG11	1:B:29:ILE:HD13	2.01	0.42
2:D:13:VAL:HG11	2:D:29:ILE:HD13	2.01	0.42
1:F:13:VAL:HG11	1:F:29:ILE:HD13	2.00	0.42
1:A:381:VAL:HG12	1:A:385:MET:HE2	2.01	0.42
2:C:366:THR:HB	2:C:370:GLY:CA	2.50	0.42
2:G:366:THR:HB	2:G:370:GLY:CA	2.49	0.42
1:A:473:ARG:HG2	6:A:891:HOH:O	2.18	0.42
2:E:133:LEU:HD12	2:E:133:LEU:HA	1.87	0.42
1:F:431:LEU:HD23	1:F:431:LEU:N	2.34	0.42
2:G:123:ALA:HB1	2:G:418:ARG:CD	2.47	0.42
2:G:21:LEU:HD13	2:G:363:LEU:HG	2.02	0.42
2:H:346:ILE:HG13	2:H:464:LEU:HD21	2.01	0.42
2:C:21:LEU:HD13	2:C:363:LEU:HG	2.01	0.42
2:H:366:THR:HB	2:H:370:GLY:CA	2.50	0.42
1:B:343:PRO:HG2	6:B:818:HOH:O	2.20	0.42
1:A:311:ILE:CG2	1:B:318:PHE:HB3	2.49	0.41
2:D:366:THR:HB	2:D:370:GLY:CA	2.50	0.41
2:G:431:LEU:N	2:G:431:LEU:HD23	2.34	0.41
1:A:435:TRP:CE3	2:C:439:MET:HE2	2.56	0.41
2:G:311:ILE:HG23	2:H:318:PHE:HB3	2.03	0.41
1:A:363:LEU:HD11	1:A:377:LEU:HB3	2.00	0.41
2:C:133:LEU:HD12	2:C:133:LEU:HA	1.93	0.41
2:C:346:ILE:HG13	2:C:464:LEU:HD21	2.02	0.41
1:F:133:LEU:HD13	1:F:166:LEU:HD22	2.03	0.41
1:B:133:LEU:HD13	1:B:166:LEU:HD22	2.03	0.41
2:C:311:ILE:HG23	2:D:318:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:ILE:HG13	2:D:464:LEU:HD21	2.02	0.41
2:H:13:VAL:HG11	2:H:29:ILE:HD13	2.01	0.41
2:C:133:LEU:HD13	2:C:166:LEU:HD22	2.03	0.41
1:F:382:VAL:HA	1:F:385:MET:HE3	2.02	0.41
1:A:374:SER:N	1:A:375:PRO:HD2	2.36	0.41
2:E:133:LEU:HD13	2:E:166:LEU:HD22	2.03	0.41
1:F:346:ILE:HG13	1:F:464:LEU:HD21	2.02	0.41
1:F:362:MET:HE2	1:F:362:MET:HB2	1.84	0.41
2:G:403:LEU:HG	2:G:486:VAL:HG11	2.03	0.41
2:H:133:LEU:HD12	2:H:133:LEU:HA	1.89	0.41
2:H:479:LEU:HD13	2:H:479:LEU:HA	1.92	0.41
2:D:240:LEU:HB2	2:D:243:LEU:HD22	2.03	0.41
2:E:123:ALA:HB1	2:E:418:ARG:CD	2.51	0.41
2:E:362:MET:HE2	2:E:362:MET:HB2	1.84	0.41
2:E:374:SER:N	2:E:375:PRO:HD2	2.36	0.41
2:G:362:MET:HE2	2:G:362:MET:HB2	1.84	0.41
1:A:133:LEU:HD13	1:A:166:LEU:HD22	2.03	0.40
1:B:240:LEU:HB2	1:B:243:LEU:HD22	2.03	0.40
2:G:133:LEU:HD13	2:G:166:LEU:HD22	2.03	0.40
2:H:133:LEU:HD13	2:H:166:LEU:HD22	2.03	0.40
2:H:362:MET:HE2	2:H:362:MET:HB2	1.80	0.40
3:H:701:FAD:H9	3:H:701:FAD:H1'2	1.85	0.40
1:A:439:MET:HE2	2:C:435:TRP:CE3	2.56	0.40
1:B:382:VAL:HA	1:B:385:MET:HE3	2.02	0.40
2:D:133:LEU:HD13	2:D:166:LEU:HD22	2.04	0.40
1:F:479:LEU:HD13	1:F:479:LEU:HA	1.92	0.40
1:F:374:SER:N	1:F:375:PRO:HD2	2.36	0.40
2:C:240:LEU:HB2	2:C:243:LEU:HD22	2.04	0.40
2:G:343:PRO:HG2	6:G:807:HOH:O	2.21	0.40
2:H:374:SER:N	2:H:375:PRO:HD2	2.37	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	478/512 (93%)	464 (97%)	13 (3%)	1 (0%)	43	52
1	B	478/512 (93%)	463 (97%)	14 (3%)	1 (0%)	43	52
1	F	479/512 (94%)	464 (97%)	14 (3%)	1 (0%)	43	52
2	C	479/512 (94%)	464 (97%)	14 (3%)	1 (0%)	43	52
2	D	474/512 (93%)	458 (97%)	15 (3%)	1 (0%)	43	52
2	E	480/512 (94%)	466 (97%)	13 (3%)	1 (0%)	43	52
2	G	480/512 (94%)	464 (97%)	15 (3%)	1 (0%)	43	52
2	H	464/512 (91%)	448 (97%)	15 (3%)	1 (0%)	43	52
All	All	3812/4096 (93%)	3691 (97%)	113 (3%)	8 (0%)	43	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	TRP
1	B	153	TRP
2	C	153	TRP
2	D	153	TRP
2	E	153	TRP
1	F	153	TRP
2	G	153	TRP
2	H	153	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/398 (94%)	355 (95%)	18 (5%)	23	29
1	B	373/398 (94%)	355 (95%)	18 (5%)	23	29
1	F	374/398 (94%)	356 (95%)	18 (5%)	23	29
2	C	374/399 (94%)	353 (94%)	21 (6%)	19	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	370/399 (93%)	354 (96%)	16 (4%)	26	34
2	E	374/399 (94%)	355 (95%)	19 (5%)	21	26
2	G	375/399 (94%)	354 (94%)	21 (6%)	19	23
2	H	365/399 (92%)	345 (94%)	20 (6%)	19	24
All	All	2978/3189 (93%)	2827 (95%)	151 (5%)	22	26

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	37	ARG
1	A	38	VAL
1	A	85	GLN
1	A	137	LYS
1	A	189	GLN
1	A	203	ARG
1	A	335	ARG
1	A	355	THR
1	A	362	MET
1	A	379	ARG
1	A	434	GLU
1	A	439	MET
1	A	440	GLU
1	A	452	ASP
1	A	457	THR
1	A	479	LEU
1	A	491	HIS
1	B	11	THR
1	B	35	ASP
1	B	38	VAL
1	B	85	GLN
1	B	137	LYS
1	B	189	GLN
1	B	203	ARG
1	B	335	ARG
1	B	355	THR
1	B	362	MET
1	B	379	ARG
1	B	434	GLU
1	B	439	MET
1	B	440	GLU

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Mol	Chain	Res	Type
1	B	452	ASP
1	B	457	THR
1	B	479	LEU
1	B	491	HIS
2	C	35	ASP
2	C	37	ARG
2	C	38	VAL
2	C	85	GLN
2	C	133	LEU
2	C	137	LYS
2	C	189	GLN
2	C	203	ARG
2	C	281[A]	CYS
2	C	281[B]	CYS
2	C	335	ARG
2	C	355	THR
2	C	362	MET
2	C	379	ARG
2	C	434	GLU
2	C	439	MET
2	C	440	GLU
2	C	449	GLU
2	C	452	ASP
2	C	457	THR
2	C	479	LEU
2	D	35	ASP
2	D	38	VAL
2	D	85	GLN
2	D	133	LEU
2	D	137	LYS
2	D	189	GLN
2	D	335	ARG
2	D	355	THR
2	D	362	MET
2	D	379	ARG
2	D	439	MET
2	D	440	GLU
2	D	449	GLU
2	D	452	ASP
2	D	457	THR
2	D	479	LEU
2	E	35	ASP

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Mol	Chain	Res	Type
2	E	37	ARG
2	E	38	VAL
2	E	85	GLN
2	E	137	LYS
2	E	189	GLN
2	E	203	ARG
2	E	281[A]	CYS
2	E	281[B]	CYS
2	E	335	ARG
2	E	355	THR
2	E	362	MET
2	E	379	ARG
2	E	434	GLU
2	E	439	MET
2	E	440	GLU
2	E	452	ASP
2	E	457	THR
2	E	479	LEU
1	F	35	ASP
1	F	37	ARG
1	F	38	VAL
1	F	85	GLN
1	F	137	LYS
1	F	189	GLN
1	F	203	ARG
1	F	335	ARG
1	F	355	THR
1	F	362	MET
1	F	379	ARG
1	F	434	GLU
1	F	439	MET
1	F	440	GLU
1	F	452	ASP
1	F	457	THR
1	F	479	LEU
1	F	491	HIS
2	G	35	ASP
2	G	37	ARG
2	G	38	VAL
2	G	77	LYS
2	G	85	GLN
2	G	133	LEU

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Mol	Chain	Res	Type
2	G	137	LYS
2	G	189	GLN
2	G	203	ARG
2	G	281[A]	CYS
2	G	281[B]	CYS
2	G	335	ARG
2	G	355	THR
2	G	362	MET
2	G	379	ARG
2	G	439	MET
2	G	440	GLU
2	G	449	GLU
2	G	452	ASP
2	G	457	THR
2	G	479	LEU
2	H	35	ASP
2	H	38	VAL
2	H	85	GLN
2	H	133	LEU
2	H	137	LYS
2	H	189	GLN
2	H	203	ARG
2	H	281[A]	CYS
2	H	281[B]	CYS
2	H	335	ARG
2	H	355	THR
2	H	362	MET
2	H	379	ARG
2	H	434	GLU
2	H	439	MET
2	H	440	GLU
2	H	449	GLU
2	H	452	ASP
2	H	457	THR
2	H	479	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	189	GLN
1	A	245	HIS

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Mol	Chain	Res	Type
1	A	330	ASN
1	B	67	HIS
1	B	78	HIS
1	B	159	ASN
1	B	189	GLN
1	B	491	HIS
2	C	159	ASN
2	C	189	GLN
2	C	330	ASN
2	C	487	HIS
2	D	67	HIS
2	D	189	GLN
2	D	487	HIS
2	E	67	HIS
2	E	159	ASN
2	E	189	GLN
2	E	330	ASN
2	E	491	HIS
1	F	10	GLN
1	F	67	HIS
1	F	159	ASN
1	F	189	GLN
1	F	245	HIS
1	F	491	HIS
2	G	159	ASN
2	G	189	GLN
2	G	487	HIS
2	H	159	ASN
2	H	189	GLN
2	H	487	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
1	GQI	A	281[A]	1	8,11,12	1.57	3 (37%)	6,12,14	1.87	2 (33%)
1	GQI	A	281[B]	1	4,5,12	1.05	0	1,5,14	0.14	0
1	GQI	F	281[A]	1	8,11,12	1.55	2 (25%)	6,12,14	1.35	1 (16%)
1	GQI	B	281[A]	1	8,11,12	1.55	3 (37%)	6,12,14	1.48	1 (16%)
1	GQI	F	281[B]	1	4,5,12	0.96	0	1,5,14	0.44	0
1	GQI	B	281[B]	1	4,5,12	1.07	0	1,5,14	0.06	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
1	GQI	A	281[A]	1	-	1/2/10/12	-
1	GQI	A	281[B]	1	-	0/1/4/12	-
1	GQI	F	281[A]	1	-	1/2/10/12	-
1	GQI	B	281[A]	1	-	1/2/10/12	-
1	GQI	F	281[B]	1	-	0/1/4/12	-
1	GQI	B	281[B]	1	-	0/1/4/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	281[A]	GQI	O3-C4	-2.93	1.22	1.30
1	A	281[A]	GQI	O3-C4	-2.72	1.23	1.30
1	A	281[A]	GQI	C3-C4	2.57	1.54	1.47
1	B	281[A]	GQI	O3-C4	-2.54	1.23	1.30
1	B	281[A]	GQI	C3-C4	2.48	1.54	1.47
1	F	281[A]	GQI	C3-C4	2.17	1.53	1.47
1	B	281[A]	GQI	O4-C	2.09	1.27	1.20
1	A	281[A]	GQI	O4-C	2.07	1.27	1.20

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281[A]	GQI	O2-C4-C3	-2.87	116.08	124.30
1	F	281[A]	GQI	O2-C4-C3	-2.40	117.43	124.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281[A]	GQI	C4-C3-N2	2.36	122.66	118.71
1	B	281[A]	GQI	C4-C3-N2	2.02	122.08	118.71

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	281[A]	GQI	N-CA-CB-S1
1	A	281[A]	GQI	N-CA-CB-S1
1	B	281[A]	GQI	N-CA-CB-S1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	I55	B	703	-	28,32,32	2.34	1 (3%)	31,46,46	2.53	8 (25%)
5	I55	E	703	-	28,32,32	3.11	2 (7%)	31,46,46	2.32	9 (29%)
4	GLY	F	702	-	4,4,4	0.99	0	3,4,4	1.87	2 (66%)
4	GLY	G	702	-	4,4,4	0.92	0	3,4,4	1.50	1 (33%)
5	I55	C	703	-	28,32,32	2.01	1 (3%)	31,46,46	2.69	10 (32%)
3	FAD	A	701	-	58,58,58	0.77	2 (3%)	85,89,89	0.85	3 (3%)
4	GLY	A	702	-	4,4,4	1.00	0	3,4,4	1.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLY	H	702	-	4,4,4	1.13	1 (25%)	3,4,4	1.27	0
4	GLY	C	702	-	4,4,4	0.94	0	3,4,4	1.64	1 (33%)
4	GLY	E	702	-	4,4,4	1.00	0	3,4,4	1.60	1 (33%)
4	GLY	B	702	-	4,4,4	0.83	0	3,4,4	1.55	1 (33%)
3	FAD	B	701	-	58,58,58	0.62	0	85,89,89	0.91	5 (5%)
5	I55	A	703	-	28,32,32	2.97	1 (3%)	31,46,46	2.35	7 (22%)
3	FAD	G	701	-	58,58,58	0.61	0	85,89,89	0.69	2 (2%)
5	I55	F	703	-	28,32,32	2.52	1 (3%)	31,46,46	2.47	8 (25%)
3	FAD	D	701	-	58,58,58	0.64	0	85,89,89	0.68	1 (1%)
4	GLY	D	702	-	4,4,4	1.18	1 (25%)	3,4,4	1.26	0
5	I55	G	703	-	28,32,32	1.89	1 (3%)	31,46,46	2.73	8 (25%)
3	FAD	H	701	-	58,58,58	0.62	0	85,89,89	0.69	2 (2%)
5	I55	D	703	-	28,32,32	3.82	1 (3%)	31,46,46	2.13	7 (22%)
3	FAD	C	701	-	58,58,58	0.61	0	85,89,89	0.70	2 (2%)
3	FAD	E	701	-	58,58,58	0.71	0	85,89,89	0.87	4 (4%)
3	FAD	F	701	-	58,58,58	0.63	0	85,89,89	0.90	4 (4%)
5	I55	H	703	-	28,32,32	3.76	1 (3%)	31,46,46	2.46	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	I55	B	703	-	-	4/14/61/61	0/3/3/3
5	I55	E	703	-	-	3/14/61/61	0/3/3/3
4	GLY	F	702	-	-	0/2/2/2	-
4	GLY	G	702	-	-	0/2/2/2	-
5	I55	C	703	-	-	1/14/61/61	0/3/3/3
3	FAD	A	701	-	-	4/34/50/50	0/6/6/6
4	GLY	A	702	-	-	0/2/2/2	-
4	GLY	H	702	-	-	0/2/2/2	-
4	GLY	C	702	-	-	0/2/2/2	-
4	GLY	E	702	-	-	0/2/2/2	-
4	GLY	B	702	-	-	0/2/2/2	-
3	FAD	B	701	-	-	3/34/50/50	0/6/6/6
5	I55	A	703	-	-	2/14/61/61	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	G	701	-	-	4/34/50/50	0/6/6/6
5	I55	F	703	-	-	3/14/61/61	0/3/3/3
3	FAD	D	701	-	-	2/34/50/50	0/6/6/6
4	GLY	D	702	-	-	0/2/2/2	-
5	I55	G	703	-	-	2/14/61/61	0/3/3/3
3	FAD	H	701	-	-	2/34/50/50	0/6/6/6
5	I55	D	703	-	-	2/14/61/61	0/3/3/3
3	FAD	C	701	-	-	4/34/50/50	0/6/6/6
3	FAD	E	701	-	-	3/34/50/50	0/6/6/6
3	FAD	F	701	-	-	5/34/50/50	0/6/6/6
5	I55	H	703	-	-	3/14/61/61	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	703	I55	C4-C3	-19.93	1.39	1.53
5	H	703	I55	C4-C3	-19.61	1.39	1.53
5	E	703	I55	C4-C3	-15.89	1.42	1.53
5	A	703	I55	C4-C3	-15.14	1.42	1.53
5	F	703	I55	C4-C3	-12.89	1.44	1.53
5	B	703	I55	C4-C3	-11.99	1.45	1.53
5	C	703	I55	C4-C3	-10.05	1.46	1.53
5	G	703	I55	C4-C3	-9.30	1.46	1.53
3	A	701	FAD	PA-O3P	2.87	1.62	1.59
5	E	703	I55	C8-C9	2.18	1.54	1.52
3	A	701	FAD	C9-C8	-2.15	1.36	1.39
4	D	702	GLY	OXT-C	-2.14	1.23	1.30
4	H	702	GLY	OXT-C	-2.07	1.24	1.30

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	703	I55	O4-C4-C3	11.08	121.87	111.20
5	C	703	I55	O4-C4-C3	10.70	121.50	111.20
5	H	703	I55	O4-C4-C3	10.37	121.19	111.20
5	A	703	I55	O4-C4-C3	9.69	120.53	111.20
5	F	703	I55	O4-C4-C3	9.14	120.00	111.20
5	E	703	I55	O4-C4-C3	9.14	120.00	111.20
5	B	703	I55	O4-C4-C3	9.10	119.97	111.20
5	D	703	I55	O4-C4-C3	8.21	119.11	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	703	I55	C4-C3-N2	7.03	121.28	111.08
5	F	703	I55	C4-C3-N2	6.44	120.43	111.08
5	G	703	I55	C4-C3-N2	6.19	120.06	111.08
5	C	703	I55	C4-C3-N2	6.15	120.02	111.08
5	A	703	I55	C4-C3-N2	5.40	118.92	111.08
5	E	703	I55	C4-C3-N2	5.34	118.83	111.08
5	H	703	I55	C4-C3-N2	5.30	118.78	111.08
5	D	703	I55	C4-C3-N2	4.83	118.09	111.08
5	G	703	I55	C15-C3-C4	3.76	116.03	109.80
5	C	703	I55	C15-C3-C4	3.71	115.94	109.80
5	F	703	I55	C15-C3-C4	3.60	115.76	109.80
5	B	703	I55	C15-C3-C4	3.49	115.58	109.80
5	C	703	I55	C15-C3-N2	3.47	117.01	110.62
3	B	701	FAD	C4'-C3'-C2'	3.28	119.02	113.57
5	G	703	I55	C15-C3-N2	3.28	116.65	110.62
3	F	701	FAD	C4'-C3'-C2'	3.23	118.94	113.57
5	E	703	I55	C15-C3-N2	3.15	116.41	110.62
5	B	703	I55	O4-C11-C12	2.89	113.61	106.44
5	B	703	I55	C9-C8-N5	2.86	112.74	109.83
5	A	703	I55	C15-C3-N2	2.84	115.84	110.62
5	G	703	I55	O4-C11-C13	2.83	115.57	109.72
3	E	701	FAD	C4'-C3'-C2'	2.74	118.14	113.57
5	C	703	I55	C6-C7-N5	-2.73	114.92	118.14
3	B	701	FAD	O4'-C4'-C5'	-2.68	104.07	109.99
5	C	703	I55	O4-C11-C13	2.66	115.23	109.72
5	D	703	I55	O4-C11-C13	2.61	115.12	109.72
5	E	703	I55	C9-C8-N5	2.60	112.48	109.83
5	F	703	I55	O4-C11-C12	2.60	112.89	106.44
5	H	703	I55	C6-C7-N5	-2.60	115.08	118.14
5	H	703	I55	C10-N6-C5	-2.56	107.89	112.17
5	H	703	I55	O4-C11-C13	2.55	115.00	109.72
3	F	701	FAD	O4'-C4'-C5'	-2.55	104.36	109.99
5	F	703	I55	C9-C8-N5	2.54	112.42	109.83
5	G	703	I55	C9-C8-N5	2.50	112.38	109.83
3	A	701	FAD	C4'-C3'-C2'	2.44	117.64	113.57
5	A	703	I55	C9-C8-N5	2.43	112.31	109.83
3	B	701	FAD	O2A-PA-O1A	2.42	123.70	112.44
3	F	701	FAD	O2A-PA-O1A	2.39	123.55	112.44
5	B	703	I55	O4-C4-N3	2.36	115.60	109.13
5	B	703	I55	C6-C7-N5	-2.34	115.38	118.14
5	B	703	I55	C10-N6-C5	-2.33	108.27	112.17
3	E	701	FAD	O2A-PA-O1A	2.33	123.27	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	703	I55	C6-C7-N5	-2.32	115.41	118.14
4	F	702	GLY	OXT-C-CA	2.32	122.60	113.38
5	G	703	I55	C10-N6-C5	-2.30	108.33	112.17
5	C	703	I55	C10-N6-C5	-2.29	108.33	112.17
5	E	703	I55	C6-C7-N5	-2.28	115.46	118.14
5	D	703	I55	C10-N6-C5	-2.27	108.38	112.17
5	D	703	I55	C9-C8-N5	2.26	112.13	109.83
3	A	701	FAD	O2A-PA-O1A	2.22	122.79	112.44
5	F	703	I55	O4-C11-C13	2.21	114.30	109.72
5	D	703	I55	C6-C7-N5	-2.21	115.54	118.14
4	C	702	GLY	OXT-C-CA	2.19	122.09	113.38
3	B	701	FAD	O4'-C4'-C3'	2.18	114.34	109.25
5	H	703	I55	O6-C14-O7	2.17	126.38	123.06
4	F	702	GLY	OXT-C-O	-2.17	117.76	123.33
3	B	701	FAD	C4-N3-C2	-2.16	121.80	125.64
4	E	702	GLY	OXT-C-CA	2.16	121.96	113.38
3	A	701	FAD	C4-N3-C2	-2.15	121.82	125.64
5	F	703	I55	O4-C4-N3	2.14	115.00	109.13
5	C	703	I55	C9-C8-N5	2.14	112.01	109.83
4	B	702	GLY	OXT-C-CA	2.14	121.89	113.38
5	A	703	I55	C10-N6-C5	-2.13	108.61	112.17
5	E	703	I55	C3-C4-N3	-2.12	105.81	109.73
5	E	703	I55	O4-C11-C12	2.12	111.69	106.44
3	C	701	FAD	C4-N3-C2	-2.10	121.91	125.64
5	F	703	I55	C10-N6-C5	-2.09	108.68	112.17
3	G	701	FAD	O2P-P-O1P	2.09	122.15	112.44
5	H	703	I55	C9-C8-N5	2.08	111.95	109.83
5	G	703	I55	C6-C7-N5	-2.08	115.69	118.14
5	C	703	I55	O4-C4-N3	2.08	114.82	109.13
5	D	703	I55	O6-C14-O7	2.06	126.22	123.06
3	E	701	FAD	C4-N3-C2	-2.06	121.98	125.64
3	D	701	FAD	C4-N3-C2	-2.05	122.00	125.64
3	E	701	FAD	O4'-C4'-C3'	2.05	114.04	109.25
4	G	702	GLY	OXT-C-CA	2.05	121.52	113.38
3	F	701	FAD	C4-N3-C2	-2.04	122.01	125.64
5	C	703	I55	O4-C11-C12	2.04	111.50	106.44
3	H	701	FAD	C4-N3-C2	-2.03	122.04	125.64
3	H	701	FAD	O2P-P-O1P	2.03	121.88	112.44
3	G	701	FAD	C4-N3-C2	-2.02	122.05	125.64
5	A	703	I55	O4-C11-C13	2.02	113.90	109.72
5	E	703	I55	C10-N6-C5	-2.01	108.80	112.17
3	C	701	FAD	O2P-P-O1P	2.01	121.81	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	703	I55	C12-C11-C13	2.01	119.03	113.38
5	E	703	I55	O4-C11-C13	2.01	113.87	109.72

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FAD	PA-O3P-P-O5'
5	B	703	I55	N6-C5-N3-C4
5	D	703	I55	C11-C13-O6-C14
5	D	703	I55	C15-C13-O6-C14
5	F	703	I55	N6-C5-N3-C4
5	H	703	I55	C11-C13-O6-C14
5	H	703	I55	C15-C13-O6-C14
5	G	703	I55	O4-C11-C12-O5
5	B	703	I55	O4-C11-C12-O5
5	E	703	I55	O4-C11-C12-O5
3	A	701	FAD	C2B-C1B-N9A-C8A
3	B	701	FAD	C2B-C1B-N9A-C8A
3	C	701	FAD	C2B-C1B-N9A-C8A
3	E	701	FAD	C2B-C1B-N9A-C8A
3	F	701	FAD	C2B-C1B-N9A-C8A
3	G	701	FAD	C2B-C1B-N9A-C8A
3	H	701	FAD	C2B-C1B-N9A-C8A
5	A	703	I55	C15-C13-O6-C14
5	B	703	I55	C15-C13-O6-C14
5	C	703	I55	C15-C13-O6-C14
5	E	703	I55	C15-C13-O6-C14
5	F	703	I55	C15-C13-O6-C14
3	D	701	FAD	C2B-C1B-N9A-C8A
3	A	701	FAD	C2'-C1'-N10-C10
3	B	701	FAD	C2'-C1'-N10-C10
3	E	701	FAD	C2'-C1'-N10-C10
3	F	701	FAD	C2'-C1'-N10-C10
3	C	701	FAD	C2B-C1B-N9A-C4A
3	G	701	FAD	C2B-C1B-N9A-C4A
3	F	701	FAD	O4B-C1B-N9A-C8A
3	G	701	FAD	O4B-C1B-N9A-C8A
5	A	703	I55	O4-C11-C12-O5
3	C	701	FAD	O4B-C1B-N9A-C8A
5	H	703	I55	O4-C11-C12-O5
3	C	701	FAD	O4B-C4B-C5B-O5B

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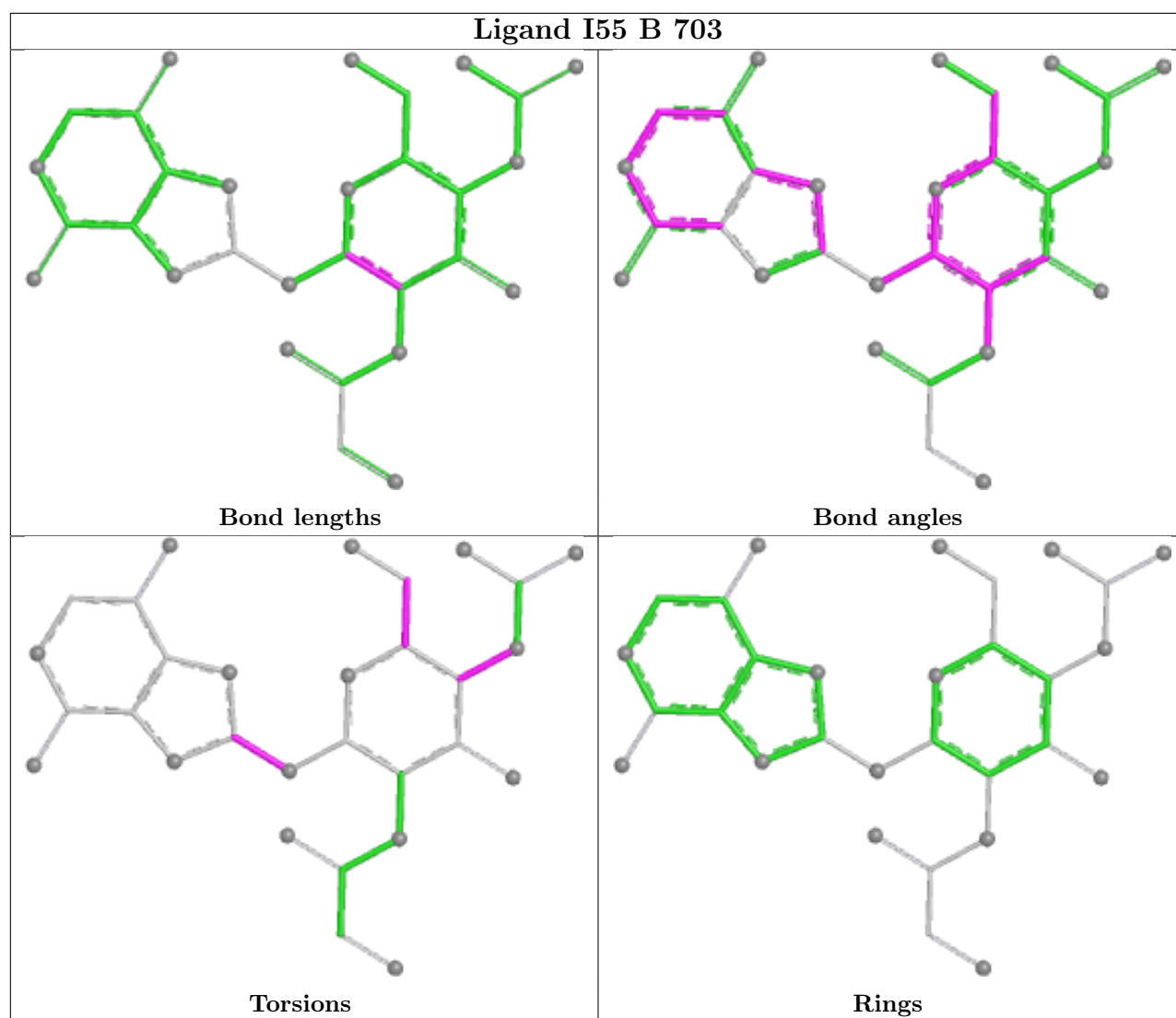
Mol	Chain	Res	Type	Atoms
5	B	703	I55	N4-C5-N3-C4
5	E	703	I55	N4-C5-N3-C4
5	F	703	I55	N4-C5-N3-C4
3	B	701	FAD	O4B-C1B-N9A-C8A
3	H	701	FAD	O4B-C1B-N9A-C8A
3	G	701	FAD	O4B-C4B-C5B-O5B
3	D	701	FAD	O4B-C1B-N9A-C8A
3	E	701	FAD	O4B-C4B-C5B-O5B
3	F	701	FAD	O4B-C4B-C5B-O5B
3	F	701	FAD	C2B-C1B-N9A-C4A
5	G	703	I55	C15-C13-O6-C14
3	A	701	FAD	O4B-C1B-N9A-C8A

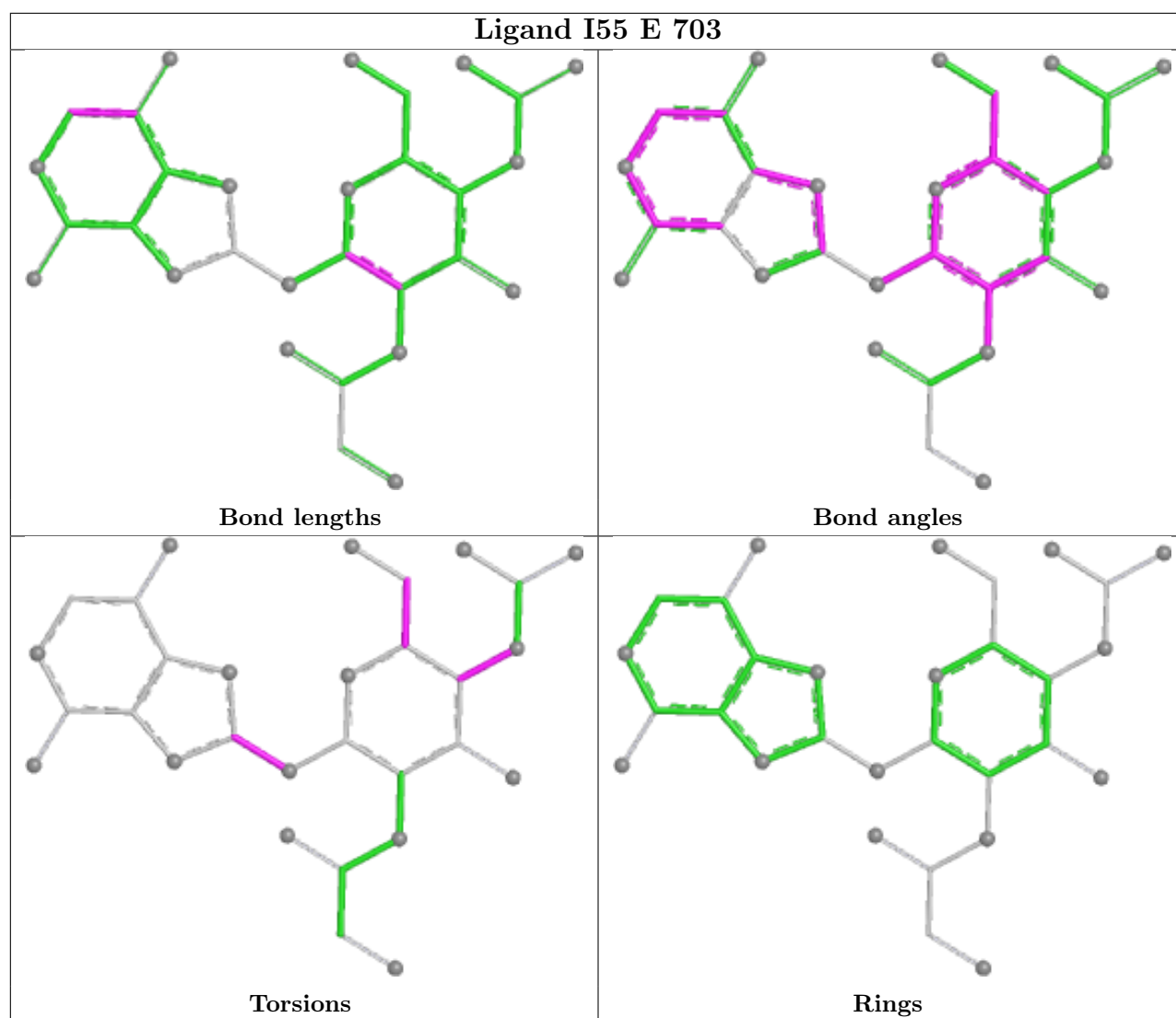
There are no ring outliers.

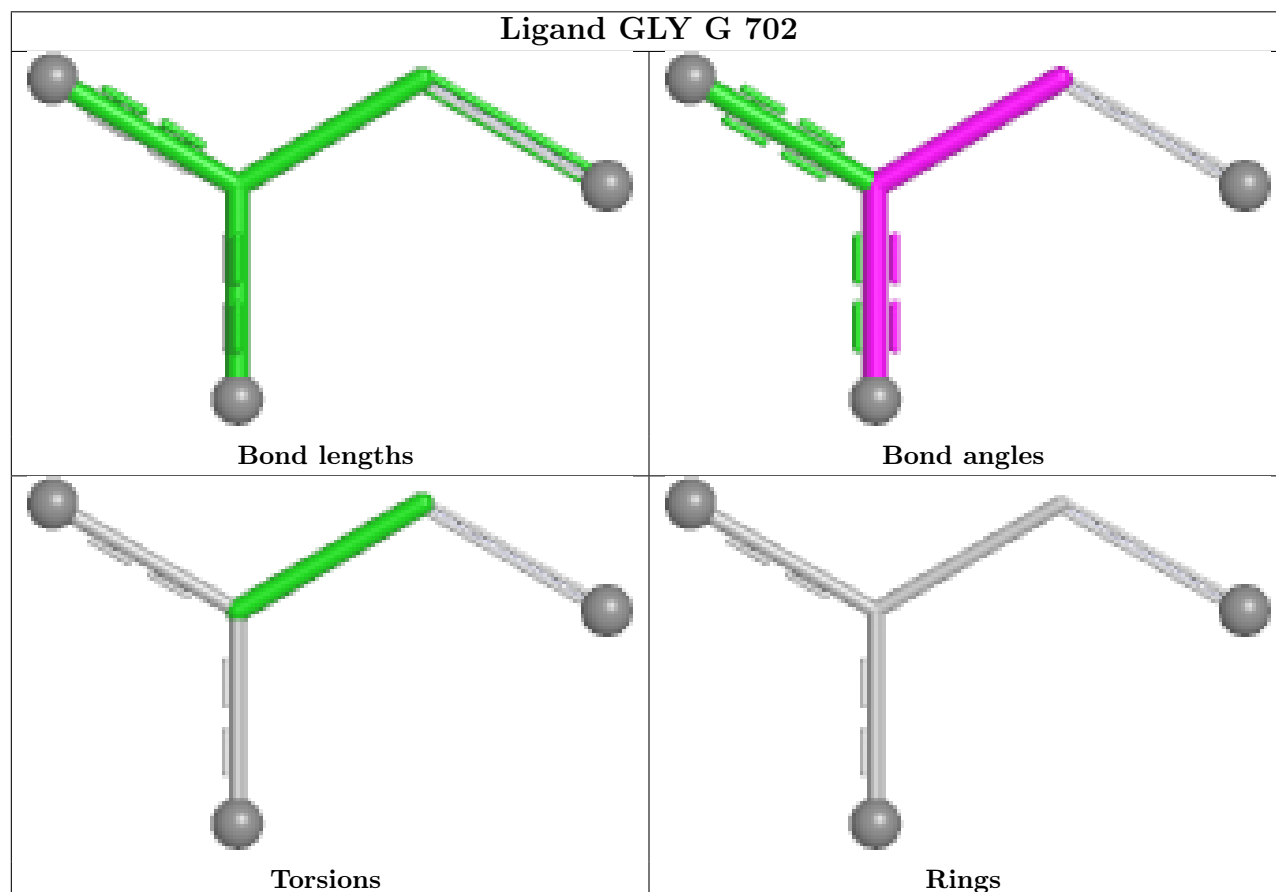
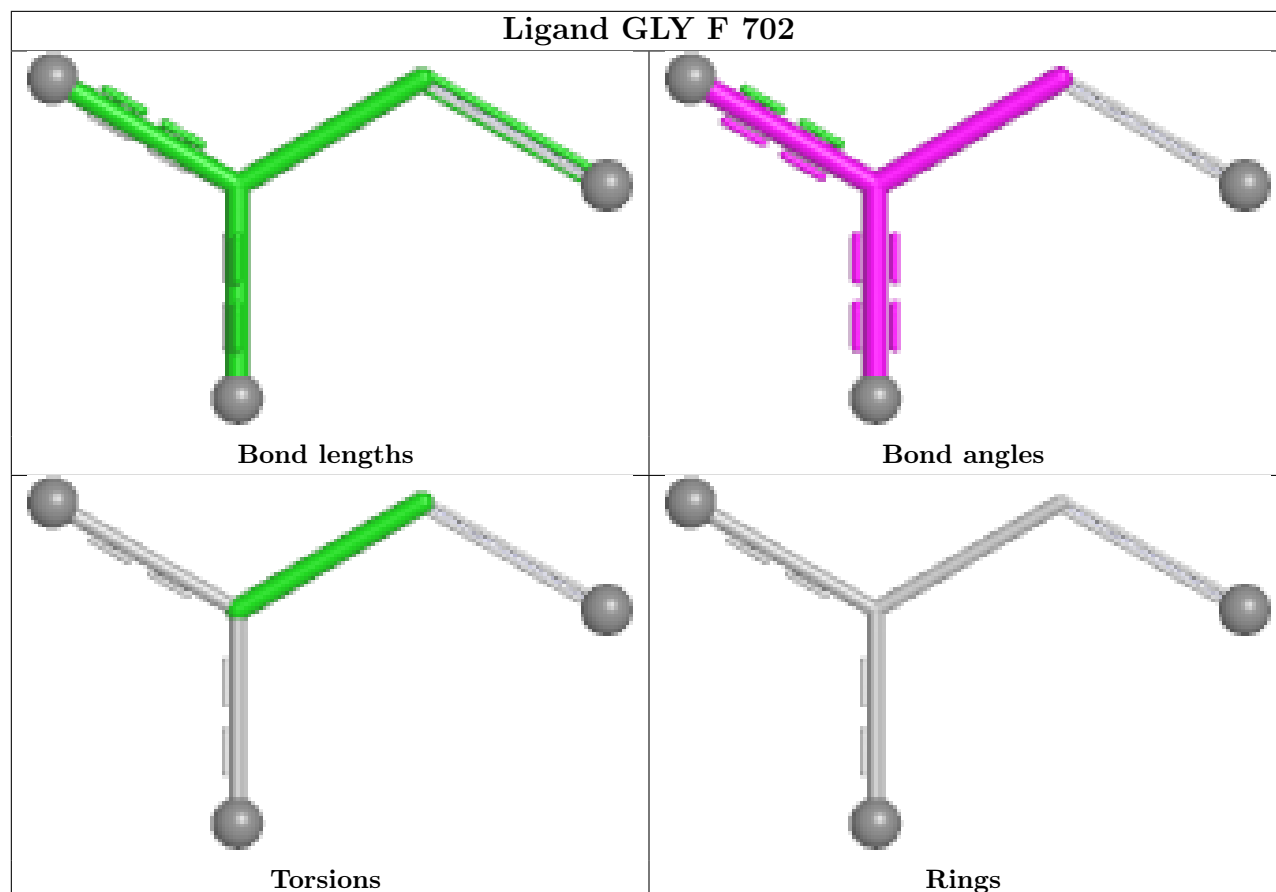
4 monomers are involved in 7 short contacts:

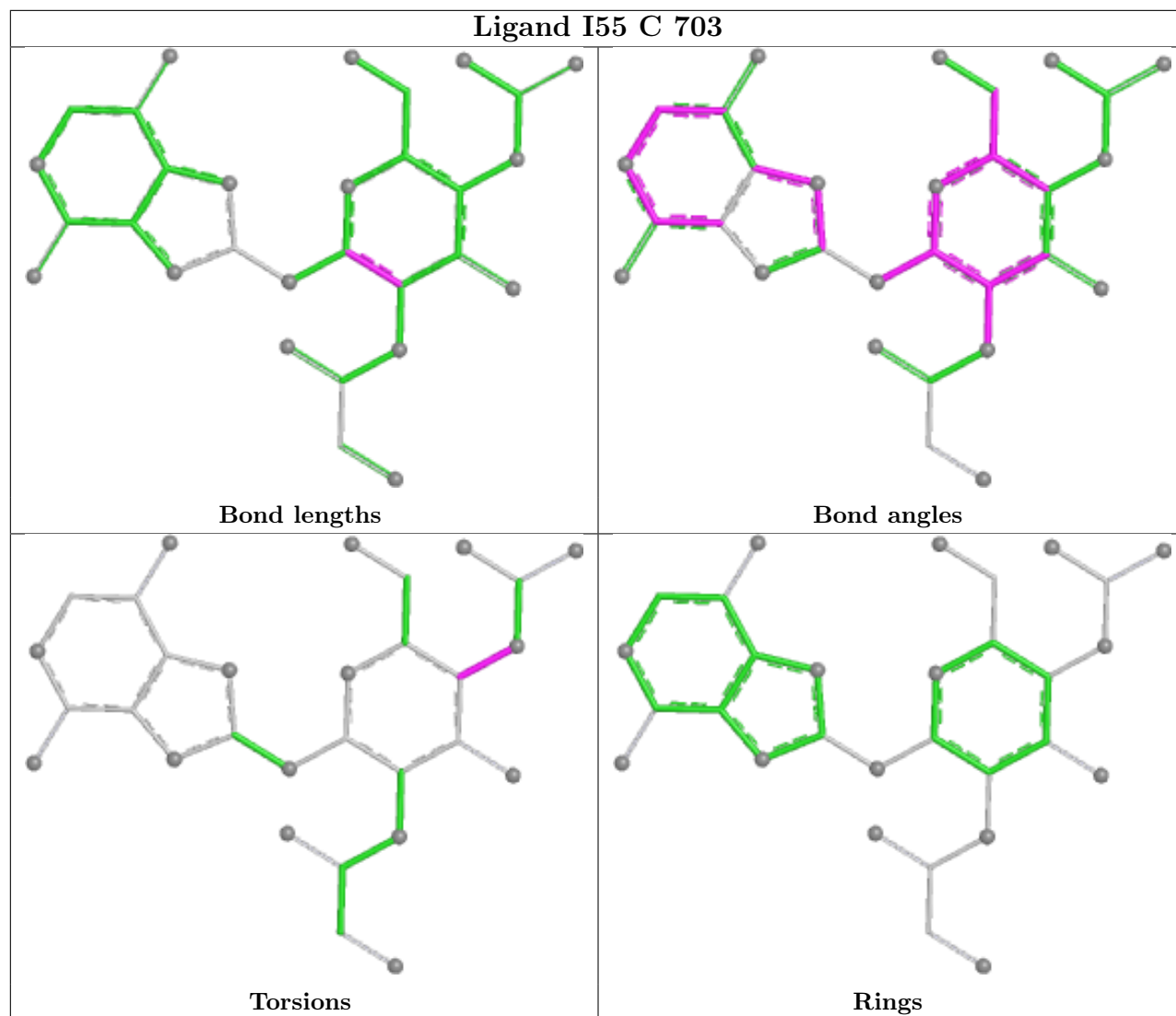
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	FAD	2	0
3	B	701	FAD	2	0
3	H	701	FAD	1	0
3	F	701	FAD	2	0

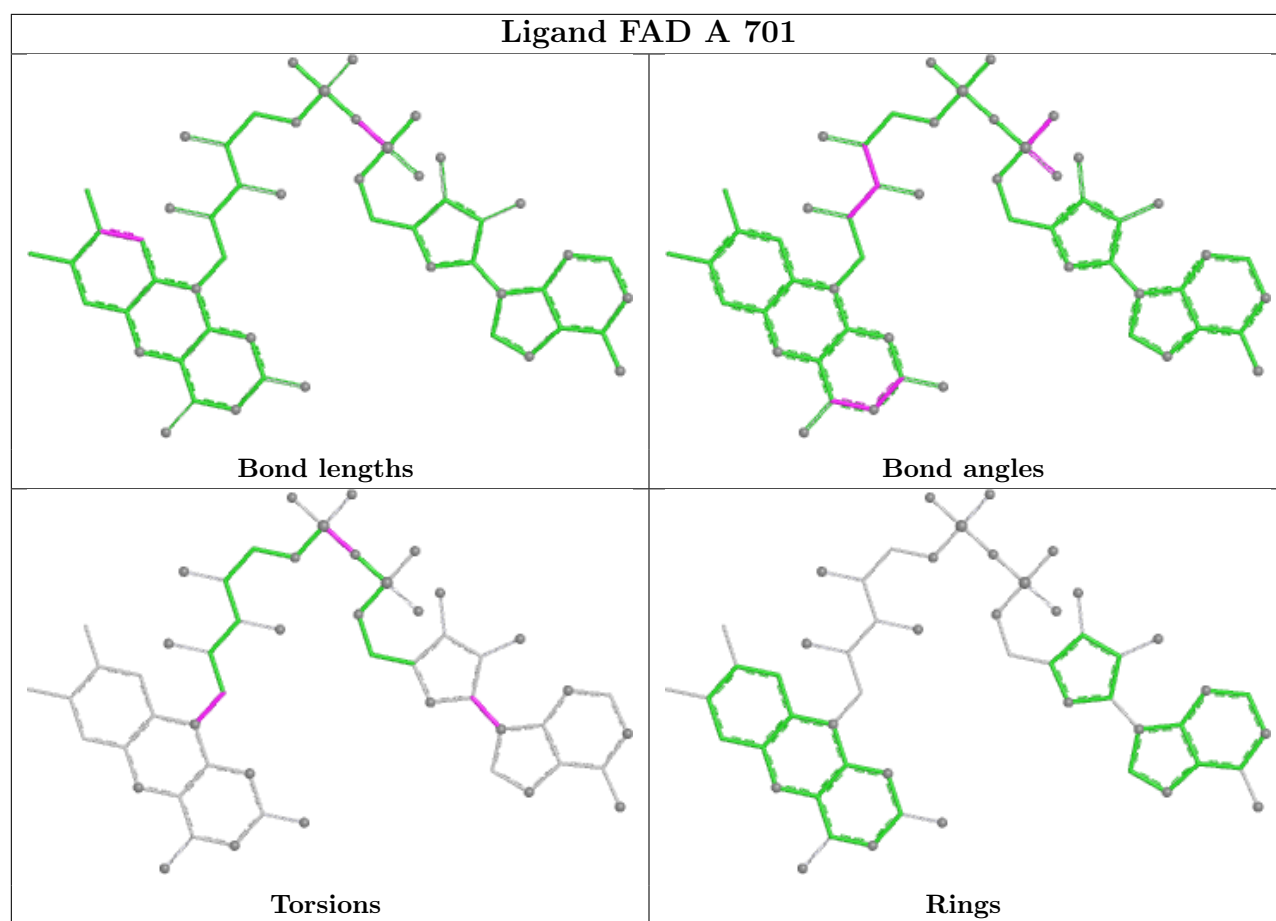
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

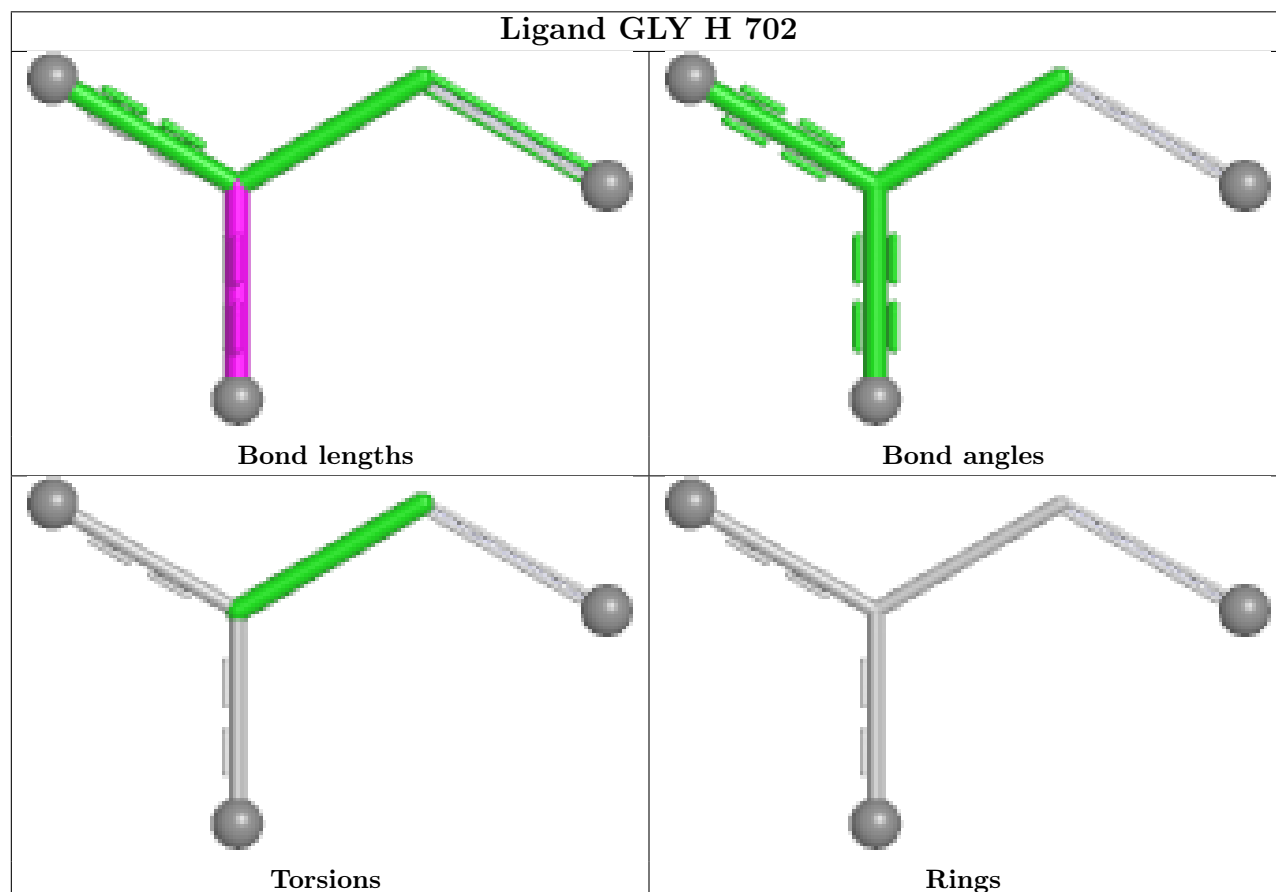
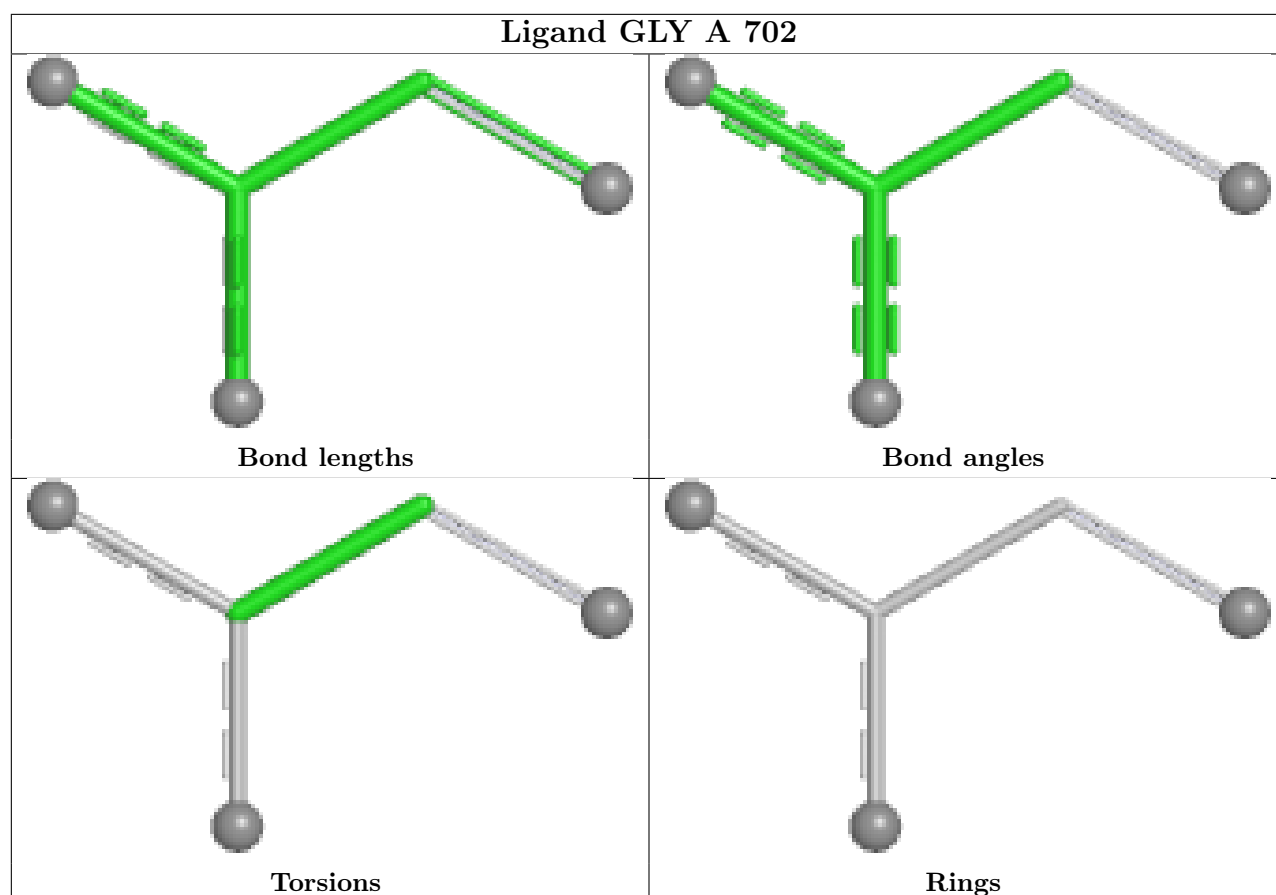


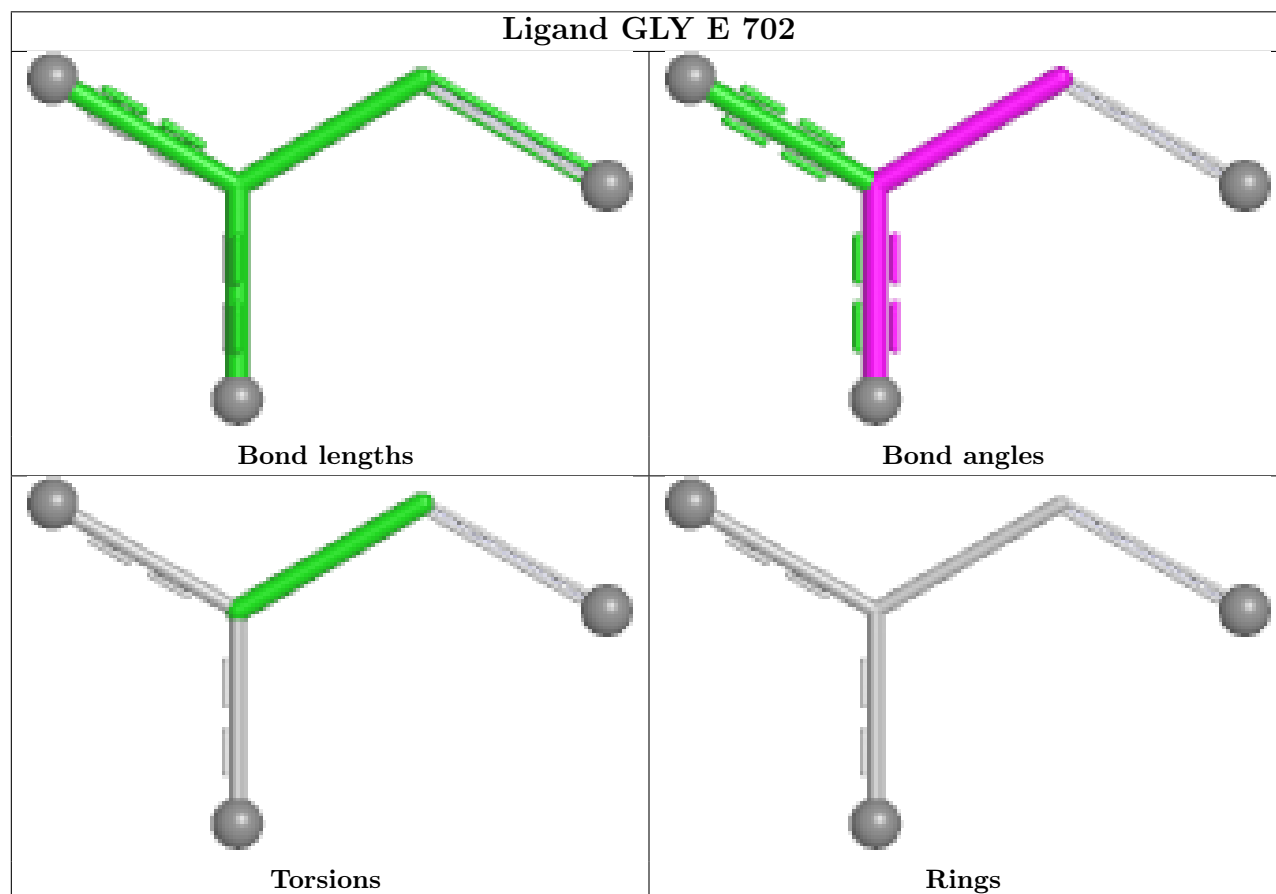
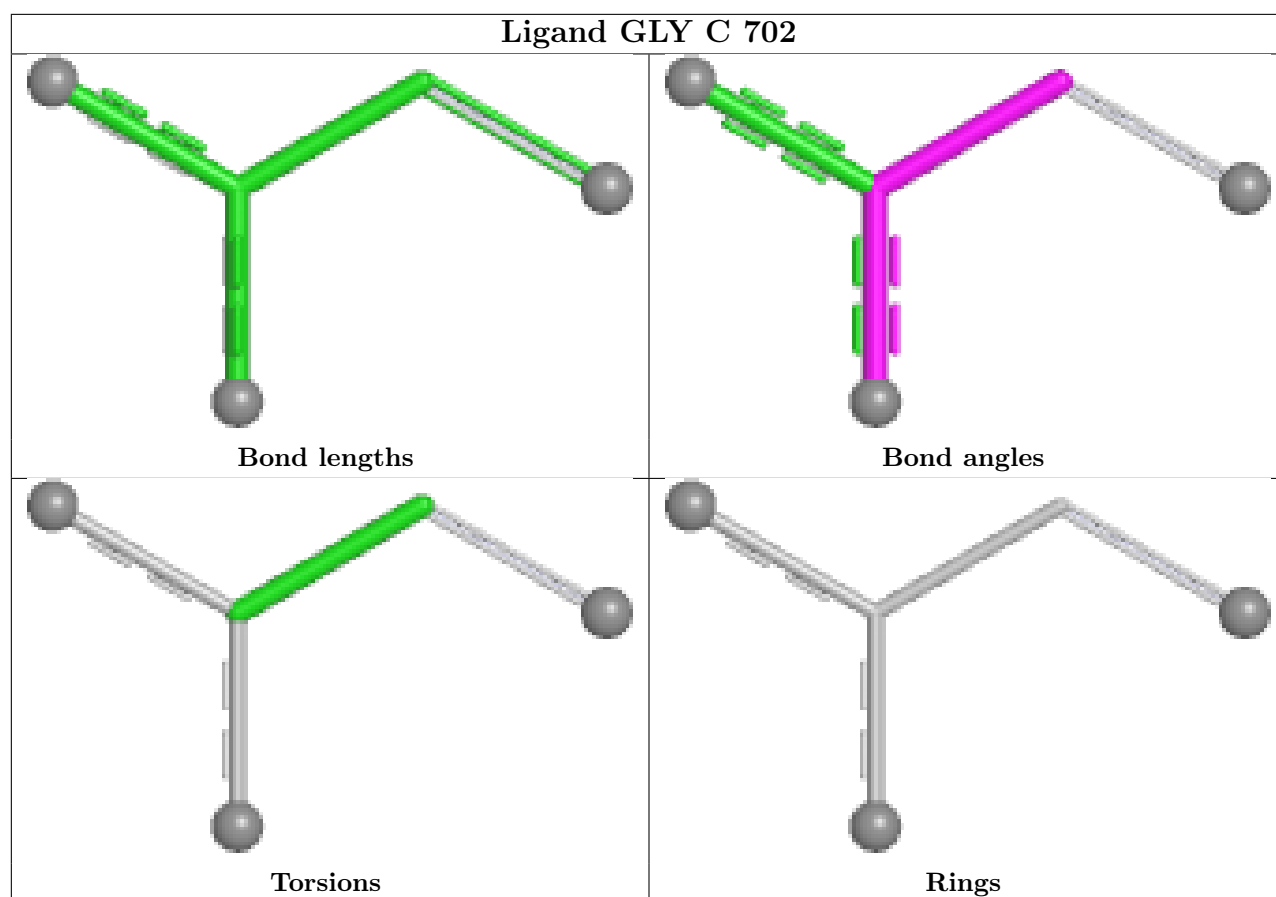


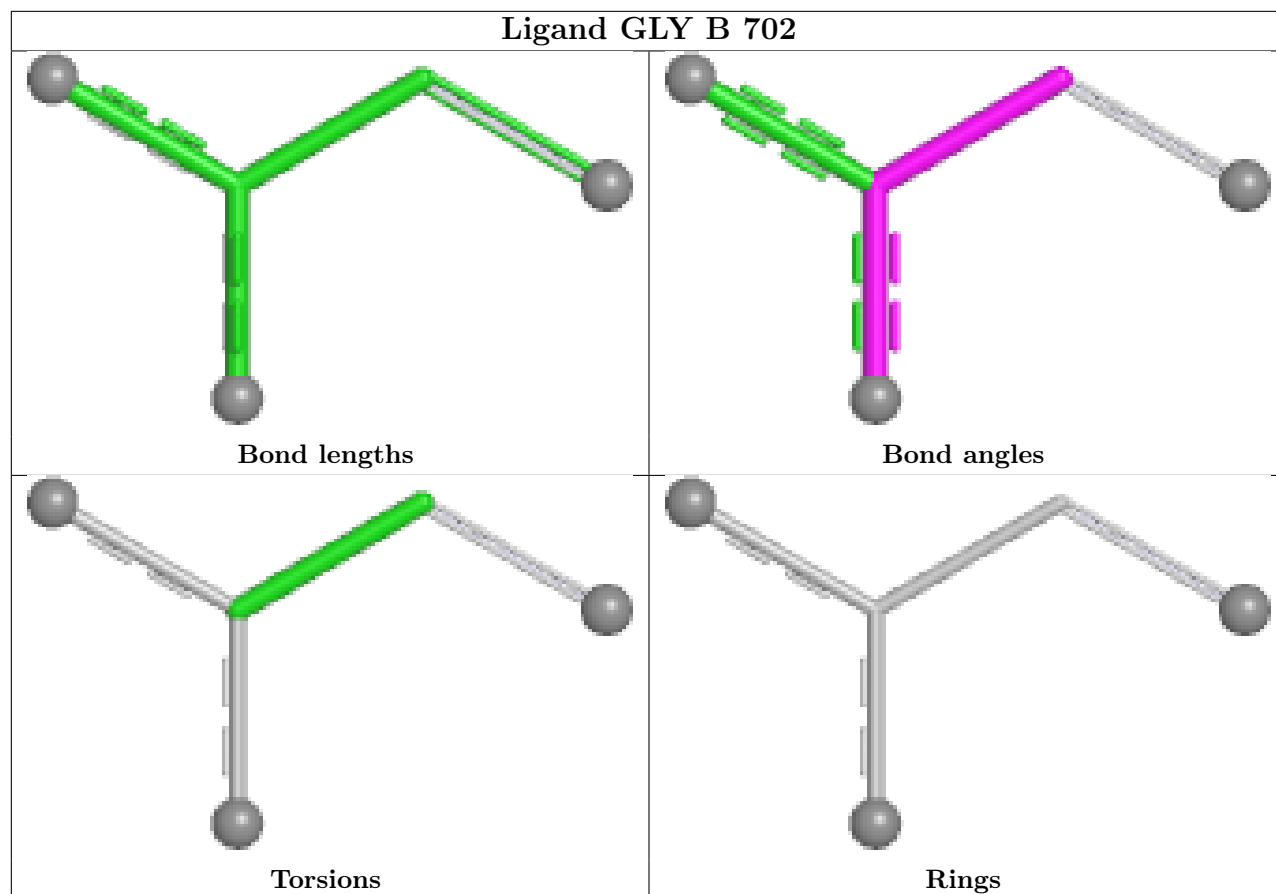


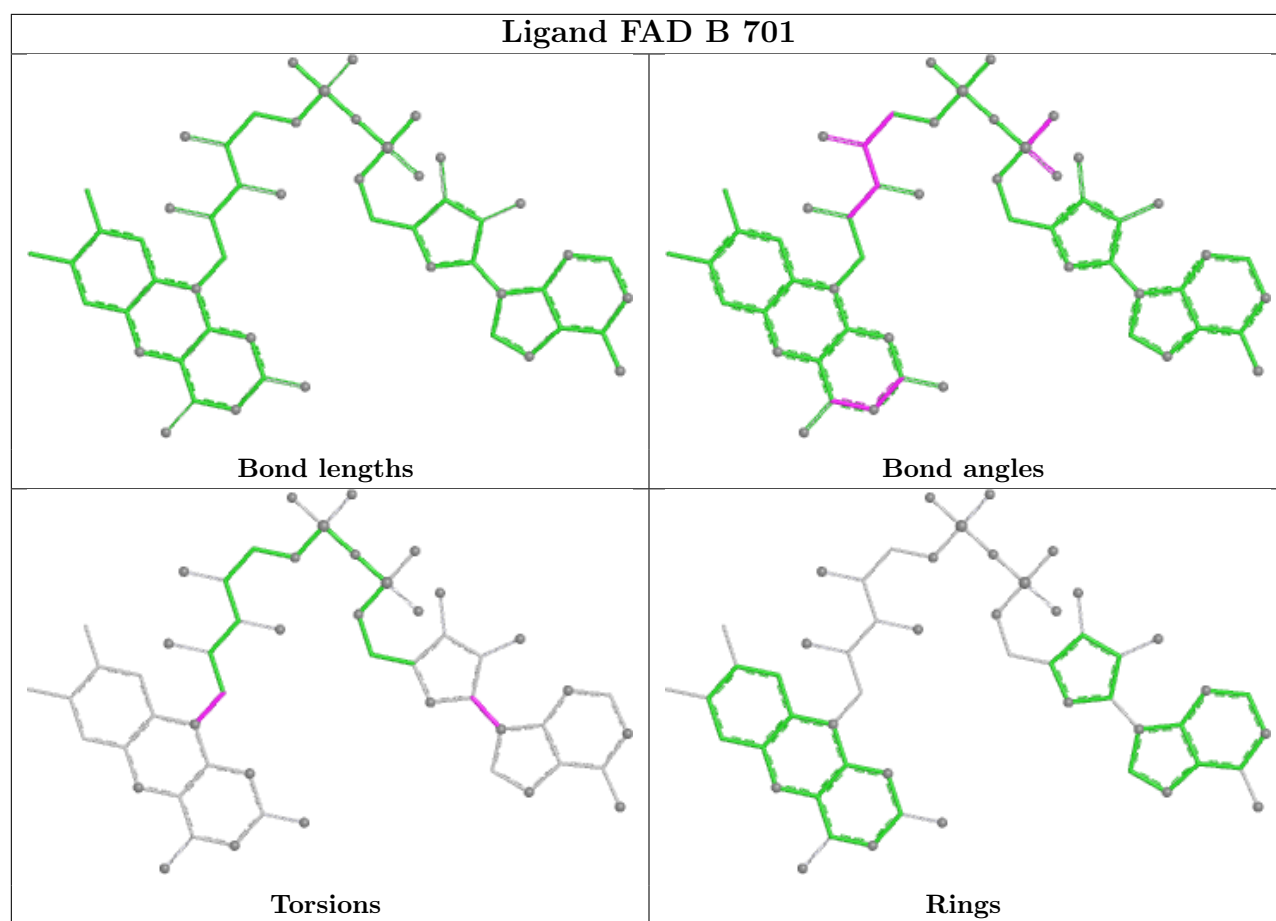


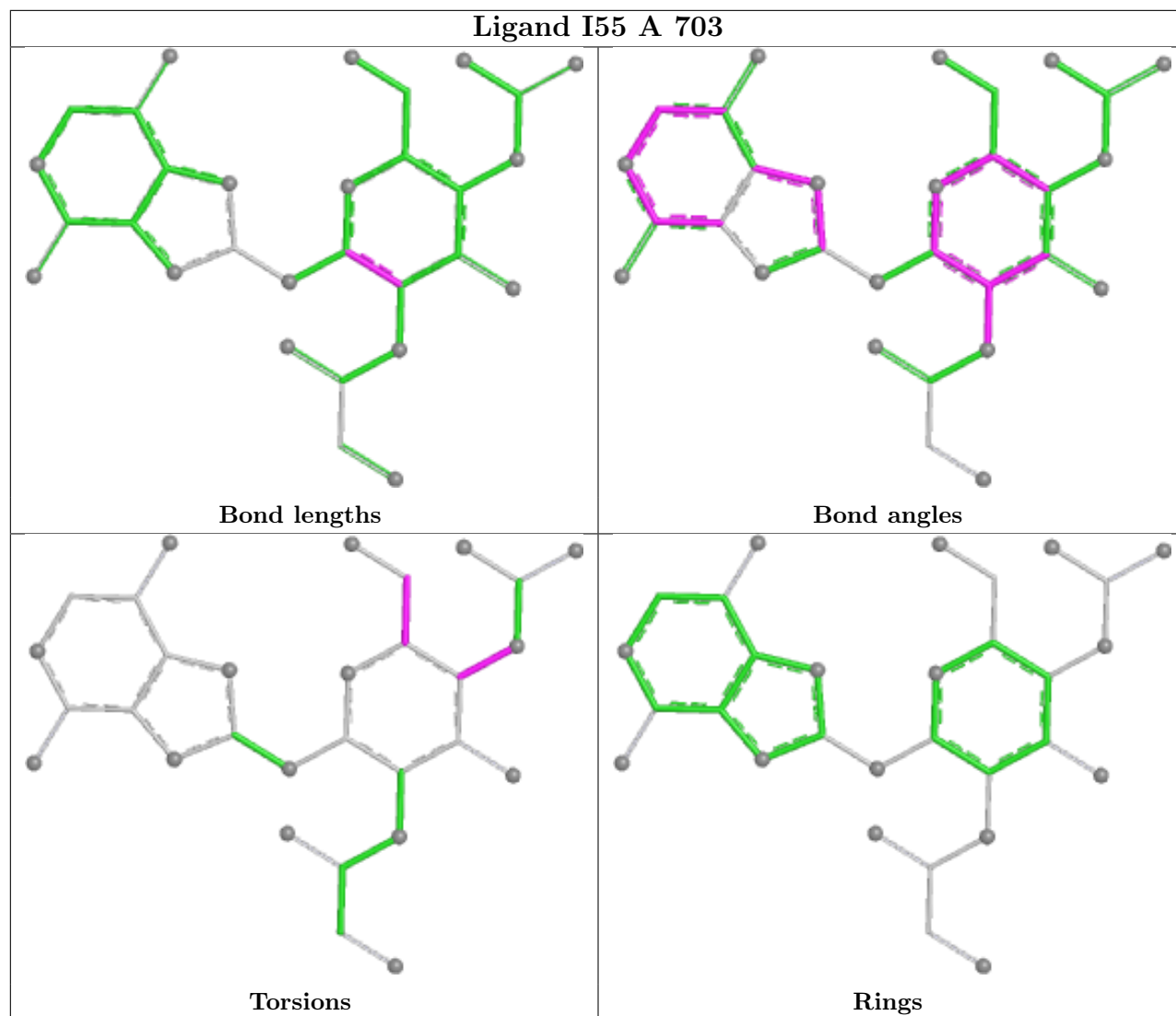


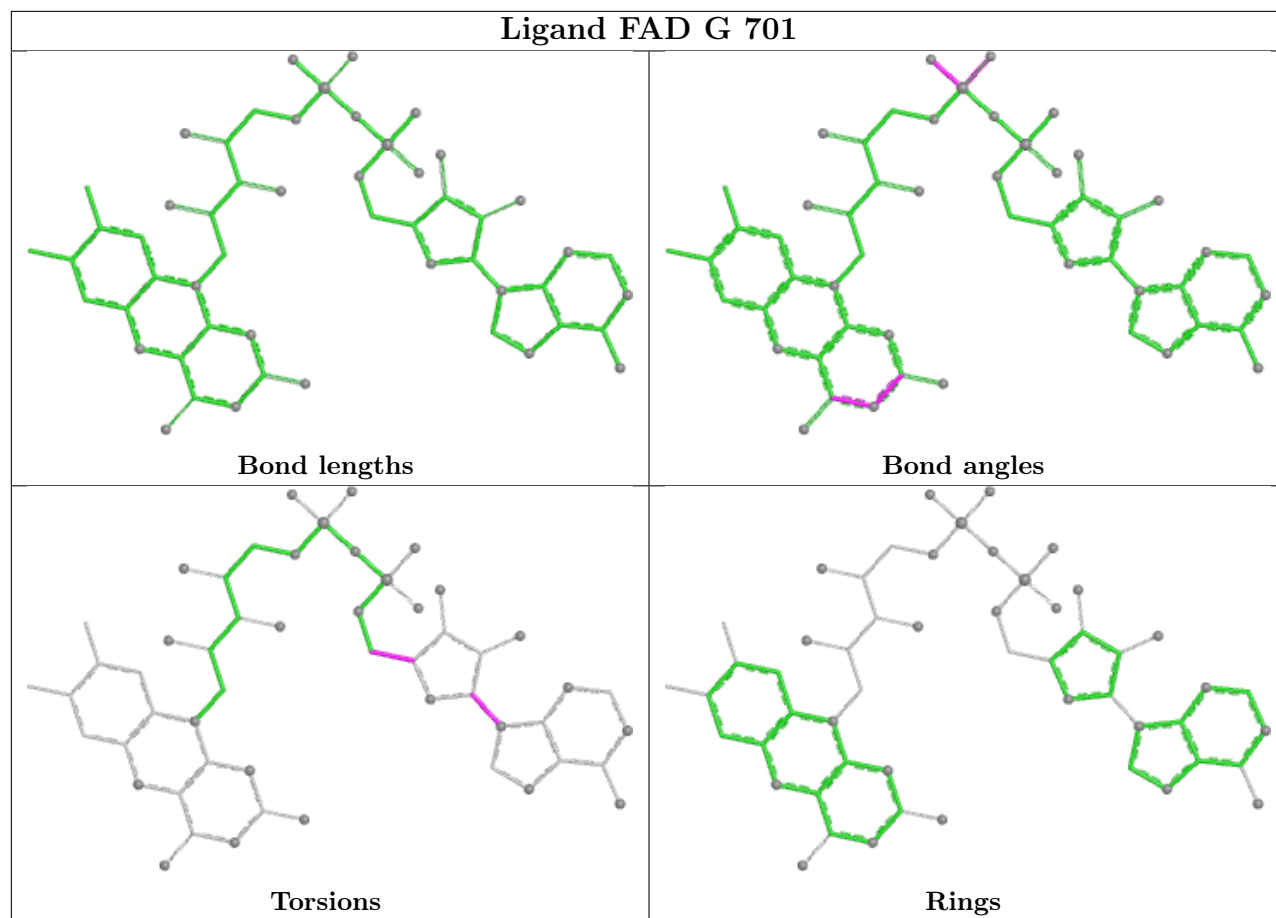


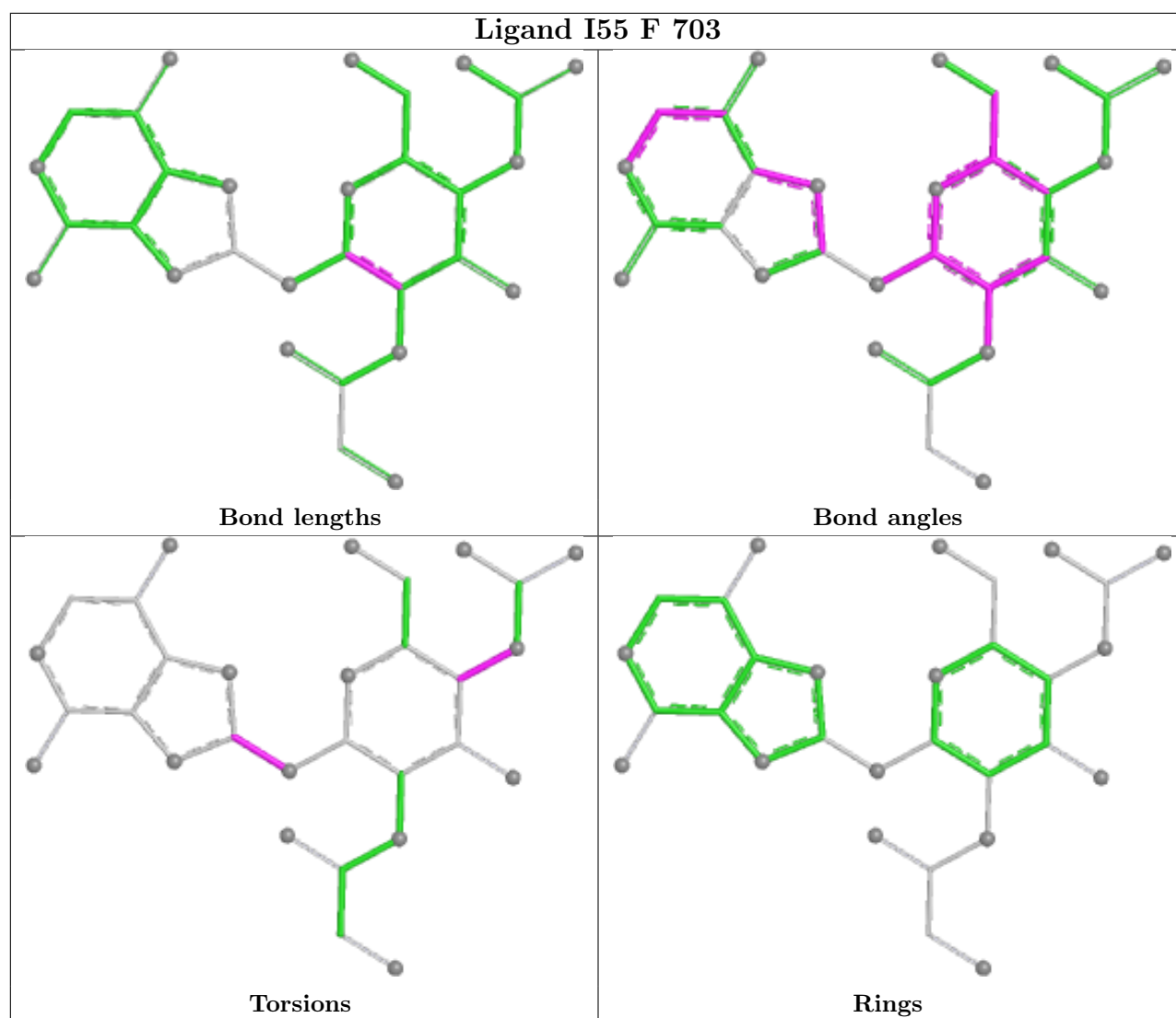


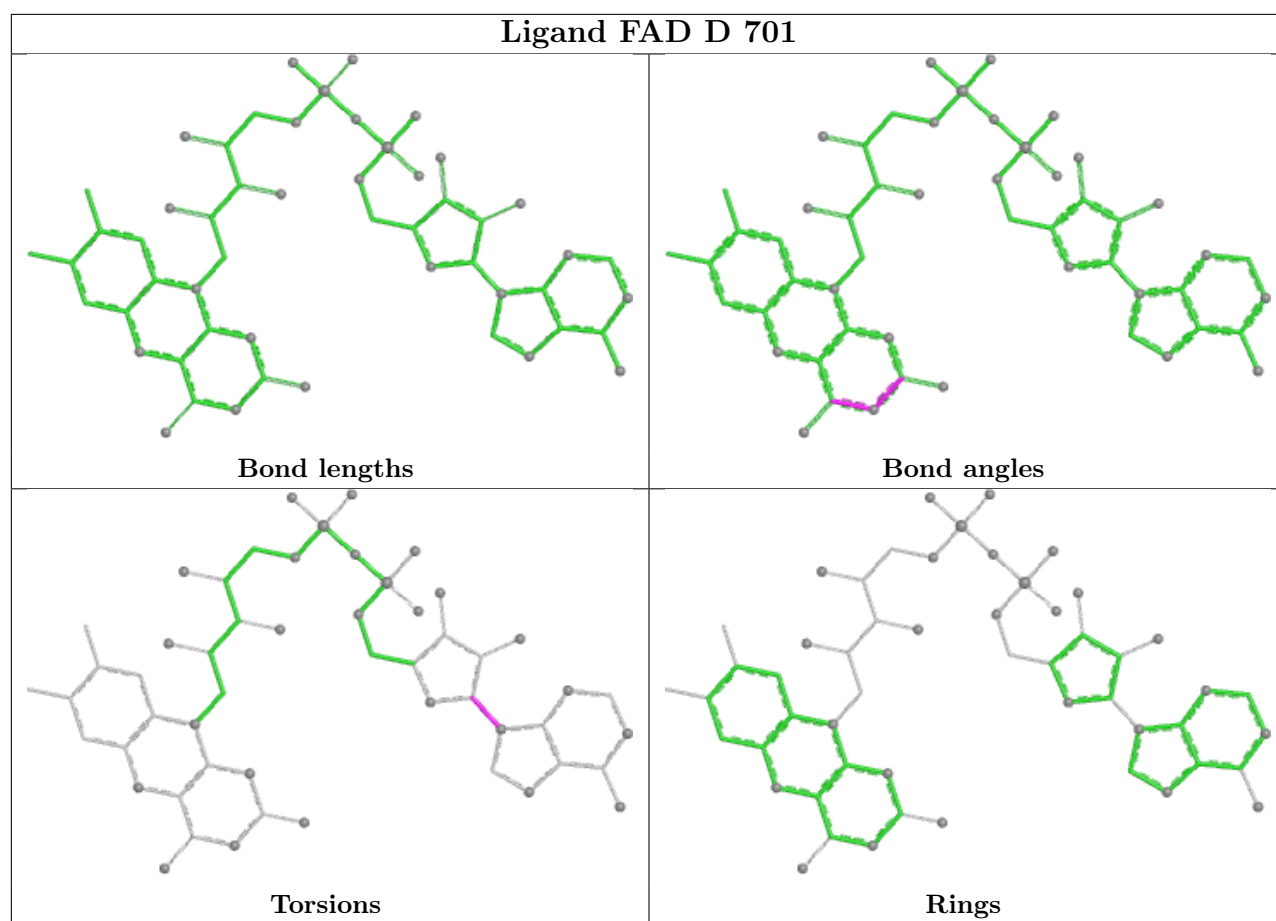


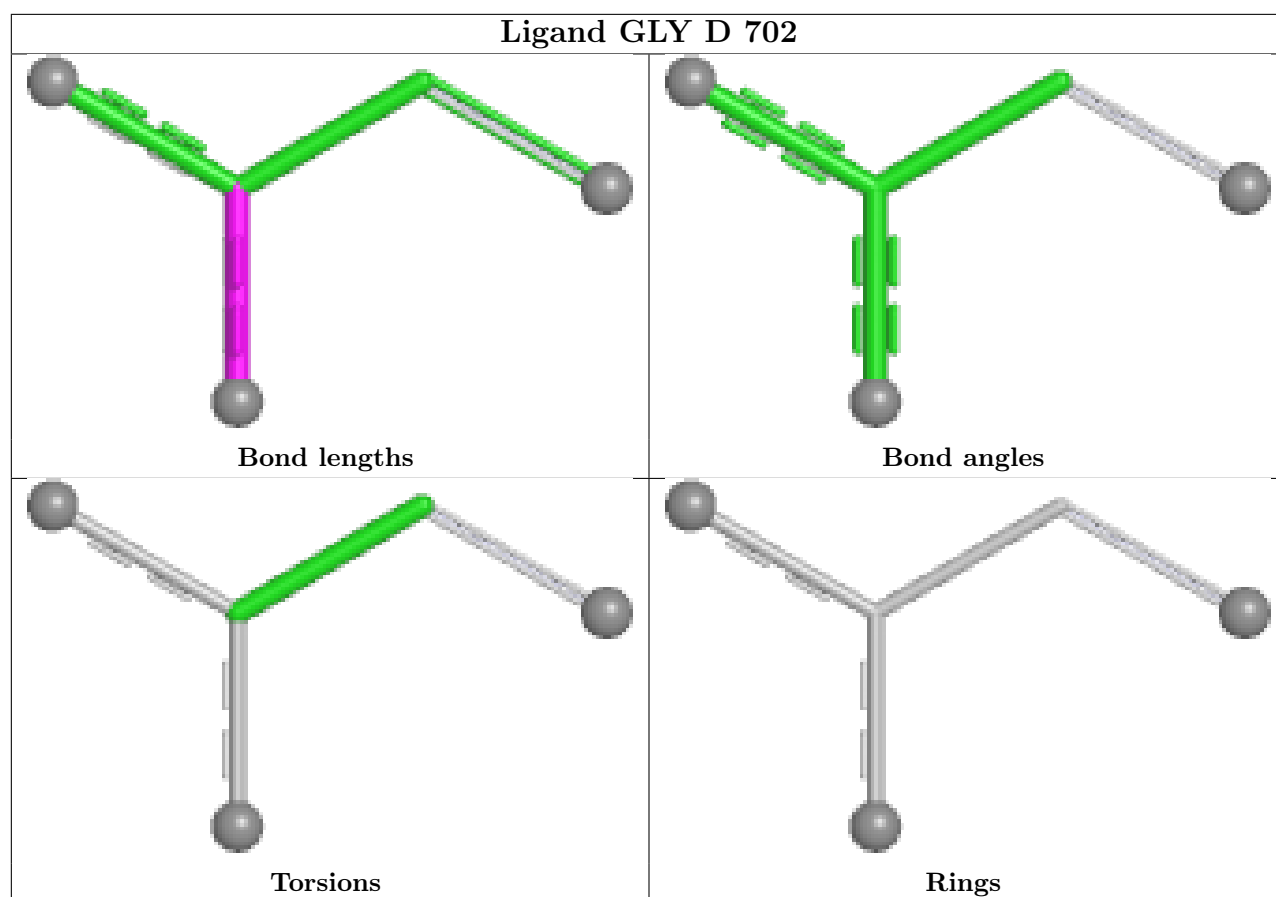


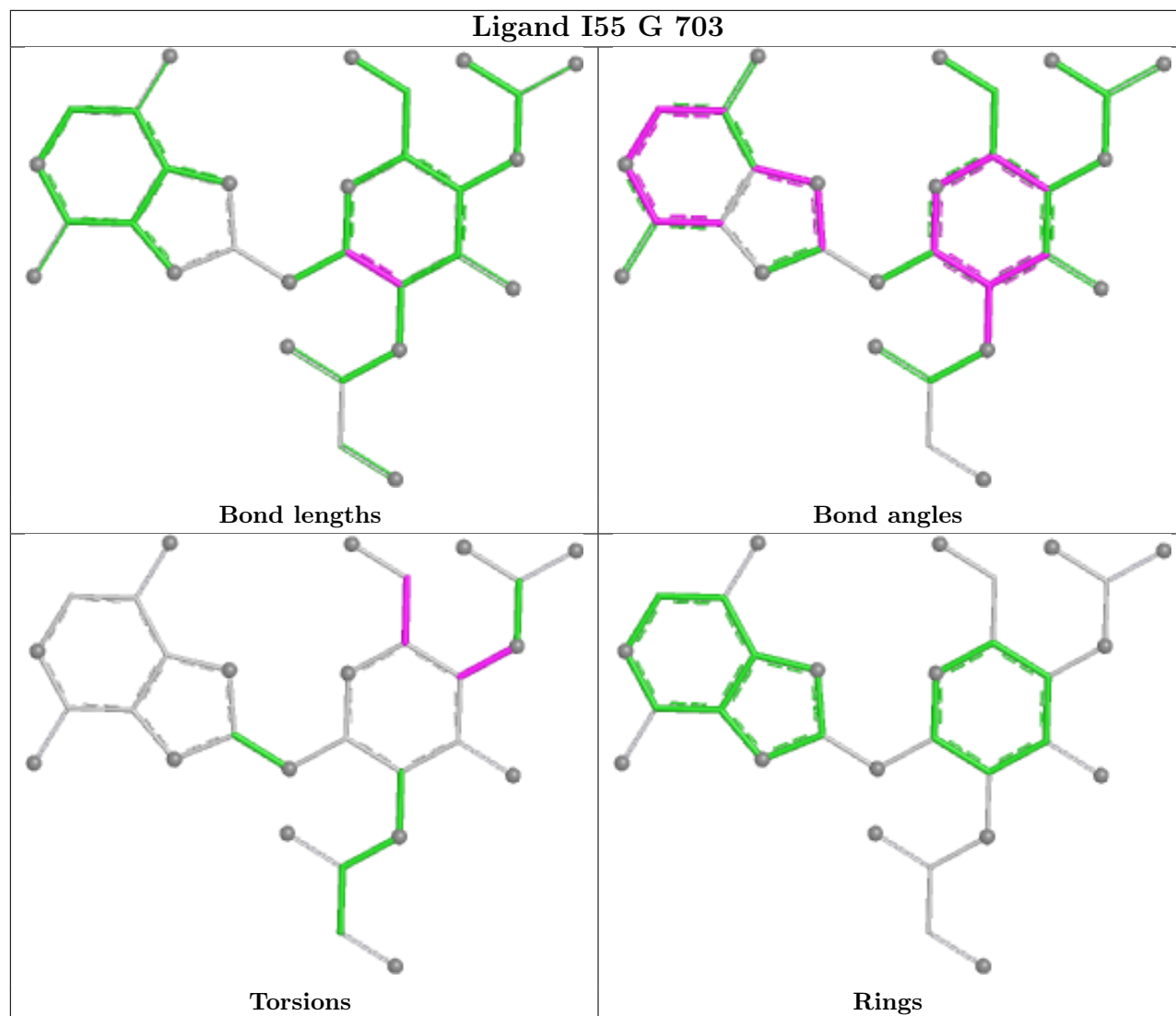


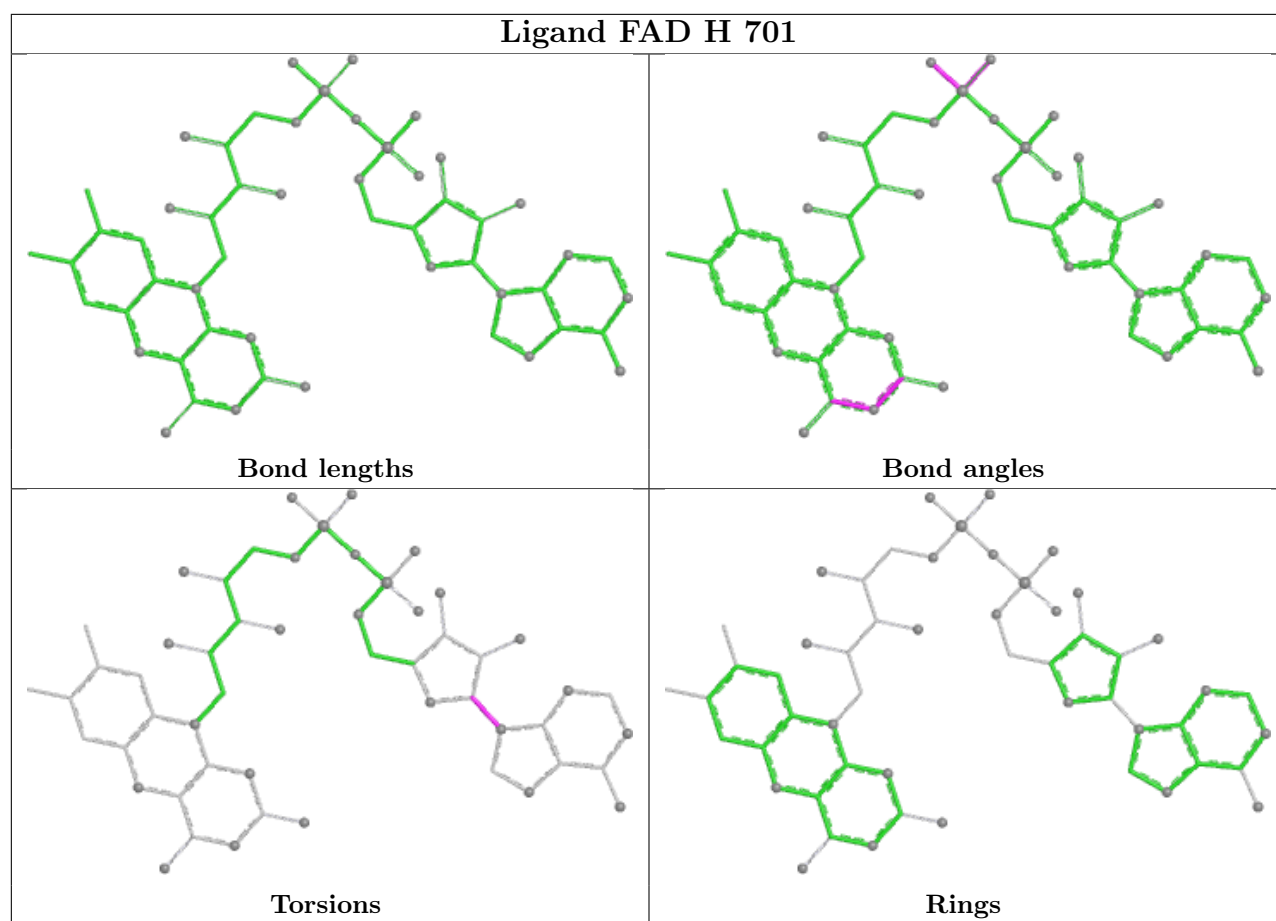


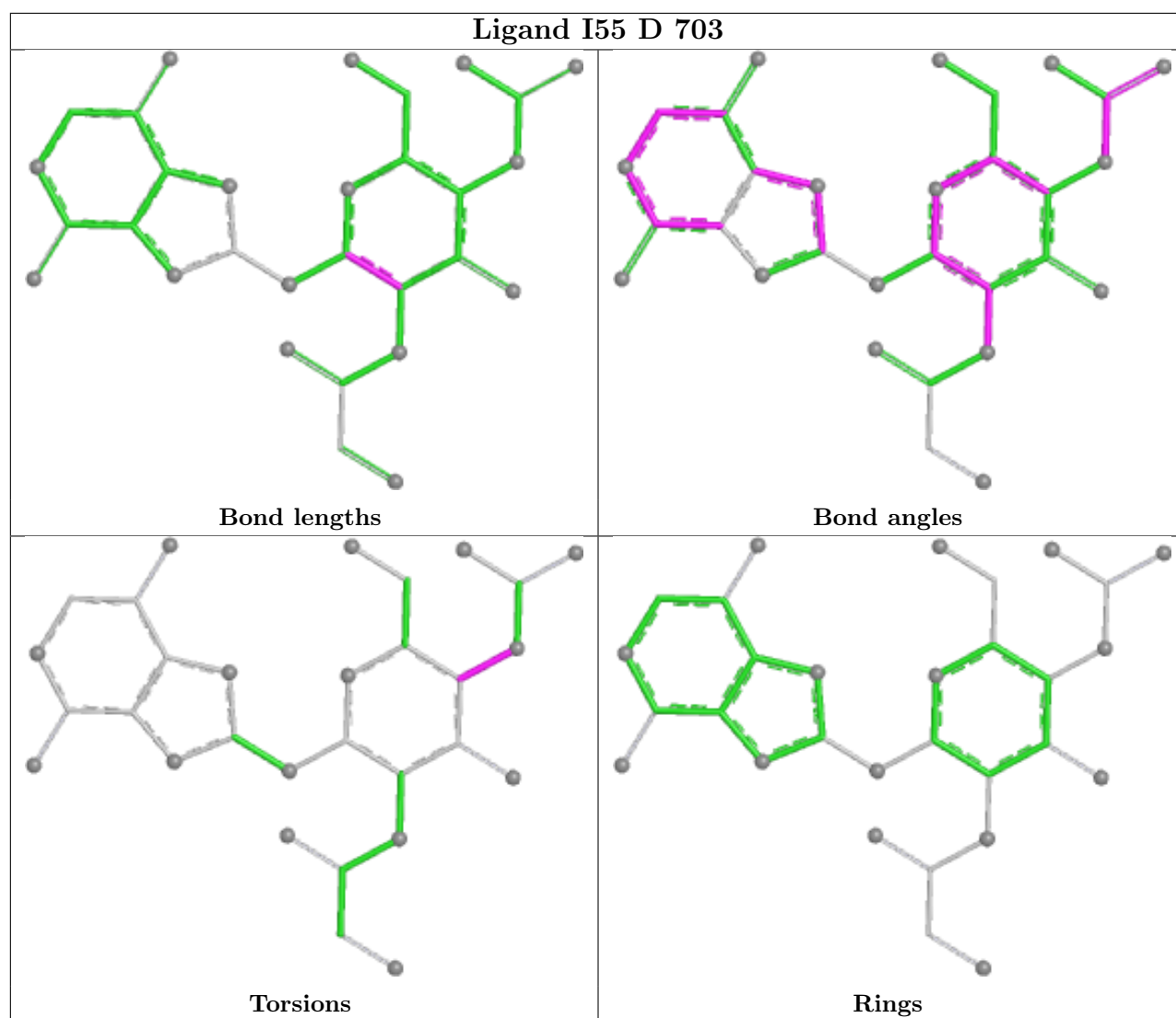


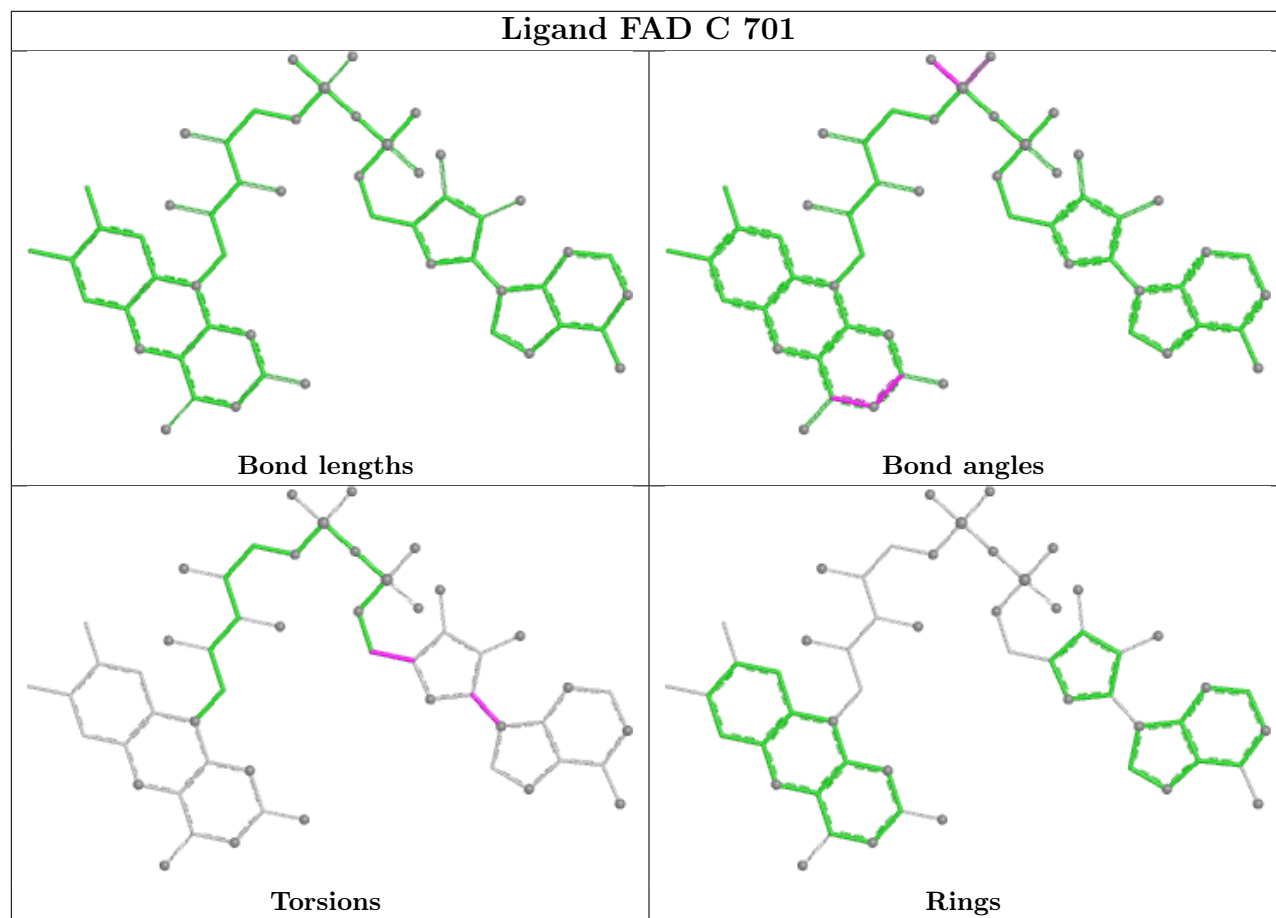


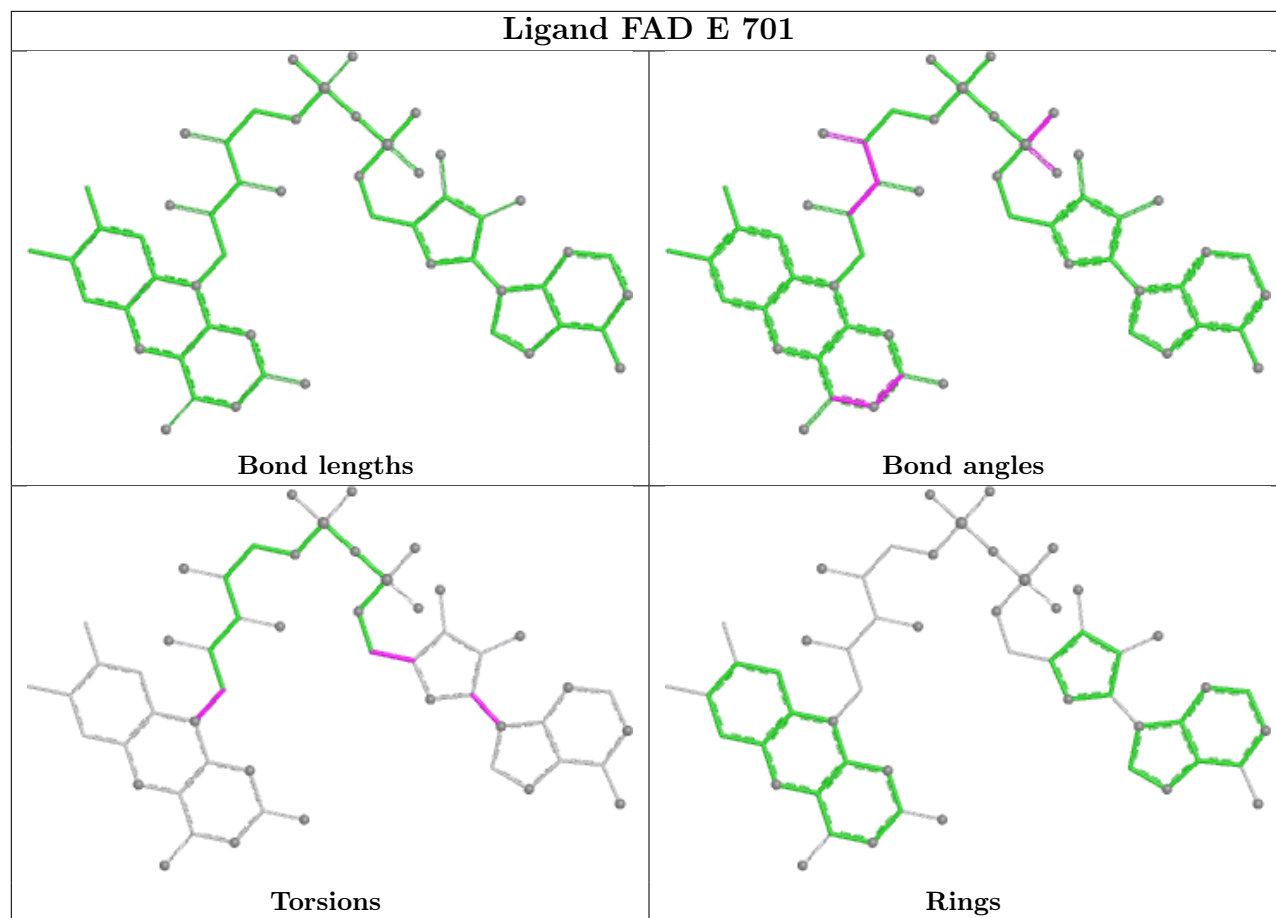




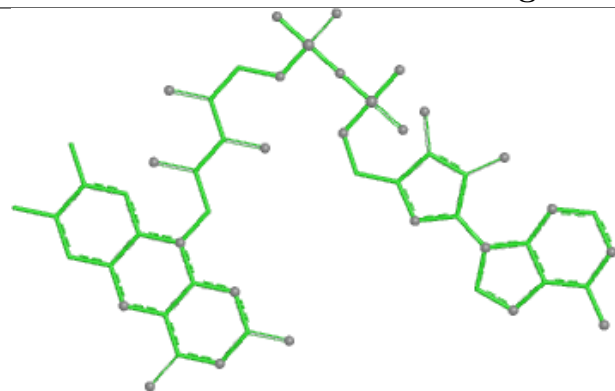




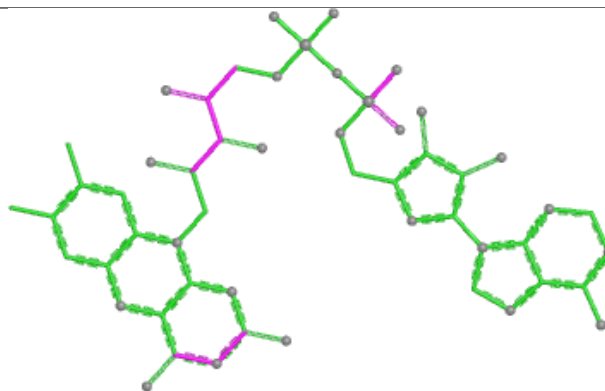




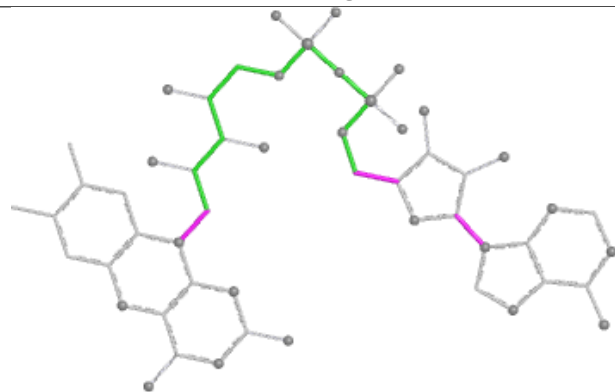
Ligand FAD F 701



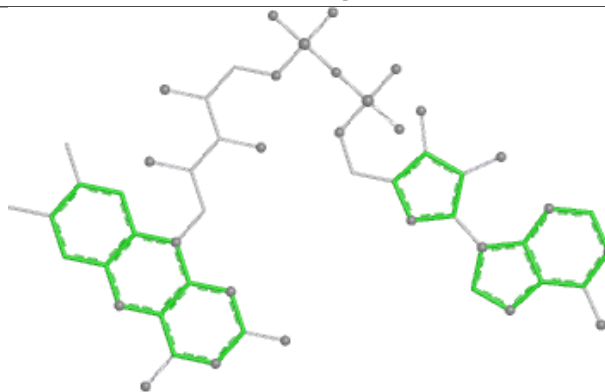
Bond lengths



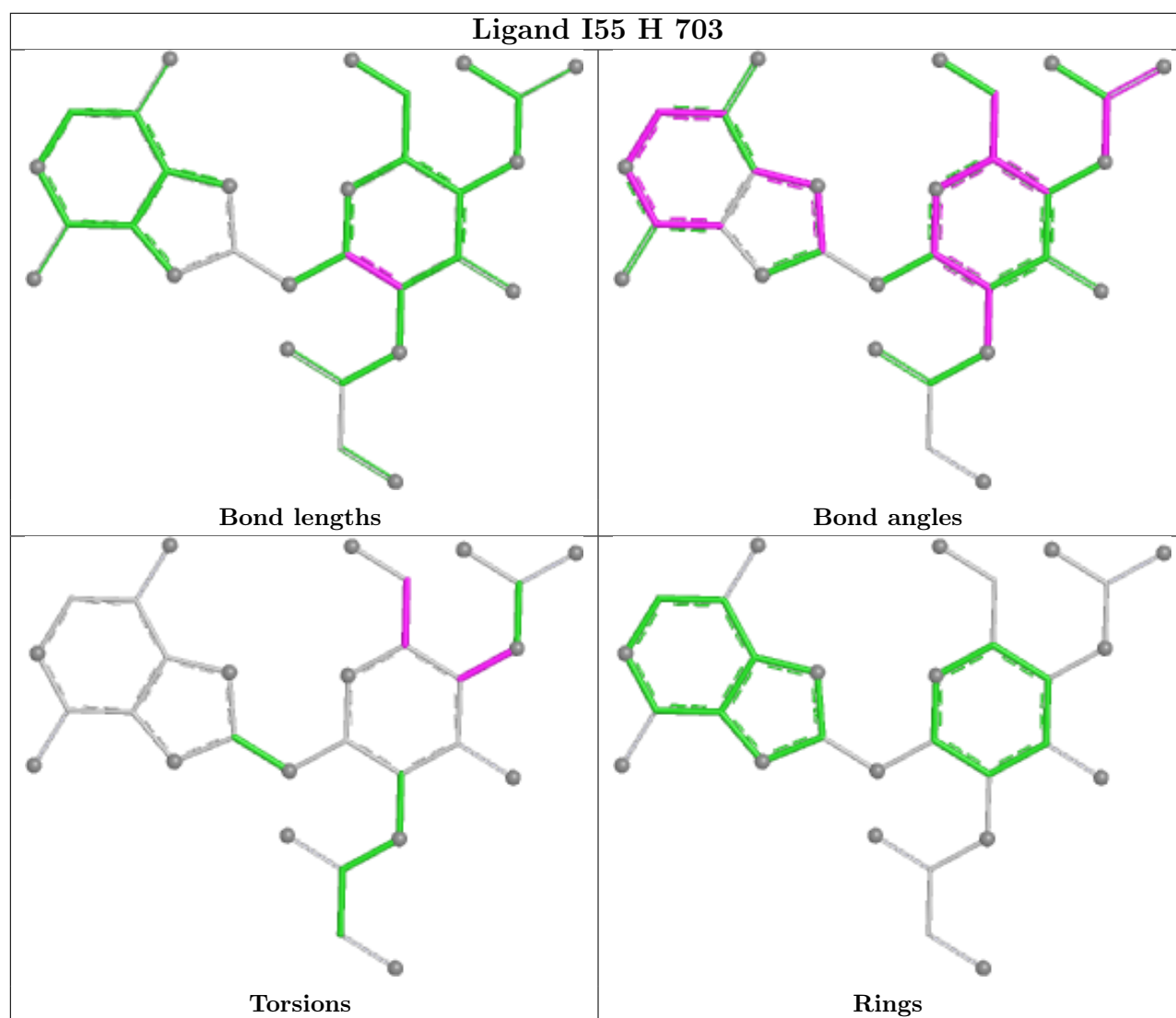
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/512 (93%)	-1.23	0 100 100	22, 38, 71, 101	0
1	B	480/512 (93%)	-1.27	0 100 100	19, 34, 64, 78	0
1	F	481/512 (93%)	-1.33	0 100 100	18, 35, 66, 80	0
2	C	480/512 (93%)	-1.27	0 100 100	19, 36, 71, 96	1 (0%)
2	D	477/512 (93%)	-1.04	0 100 100	24, 56, 100, 126	1 (0%)
2	E	481/512 (93%)	-1.25	0 100 100	20, 38, 73, 102	1 (0%)
2	G	481/512 (93%)	-1.27	0 100 100	17, 37, 71, 93	1 (0%)
2	H	469/512 (91%)	-0.98	0 100 100	24, 54, 99, 117	1 (0%)
All	All	3829/4096 (93%)	-1.20	0 100 100	17, 40, 84, 126	5 (0%)

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	GQI	A	281[A]	12/13	0.98	0.06	36,37,40,46	12
1	GQI	A	281[B]	6/13	0.98	0.06	31,32,33,33	6
1	GQI	B	281[A]	12/13	0.98	0.08	32,37,41,42	12
1	GQI	B	281[B]	6/13	0.98	0.08	22,24,26,26	6
1	GQI	F	281[A]	12/13	0.98	0.06	35,38,43,44	12
1	GQI	F	281[B]	6/13	0.98	0.06	25,27,29,29	6

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

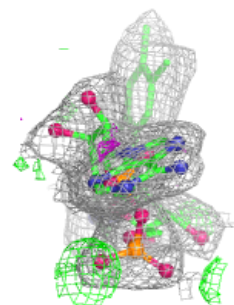
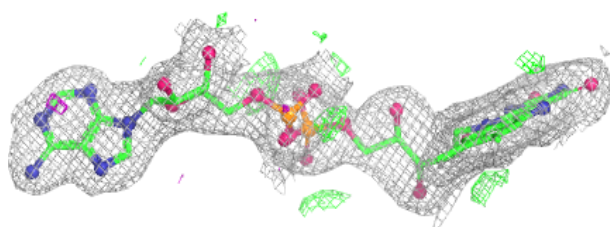
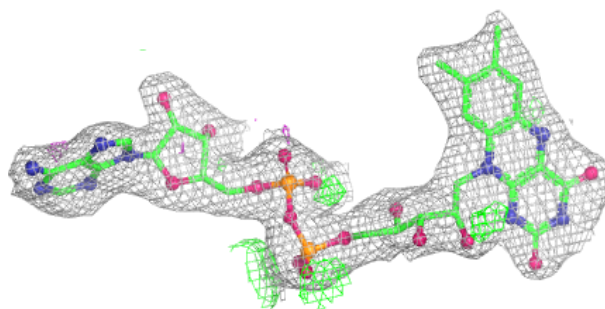
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FAD	A	701	53/53	0.99	0.03	28,32,36,40	0
3	FAD	B	701	53/53	0.99	0.03	22,28,32,33	0
3	FAD	C	701	53/53	0.99	0.04	40,51,61,63	0
3	FAD	D	701	53/53	0.99	0.04	50,59,76,78	0
3	FAD	E	701	53/53	0.99	0.03	29,32,35,40	0
3	FAD	F	701	53/53	0.99	0.03	22,27,32,34	0
3	FAD	G	701	53/53	0.99	0.04	39,51,61,64	0
3	FAD	H	701	53/53	0.99	0.04	51,59,74,75	0
4	GLY	A	702	5/5	0.99	0.04	38,42,48,51	0
4	GLY	B	702	5/5	0.99	0.04	33,33,35,35	0
4	GLY	C	702	5/5	0.99	0.06	43,46,51,52	0
4	GLY	D	702	5/5	0.99	0.04	55,57,60,61	0
4	GLY	E	702	5/5	0.99	0.03	39,40,44,45	0
4	GLY	F	702	5/5	0.99	0.05	31,33,34,35	0
4	GLY	G	702	5/5	0.99	0.06	45,50,55,59	0
4	GLY	H	702	5/5	0.99	0.05	54,59,64,65	0
5	I55	A	703	30/30	0.99	0.03	27,34,45,49	0
5	I55	B	703	30/30	0.99	0.04	29,40,47,51	0
5	I55	C	703	30/30	0.99	0.04	33,42,52,53	0
5	I55	D	703	30/30	0.99	0.04	40,48,53,55	0
5	I55	E	703	30/30	0.99	0.03	26,33,41,48	0
5	I55	F	703	30/30	0.99	0.03	27,42,48,51	0
5	I55	G	703	30/30	0.99	0.04	33,45,51,52	0
5	I55	H	703	30/30	0.99	0.04	39,48,53,54	0

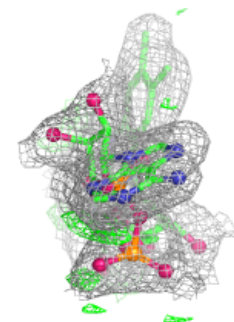
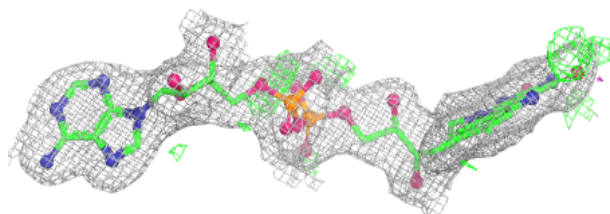
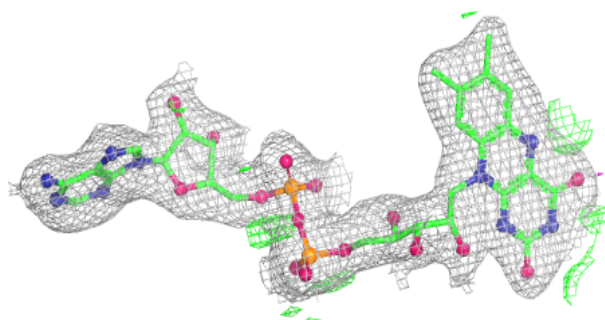
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 701:

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

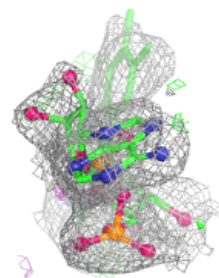
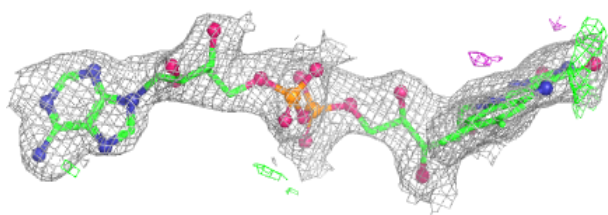
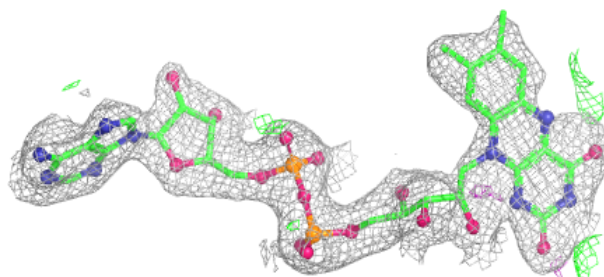
**Electron density around FAD B 701:**

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and green (positive)

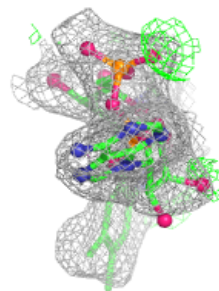
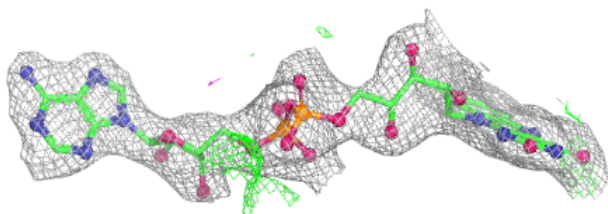
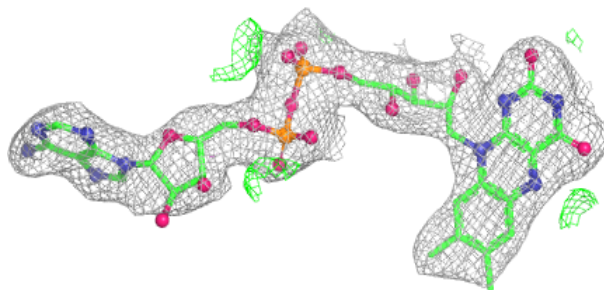


Electron density around FAD C 701:

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

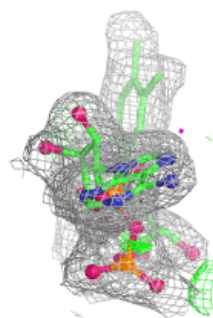
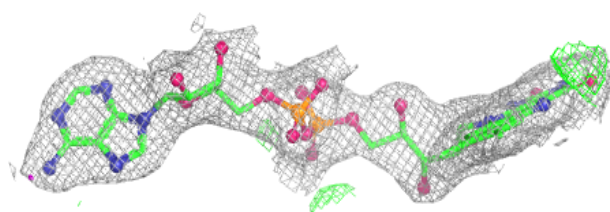
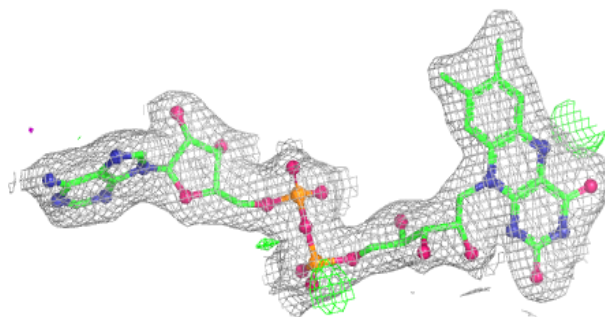
**Electron density around FAD D 701:**

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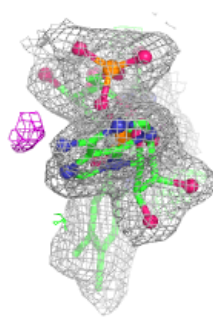
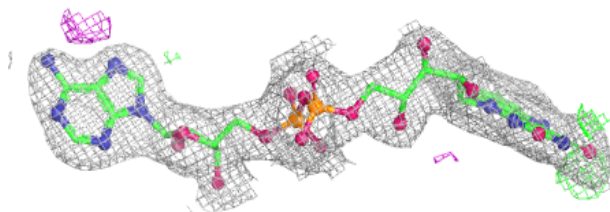
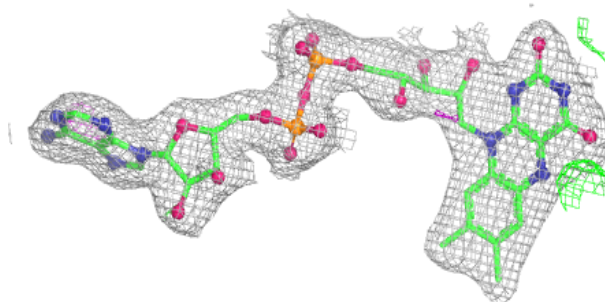


Electron density around FAD E 701:

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and green (positive)

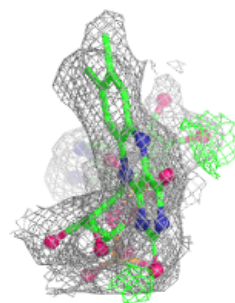
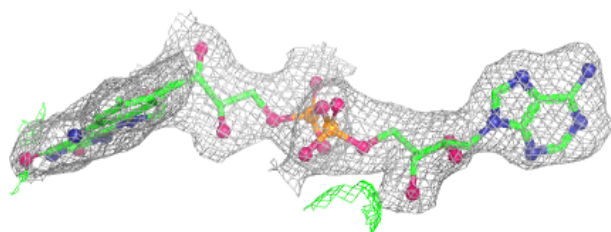
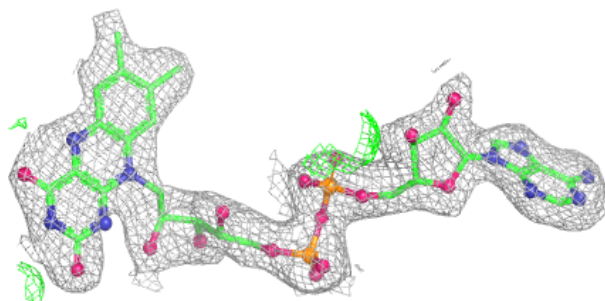
**Electron density around FAD F 701:**

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and green (positive)

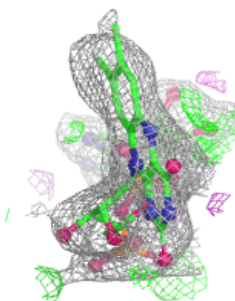
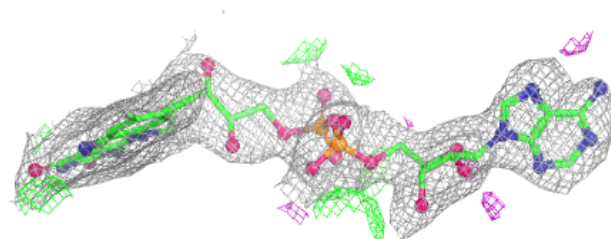
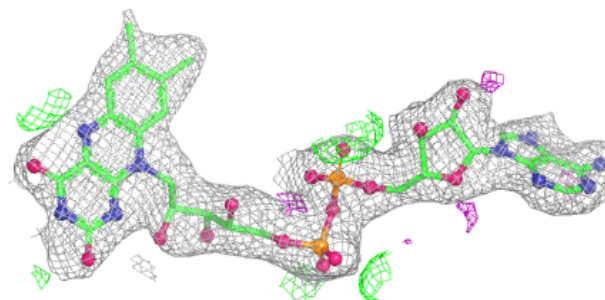


Electron density around FAD G 701:

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and green (positive)

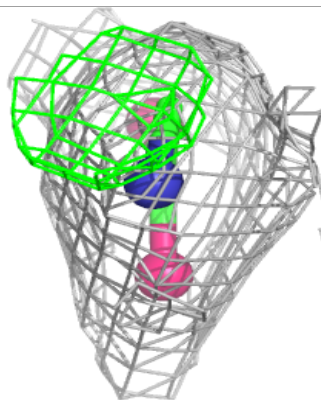
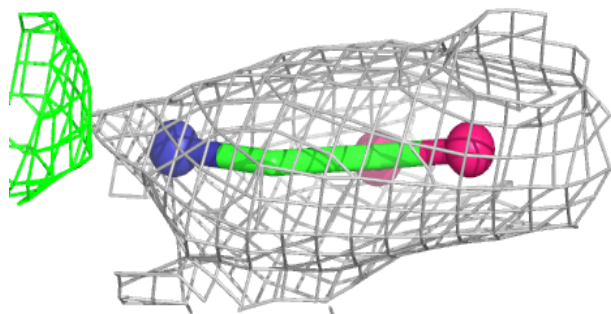
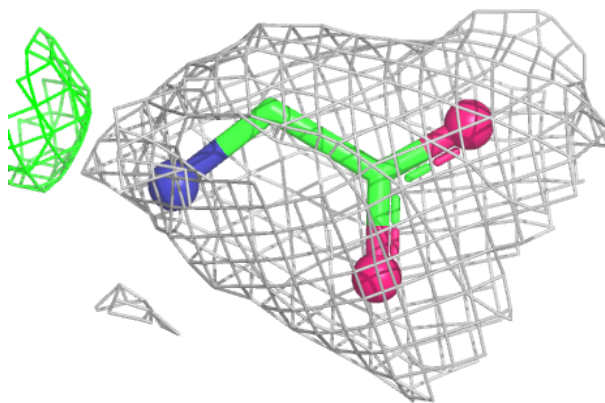
**Electron density around FAD H 701:**

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and green (positive)

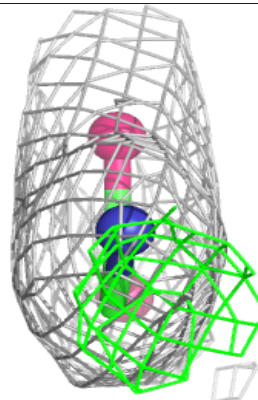
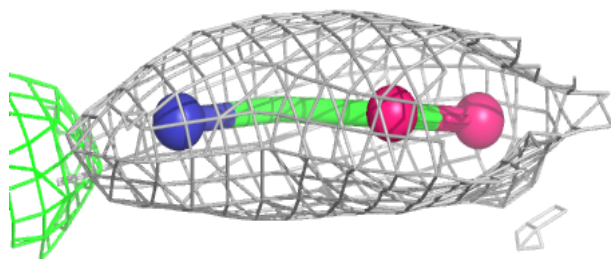
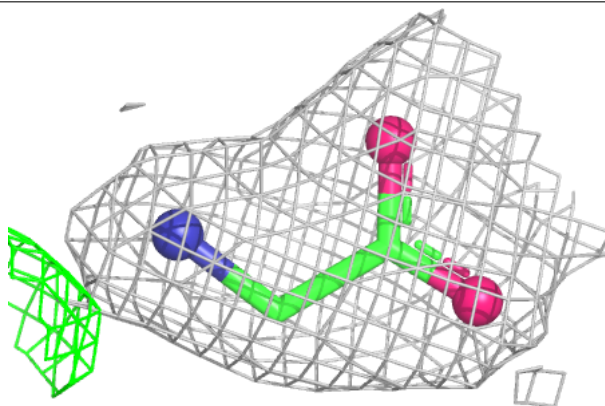


Electron density around GLY A 702:

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and green (positive)

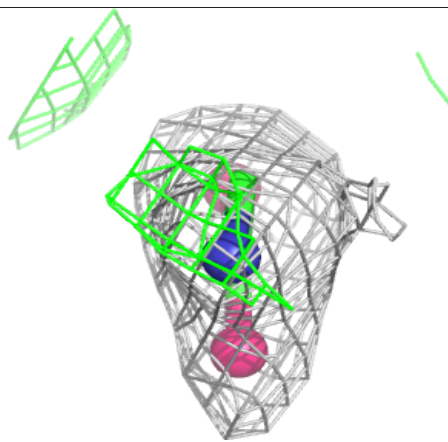
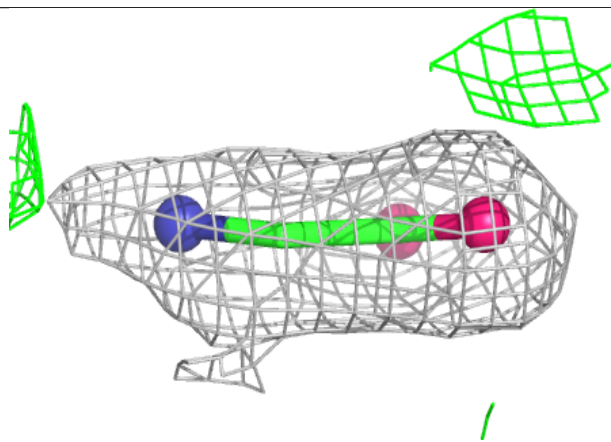
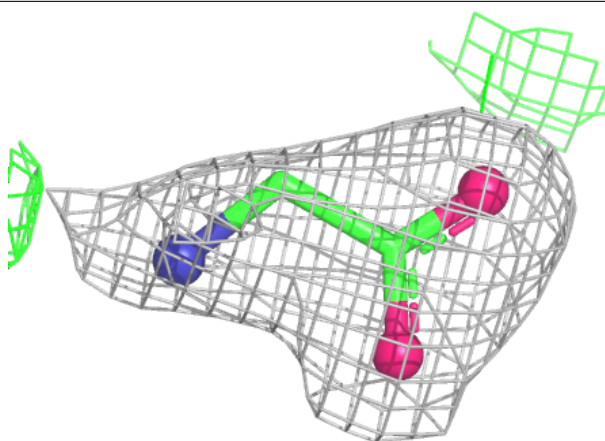
**Electron density around GLY B 702:**

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and green (positive)



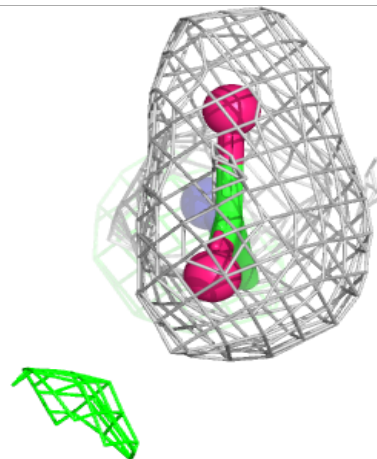
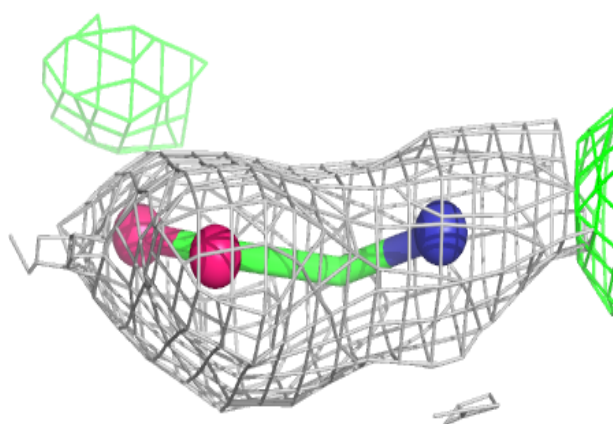
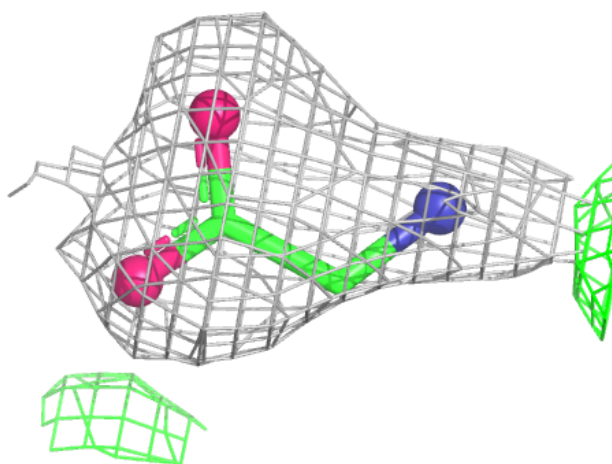
Electron density around GLY C 702:

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and green (positive)



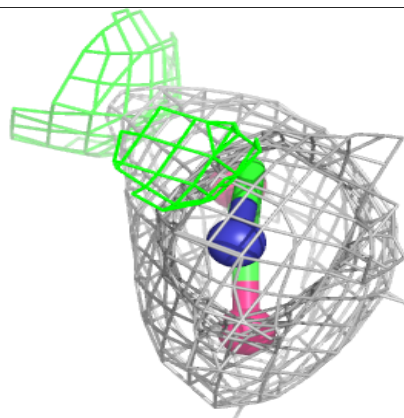
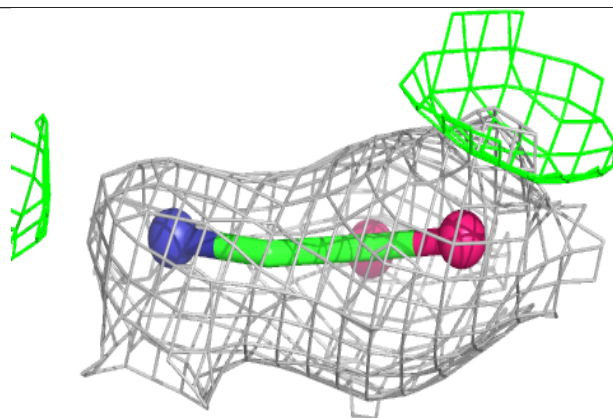
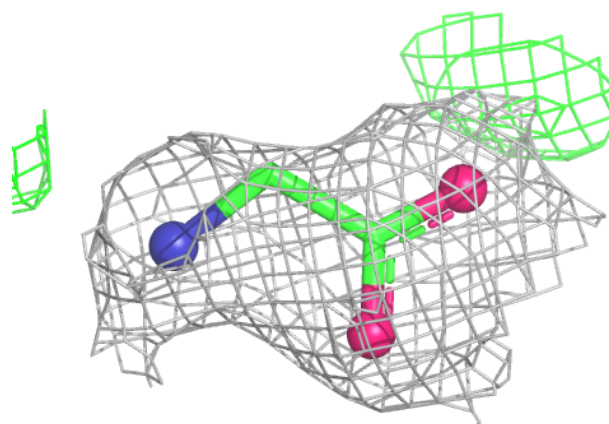
Electron density around GLY D 702:

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and green (positive)

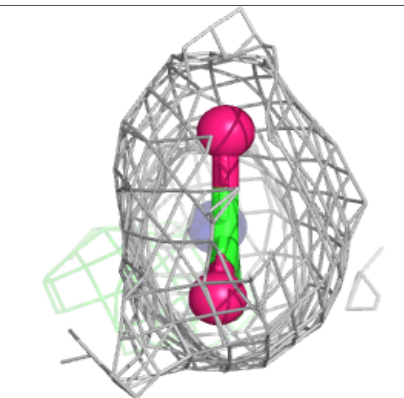
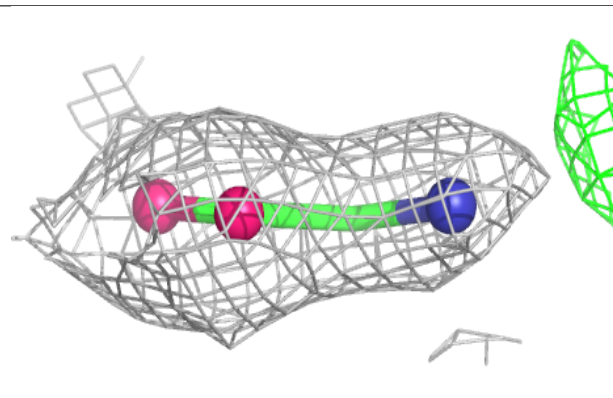
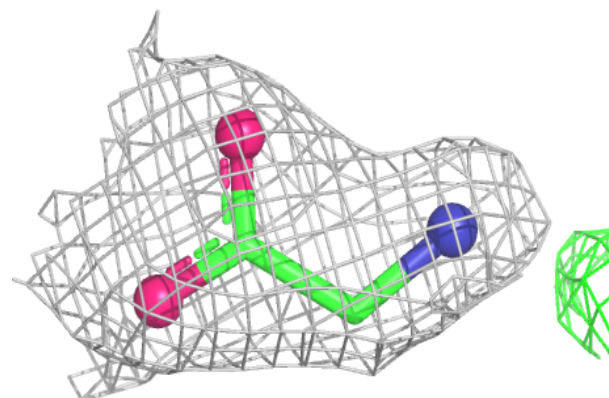


Electron density around GLY E 702:

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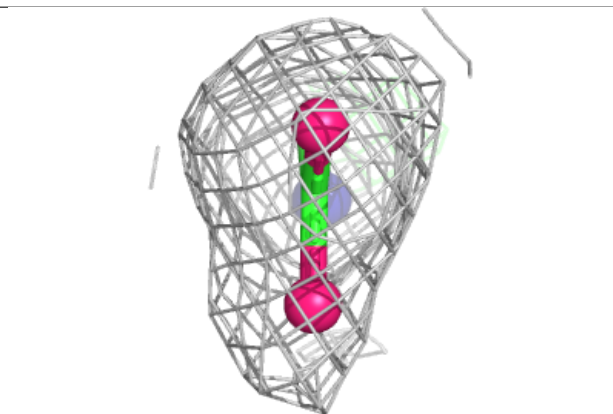
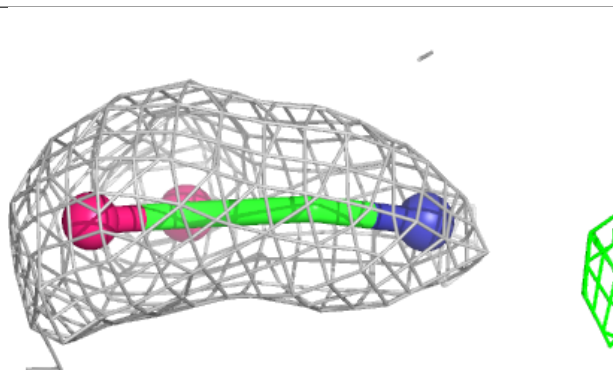
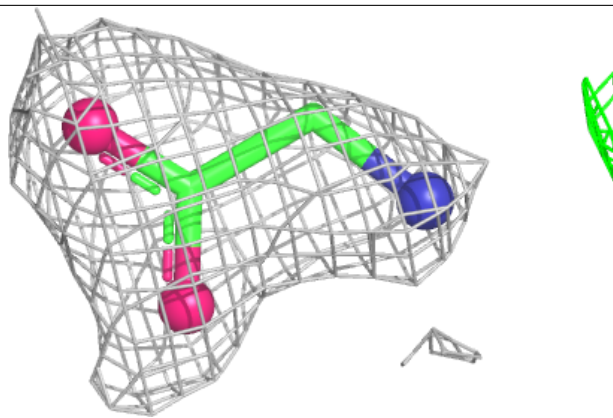
**Electron density around GLY F 702:**

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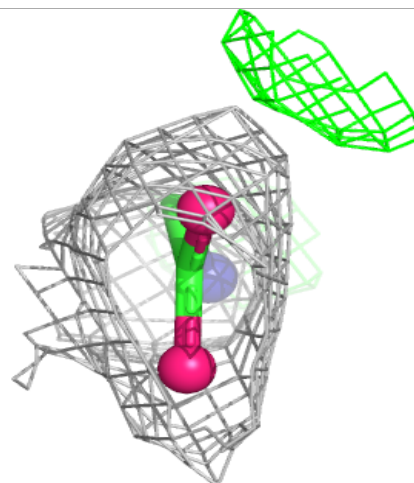
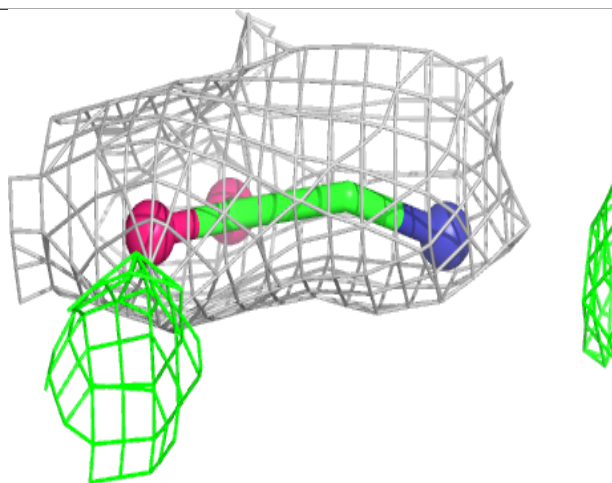
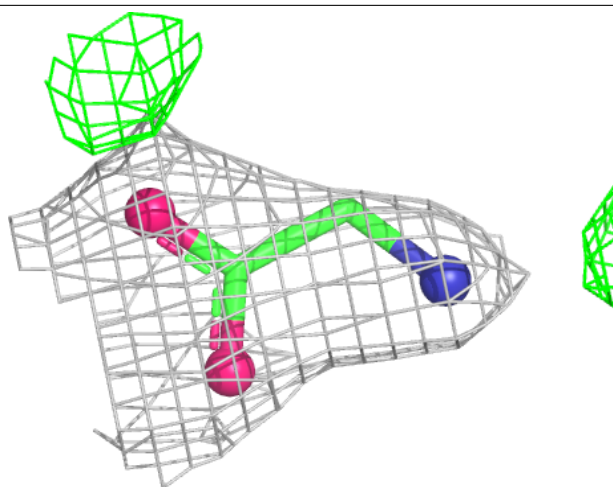
Electron density around GLY G 702:

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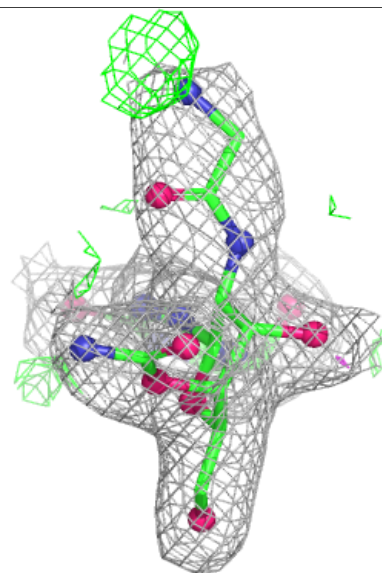
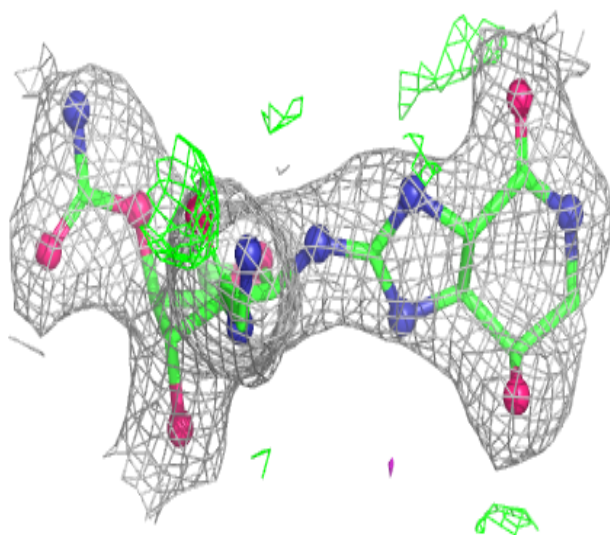
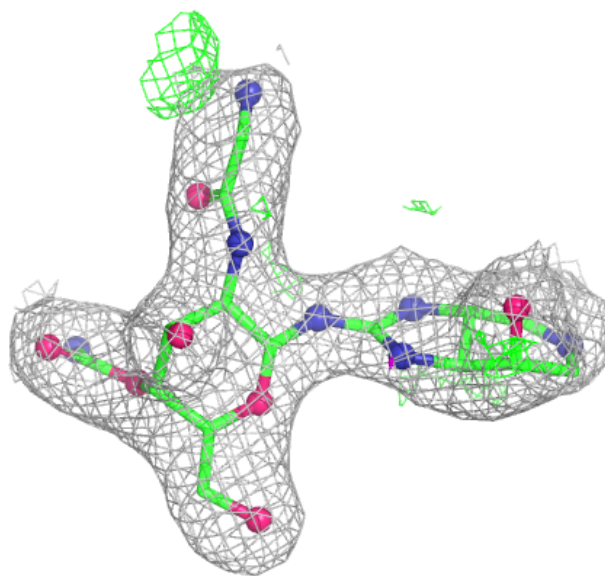
Electron density around GLY H 702:

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and green (positive)



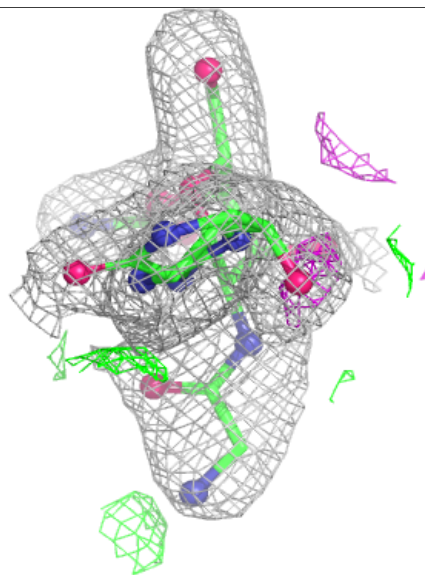
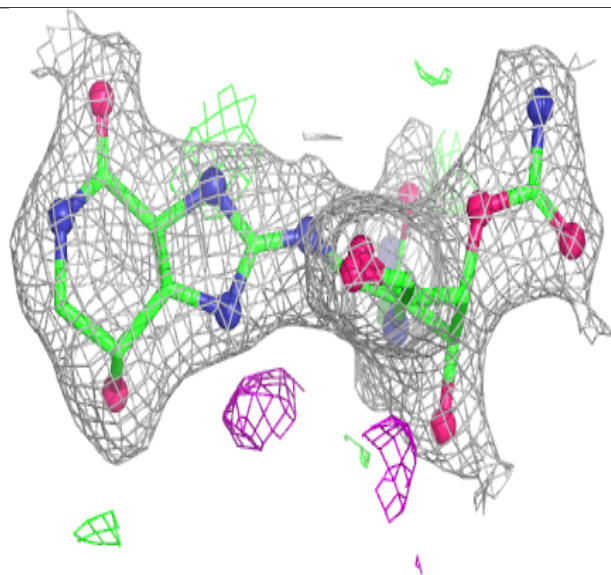
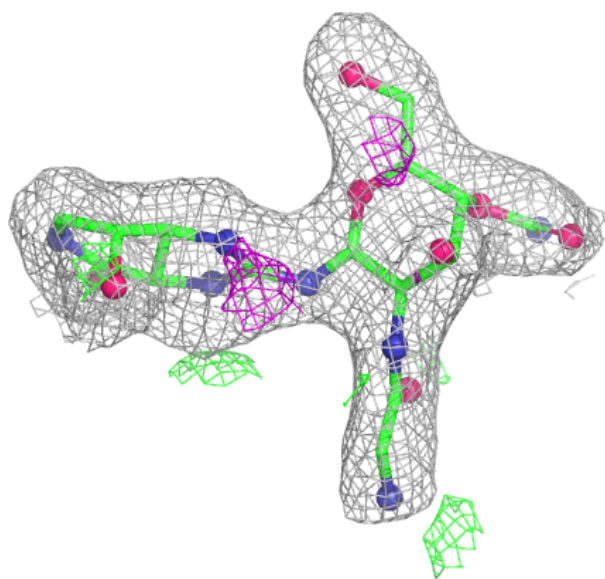
Electron density around I55 A 703:

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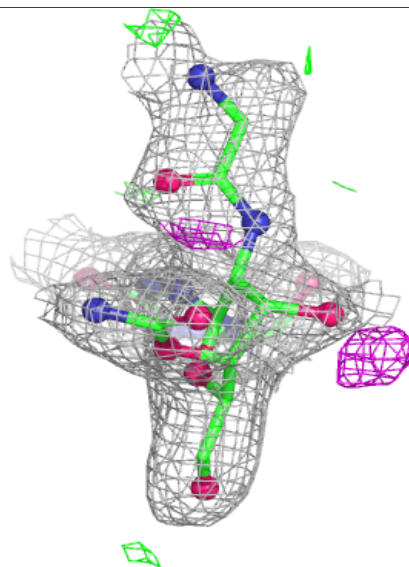
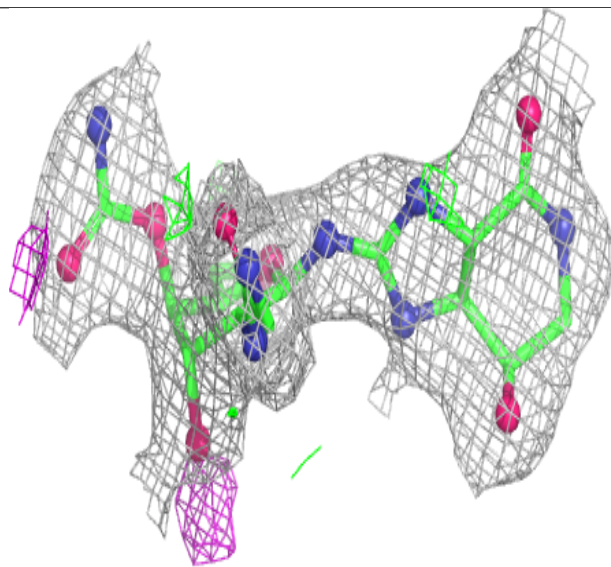
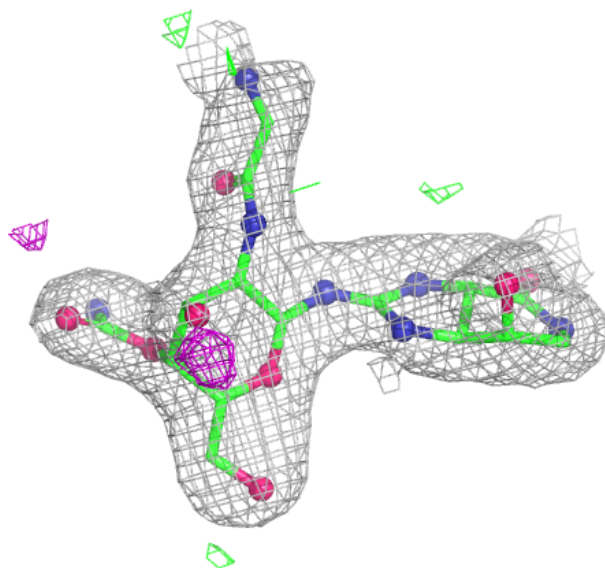
Electron density around I55 B 703:

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and green (positive)



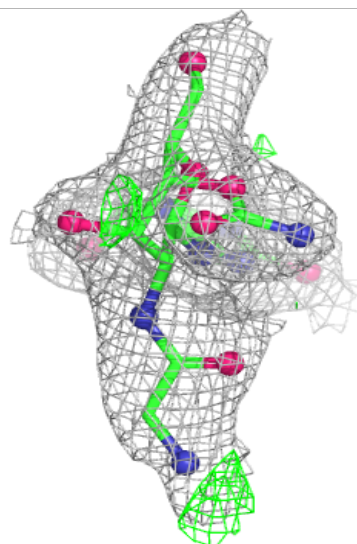
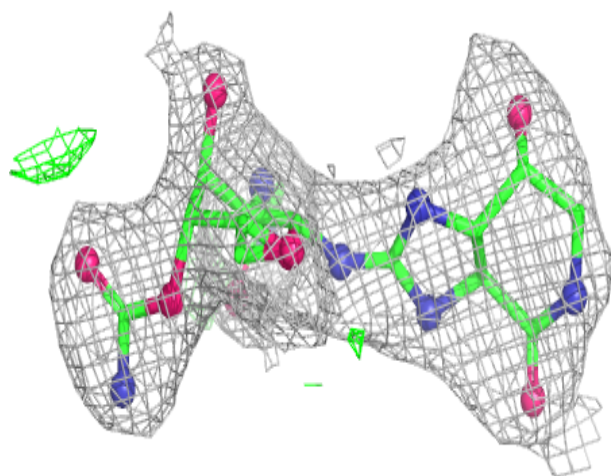
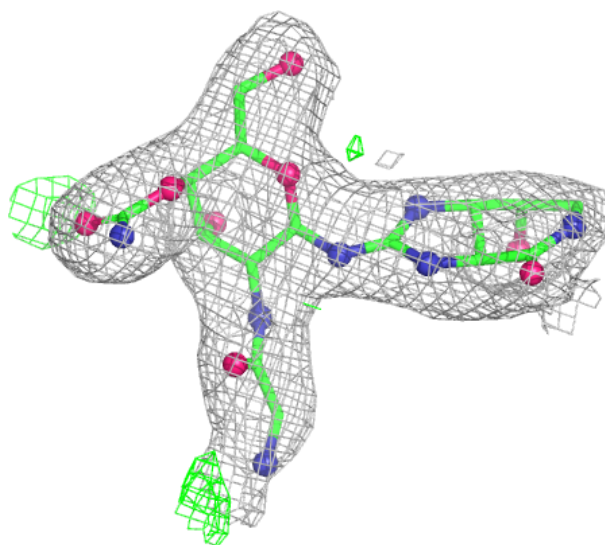
Electron density around I55 C 703:

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and green (positive)



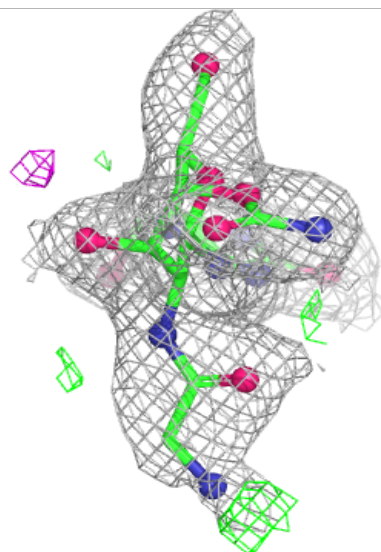
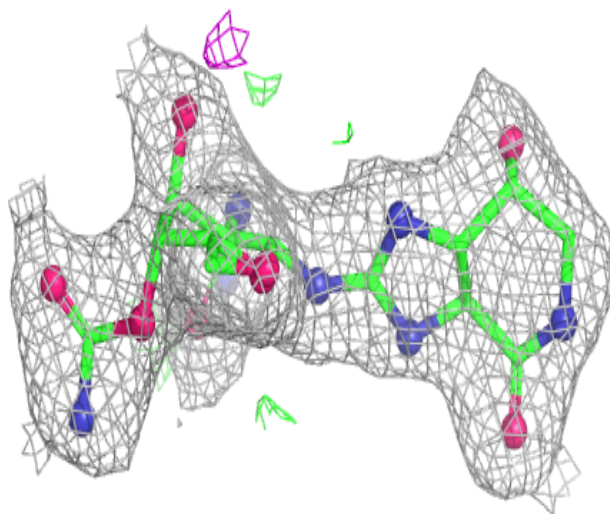
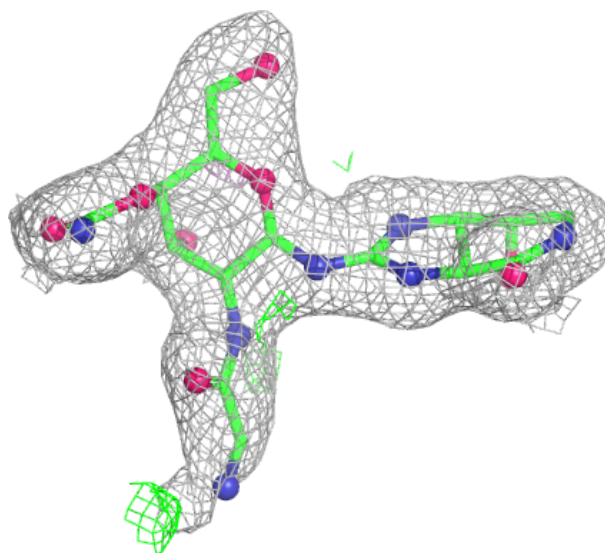
Electron density around I55 D 703:

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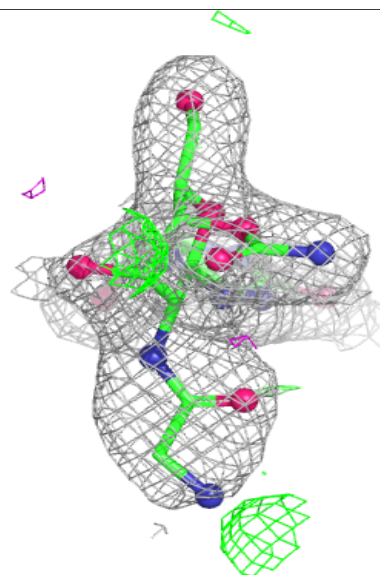
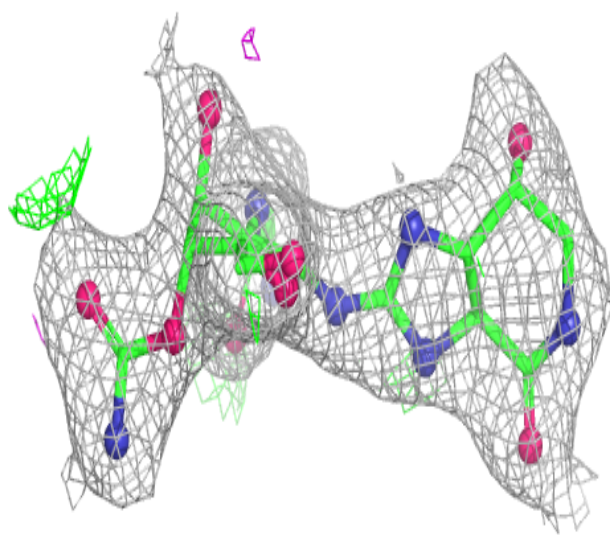
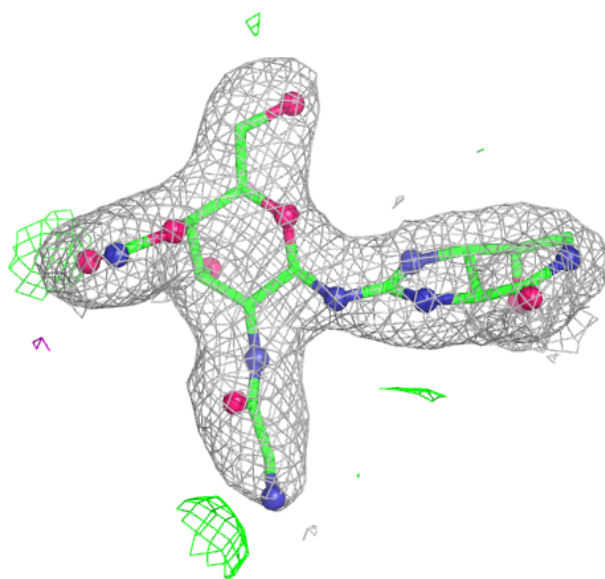
Electron density around I55 E 703:

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and green (positive)



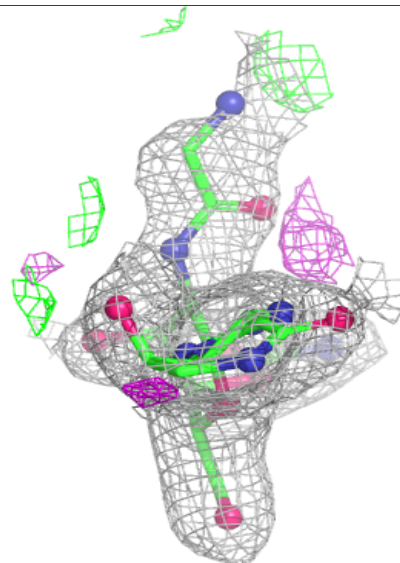
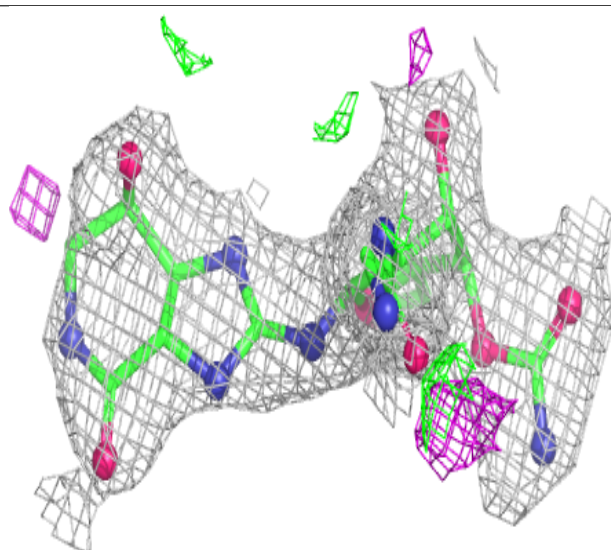
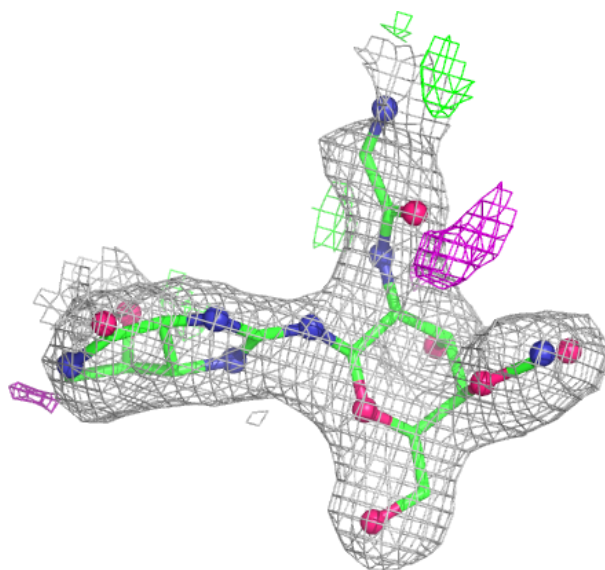
Electron density around I55 F 703:

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and green (positive)



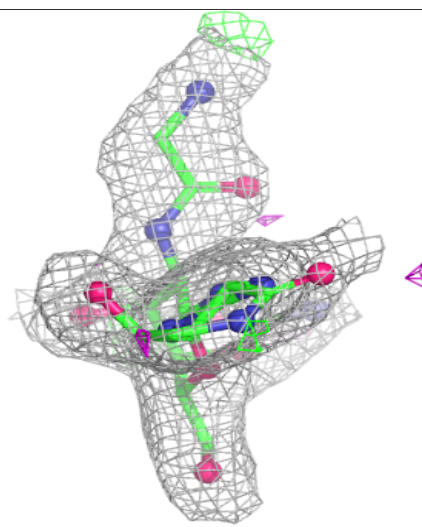
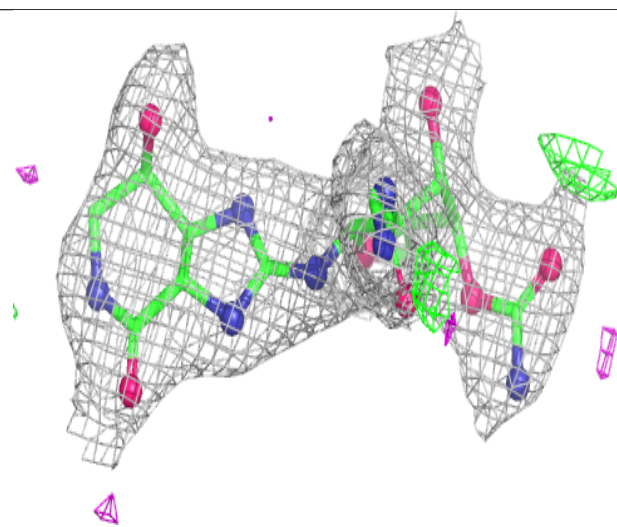
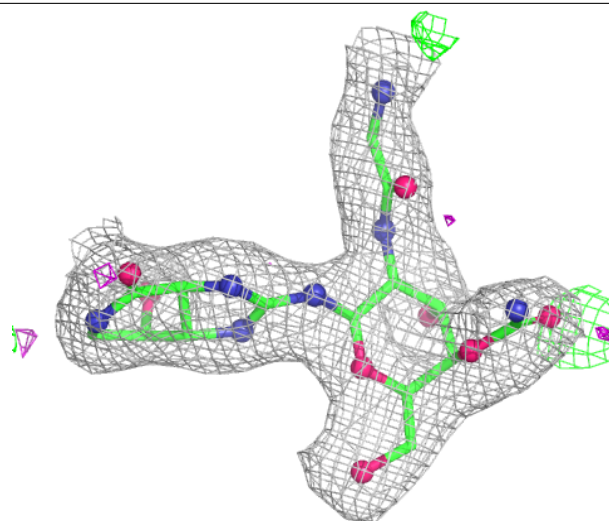
Electron density around I55 G 703:

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



Electron density around I55 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.