



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 24, 2026 – 01:52 AM UTC

PDB ID : 4EIL / pdb\_00004eil  
Title : Crystal Structure of the loop truncated Toxoplasma gondii TS-DHFR  
Authors : Sharma, H.  
Deposited on : 2012-04-05  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

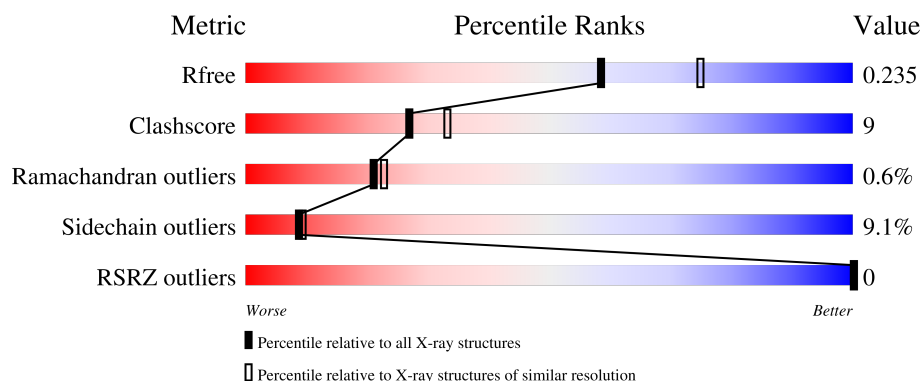
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	566	 69% 18% • 10%
1	B	566	 66% 18% • 13%
1	C	566	 69% 18% • 10%
1	D	566	 64% 19% • 13%
1	E	566	 72% 16% • 10%

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Mol	Chain	Length	Quality of chain
1	F	566	
1	G	566	
1	H	566	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	B	701	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35087 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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	B	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	C	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	D	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	E	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	F	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	G	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	H	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			

There are 352 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	ASN	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	TRP	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	THR	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ASP	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	GLN	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	CYS	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	ASN	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	TRP	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP Q07422
B	?	-	THR	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ASP	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	GLN	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	CYS	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
C	?	-	ARG	deletion	UNP Q07422
C	?	-	LEU	deletion	UNP Q07422
C	?	-	ASN	deletion	UNP Q07422
C	?	-	GLY	deletion	UNP Q07422
C	?	-	TRP	deletion	UNP Q07422
C	?	-	LEU	deletion	UNP Q07422
C	?	-	PRO	deletion	UNP Q07422
C	?	-	ARG	deletion	UNP Q07422
C	?	-	LYS	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	deletion	UNP Q07422
C	?	-	ALA	deletion	UNP Q07422
C	?	-	LYS	deletion	UNP Q07422
C	?	-	THR	deletion	UNP Q07422
C	?	-	GLY	deletion	UNP Q07422
C	?	-	ASP	deletion	UNP Q07422
C	?	-	SER	deletion	UNP Q07422
C	?	-	GLY	deletion	UNP Q07422
C	?	-	LEU	deletion	UNP Q07422
C	?	-	PRO	deletion	UNP Q07422
C	?	-	SER	deletion	UNP Q07422
C	?	-	PRO	deletion	UNP Q07422
C	?	-	SER	deletion	UNP Q07422
C	?	-	VAL	deletion	UNP Q07422
C	?	-	GLY	deletion	UNP Q07422
C	?	-	LYS	deletion	UNP Q07422
C	?	-	GLN	deletion	UNP Q07422
C	?	-	ALA	deletion	UNP Q07422
C	?	-	ALA	deletion	UNP Q07422
C	?	-	ALA	deletion	UNP Q07422
C	?	-	PRO	deletion	UNP Q07422
C	?	-	ALA	deletion	UNP Q07422
C	?	-	GLU	deletion	UNP Q07422
C	?	-	SER	deletion	UNP Q07422
C	?	-	VAL	deletion	UNP Q07422
C	?	-	PHE	deletion	UNP Q07422
C	?	-	VAL	deletion	UNP Q07422
C	?	-	PRO	deletion	UNP Q07422
C	?	-	PHE	deletion	UNP Q07422
C	?	-	CYS	deletion	UNP Q07422
C	?	-	PRO	deletion	UNP Q07422
C	?	-	GLU	deletion	UNP Q07422
C	?	-	LEU	deletion	UNP Q07422
C	?	-	GLY	deletion	UNP Q07422
C	?	-	ARG	deletion	UNP Q07422
D	?	-	ARG	deletion	UNP Q07422
D	?	-	LEU	deletion	UNP Q07422
D	?	-	ASN	deletion	UNP Q07422
D	?	-	GLY	deletion	UNP Q07422
D	?	-	TRP	deletion	UNP Q07422
D	?	-	LEU	deletion	UNP Q07422
D	?	-	PRO	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ARG	deletion	UNP Q07422
D	?	-	LYS	deletion	UNP Q07422
D	?	-	PHE	deletion	UNP Q07422
D	?	-	ALA	deletion	UNP Q07422
D	?	-	LYS	deletion	UNP Q07422
D	?	-	THR	deletion	UNP Q07422
D	?	-	GLY	deletion	UNP Q07422
D	?	-	ASP	deletion	UNP Q07422
D	?	-	SER	deletion	UNP Q07422
D	?	-	GLY	deletion	UNP Q07422
D	?	-	LEU	deletion	UNP Q07422
D	?	-	PRO	deletion	UNP Q07422
D	?	-	SER	deletion	UNP Q07422
D	?	-	PRO	deletion	UNP Q07422
D	?	-	SER	deletion	UNP Q07422
D	?	-	VAL	deletion	UNP Q07422
D	?	-	GLY	deletion	UNP Q07422
D	?	-	LYS	deletion	UNP Q07422
D	?	-	GLN	deletion	UNP Q07422
D	?	-	ALA	deletion	UNP Q07422
D	?	-	ALA	deletion	UNP Q07422
D	?	-	ALA	deletion	UNP Q07422
D	?	-	PRO	deletion	UNP Q07422
D	?	-	ALA	deletion	UNP Q07422
D	?	-	GLU	deletion	UNP Q07422
D	?	-	SER	deletion	UNP Q07422
D	?	-	VAL	deletion	UNP Q07422
D	?	-	PHE	deletion	UNP Q07422
D	?	-	VAL	deletion	UNP Q07422
D	?	-	PRO	deletion	UNP Q07422
D	?	-	PHE	deletion	UNP Q07422
D	?	-	CYS	deletion	UNP Q07422
D	?	-	PRO	deletion	UNP Q07422
D	?	-	GLU	deletion	UNP Q07422
D	?	-	LEU	deletion	UNP Q07422
D	?	-	GLY	deletion	UNP Q07422
D	?	-	ARG	deletion	UNP Q07422
E	?	-	ARG	deletion	UNP Q07422
E	?	-	LEU	deletion	UNP Q07422
E	?	-	ASN	deletion	UNP Q07422
E	?	-	GLY	deletion	UNP Q07422
E	?	-	TRP	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP Q07422
E	?	-	PRO	deletion	UNP Q07422
E	?	-	ARG	deletion	UNP Q07422
E	?	-	LYS	deletion	UNP Q07422
E	?	-	PHE	deletion	UNP Q07422
E	?	-	ALA	deletion	UNP Q07422
E	?	-	LYS	deletion	UNP Q07422
E	?	-	THR	deletion	UNP Q07422
E	?	-	GLY	deletion	UNP Q07422
E	?	-	ASP	deletion	UNP Q07422
E	?	-	SER	deletion	UNP Q07422
E	?	-	GLY	deletion	UNP Q07422
E	?	-	LEU	deletion	UNP Q07422
E	?	-	PRO	deletion	UNP Q07422
E	?	-	SER	deletion	UNP Q07422
E	?	-	PRO	deletion	UNP Q07422
E	?	-	SER	deletion	UNP Q07422
E	?	-	VAL	deletion	UNP Q07422
E	?	-	GLY	deletion	UNP Q07422
E	?	-	LYS	deletion	UNP Q07422
E	?	-	GLN	deletion	UNP Q07422
E	?	-	ALA	deletion	UNP Q07422
E	?	-	ALA	deletion	UNP Q07422
E	?	-	ALA	deletion	UNP Q07422
E	?	-	PRO	deletion	UNP Q07422
E	?	-	ALA	deletion	UNP Q07422
E	?	-	GLU	deletion	UNP Q07422
E	?	-	SER	deletion	UNP Q07422
E	?	-	VAL	deletion	UNP Q07422
E	?	-	PHE	deletion	UNP Q07422
E	?	-	VAL	deletion	UNP Q07422
E	?	-	PRO	deletion	UNP Q07422
E	?	-	PHE	deletion	UNP Q07422
E	?	-	CYS	deletion	UNP Q07422
E	?	-	PRO	deletion	UNP Q07422
E	?	-	GLU	deletion	UNP Q07422
E	?	-	LEU	deletion	UNP Q07422
E	?	-	GLY	deletion	UNP Q07422
E	?	-	ARG	deletion	UNP Q07422
F	?	-	ARG	deletion	UNP Q07422
F	?	-	LEU	deletion	UNP Q07422
F	?	-	ASN	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLY	deletion	UNP Q07422
F	?	-	TRP	deletion	UNP Q07422
F	?	-	LEU	deletion	UNP Q07422
F	?	-	PRO	deletion	UNP Q07422
F	?	-	ARG	deletion	UNP Q07422
F	?	-	LYS	deletion	UNP Q07422
F	?	-	PHE	deletion	UNP Q07422
F	?	-	ALA	deletion	UNP Q07422
F	?	-	LYS	deletion	UNP Q07422
F	?	-	THR	deletion	UNP Q07422
F	?	-	GLY	deletion	UNP Q07422
F	?	-	ASP	deletion	UNP Q07422
F	?	-	SER	deletion	UNP Q07422
F	?	-	GLY	deletion	UNP Q07422
F	?	-	LEU	deletion	UNP Q07422
F	?	-	PRO	deletion	UNP Q07422
F	?	-	SER	deletion	UNP Q07422
F	?	-	PRO	deletion	UNP Q07422
F	?	-	SER	deletion	UNP Q07422
F	?	-	VAL	deletion	UNP Q07422
F	?	-	GLY	deletion	UNP Q07422
F	?	-	LYS	deletion	UNP Q07422
F	?	-	GLN	deletion	UNP Q07422
F	?	-	ALA	deletion	UNP Q07422
F	?	-	ALA	deletion	UNP Q07422
F	?	-	ALA	deletion	UNP Q07422
F	?	-	PRO	deletion	UNP Q07422
F	?	-	ALA	deletion	UNP Q07422
F	?	-	GLU	deletion	UNP Q07422
F	?	-	SER	deletion	UNP Q07422
F	?	-	VAL	deletion	UNP Q07422
F	?	-	PHE	deletion	UNP Q07422
F	?	-	VAL	deletion	UNP Q07422
F	?	-	PRO	deletion	UNP Q07422
F	?	-	PHE	deletion	UNP Q07422
F	?	-	CYS	deletion	UNP Q07422
F	?	-	PRO	deletion	UNP Q07422
F	?	-	GLU	deletion	UNP Q07422
F	?	-	LEU	deletion	UNP Q07422
F	?	-	GLY	deletion	UNP Q07422
F	?	-	ARG	deletion	UNP Q07422
G	?	-	ARG	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LEU	deletion	UNP Q07422
G	?	-	ASN	deletion	UNP Q07422
G	?	-	GLY	deletion	UNP Q07422
G	?	-	TRP	deletion	UNP Q07422
G	?	-	LEU	deletion	UNP Q07422
G	?	-	PRO	deletion	UNP Q07422
G	?	-	ARG	deletion	UNP Q07422
G	?	-	LYS	deletion	UNP Q07422
G	?	-	PHE	deletion	UNP Q07422
G	?	-	ALA	deletion	UNP Q07422
G	?	-	LYS	deletion	UNP Q07422
G	?	-	THR	deletion	UNP Q07422
G	?	-	GLY	deletion	UNP Q07422
G	?	-	ASP	deletion	UNP Q07422
G	?	-	SER	deletion	UNP Q07422
G	?	-	GLY	deletion	UNP Q07422
G	?	-	LEU	deletion	UNP Q07422
G	?	-	PRO	deletion	UNP Q07422
G	?	-	SER	deletion	UNP Q07422
G	?	-	PRO	deletion	UNP Q07422
G	?	-	SER	deletion	UNP Q07422
G	?	-	VAL	deletion	UNP Q07422
G	?	-	GLY	deletion	UNP Q07422
G	?	-	LYS	deletion	UNP Q07422
G	?	-	GLN	deletion	UNP Q07422
G	?	-	ALA	deletion	UNP Q07422
G	?	-	ALA	deletion	UNP Q07422
G	?	-	ALA	deletion	UNP Q07422
G	?	-	PRO	deletion	UNP Q07422
G	?	-	ALA	deletion	UNP Q07422
G	?	-	GLU	deletion	UNP Q07422
G	?	-	SER	deletion	UNP Q07422
G	?	-	VAL	deletion	UNP Q07422
G	?	-	PHE	deletion	UNP Q07422
G	?	-	VAL	deletion	UNP Q07422
G	?	-	PRO	deletion	UNP Q07422
G	?	-	PHE	deletion	UNP Q07422
G	?	-	CYS	deletion	UNP Q07422
G	?	-	PRO	deletion	UNP Q07422
G	?	-	GLU	deletion	UNP Q07422
G	?	-	LEU	deletion	UNP Q07422
G	?	-	GLY	deletion	UNP Q07422

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ARG	deletion	UNP Q07422
H	?	-	ARG	deletion	UNP Q07422
H	?	-	LEU	deletion	UNP Q07422
H	?	-	ASN	deletion	UNP Q07422
H	?	-	GLY	deletion	UNP Q07422
H	?	-	TRP	deletion	UNP Q07422
H	?	-	LEU	deletion	UNP Q07422
H	?	-	PRO	deletion	UNP Q07422
H	?	-	ARG	deletion	UNP Q07422
H	?	-	LYS	deletion	UNP Q07422
H	?	-	PHE	deletion	UNP Q07422
H	?	-	ALA	deletion	UNP Q07422
H	?	-	LYS	deletion	UNP Q07422
H	?	-	THR	deletion	UNP Q07422
H	?	-	GLY	deletion	UNP Q07422
H	?	-	ASP	deletion	UNP Q07422
H	?	-	SER	deletion	UNP Q07422
H	?	-	GLY	deletion	UNP Q07422
H	?	-	LEU	deletion	UNP Q07422
H	?	-	PRO	deletion	UNP Q07422
H	?	-	SER	deletion	UNP Q07422
H	?	-	PRO	deletion	UNP Q07422
H	?	-	SER	deletion	UNP Q07422
H	?	-	VAL	deletion	UNP Q07422
H	?	-	GLY	deletion	UNP Q07422
H	?	-	LYS	deletion	UNP Q07422
H	?	-	GLN	deletion	UNP Q07422
H	?	-	ALA	deletion	UNP Q07422
H	?	-	ALA	deletion	UNP Q07422
H	?	-	ALA	deletion	UNP Q07422
H	?	-	PRO	deletion	UNP Q07422
H	?	-	ALA	deletion	UNP Q07422
H	?	-	GLU	deletion	UNP Q07422
H	?	-	SER	deletion	UNP Q07422
H	?	-	VAL	deletion	UNP Q07422
H	?	-	PHE	deletion	UNP Q07422
H	?	-	VAL	deletion	UNP Q07422
H	?	-	PRO	deletion	UNP Q07422
H	?	-	PHE	deletion	UNP Q07422
H	?	-	CYS	deletion	UNP Q07422
H	?	-	PRO	deletion	UNP Q07422
H	?	-	GLU	deletion	UNP Q07422

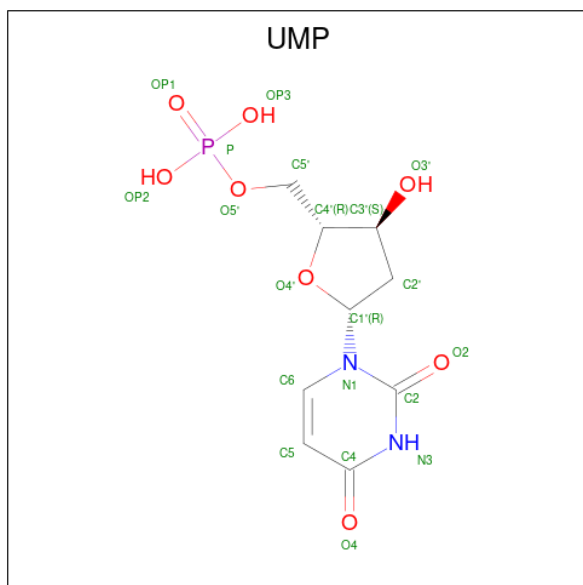
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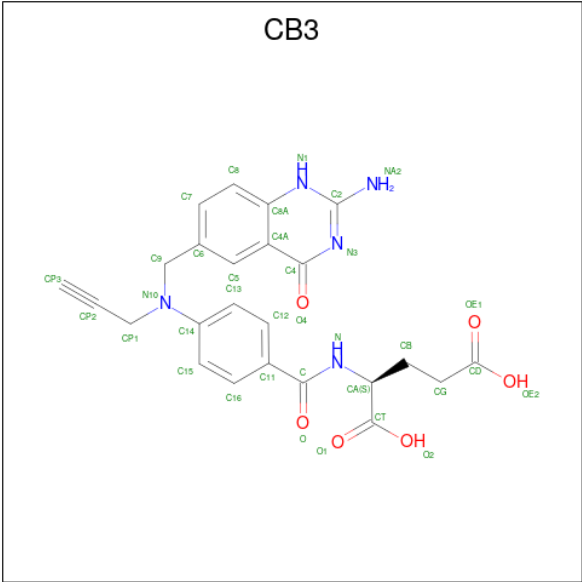
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP Q07422
H	?	-	GLY	deletion	UNP Q07422
H	?	-	ARG	deletion	UNP Q07422

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula:  $C_9H_{13}N_2O_8P$ ).



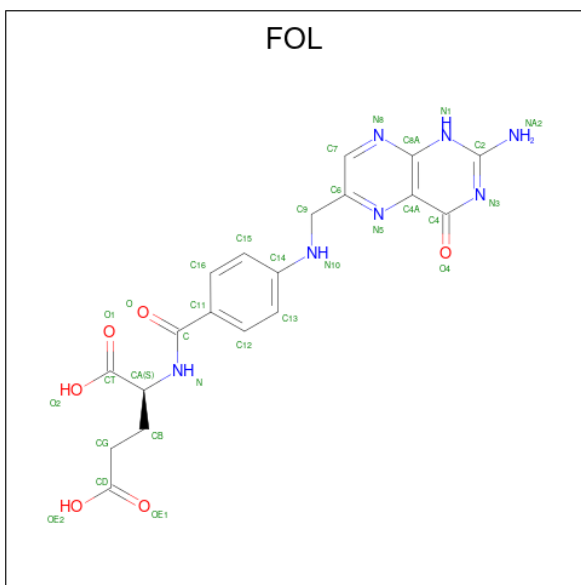
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	G	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	H	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula:  $C_{24}H_{23}N_5O_6$ ).



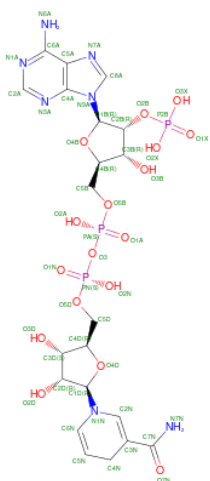
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		
3	F	1	Total	C	N	O	0	0
			35	24	5	6		
3	G	1	Total	C	N	O	0	0
			35	24	5	6		
3	H	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is FOLIC ACID (CCD ID: FOL) (formula: C<sub>19</sub>H<sub>19</sub>N<sub>7</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 32	C 19	N 7	O 6	0	0
4	B	1	Total 32	C 19	N 7	O 6	0	0
4	C	1	Total 32	C 19	N 7	O 6	0	0
4	D	1	Total 32	C 19	N 7	O 6	0	0
4	E	1	Total 32	C 19	N 7	O 6	0	0
4	F	1	Total 32	C 19	N 7	O 6	0	0
4	G	1	Total 32	C 19	N 7	O 6	0	0
4	H	1	Total 32	C 19	N 7	O 6	0	0

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$ ).



- Molecule 6 is water.

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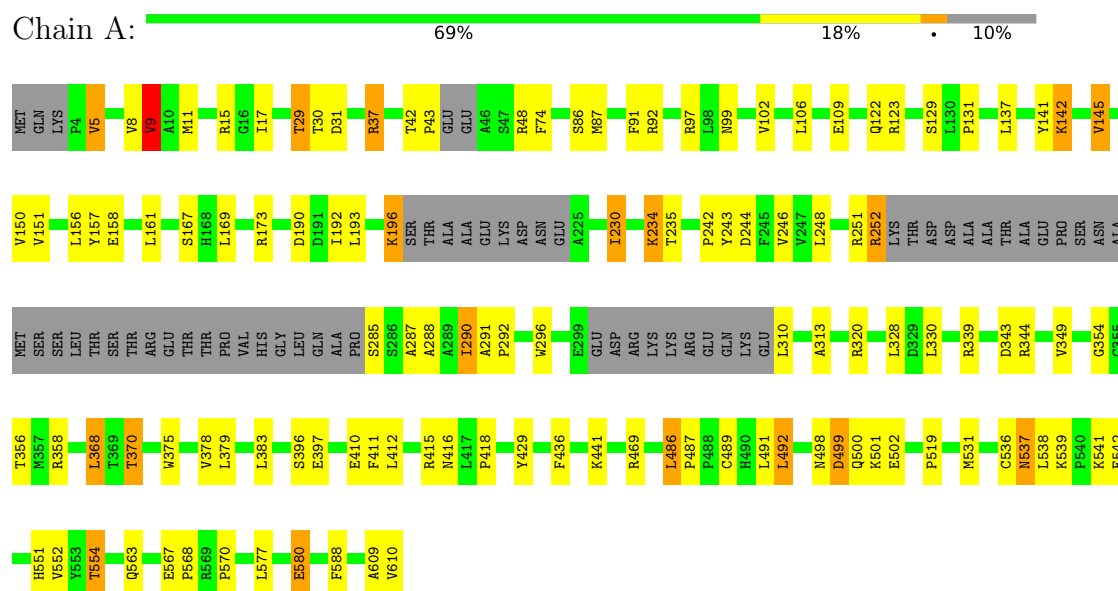
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	220	Total 220	O 220	0	0
6	F	242	Total 242	O 242	0	0
6	G	221	Total 221	O 221	0	0
6	H	215	Total 215	O 215	0	0

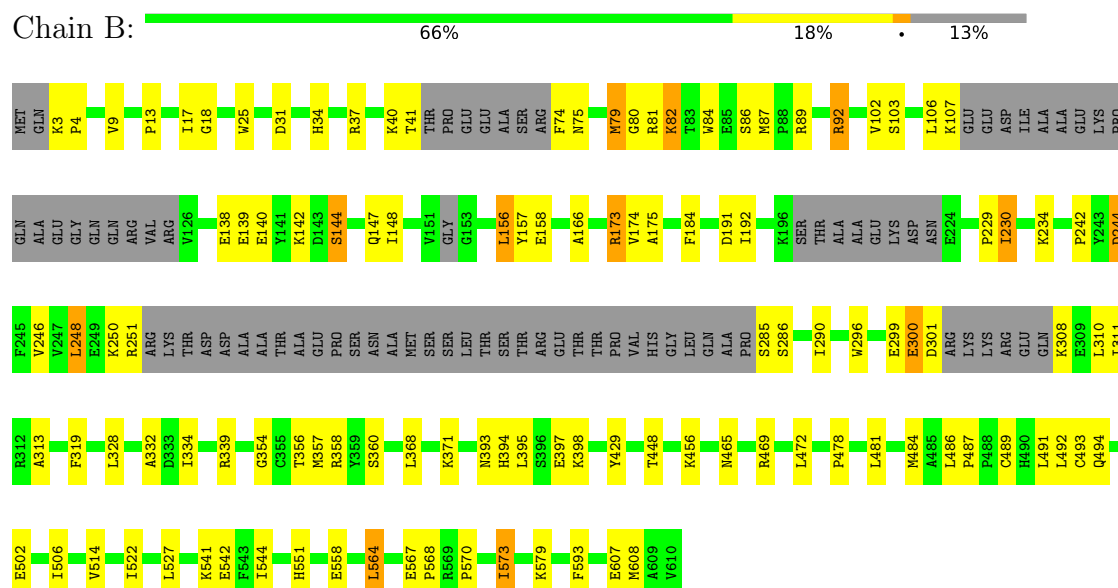
### 3 Residue-property plots

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: Bifunctional dihydrofolate reductase-thymidylate synthase

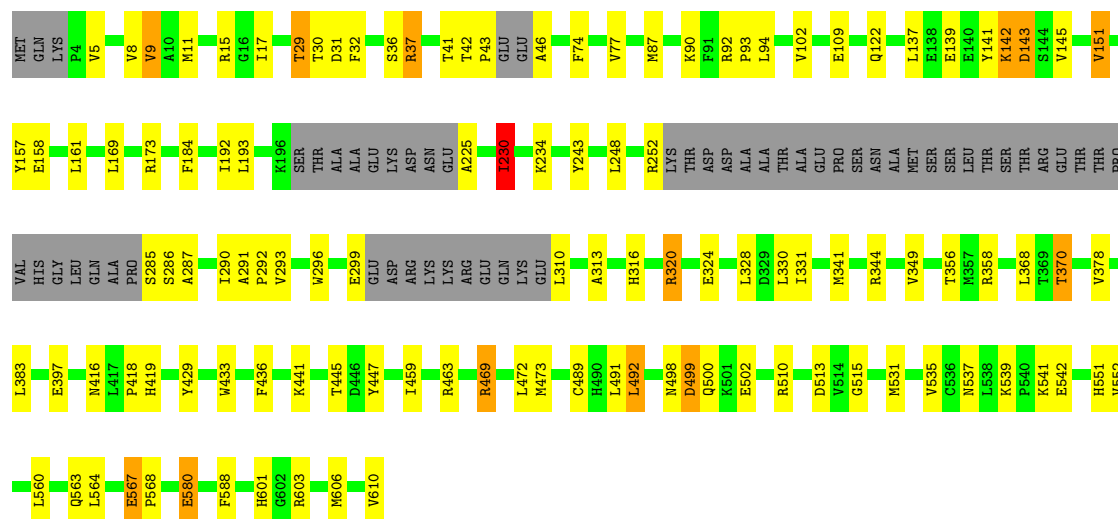


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



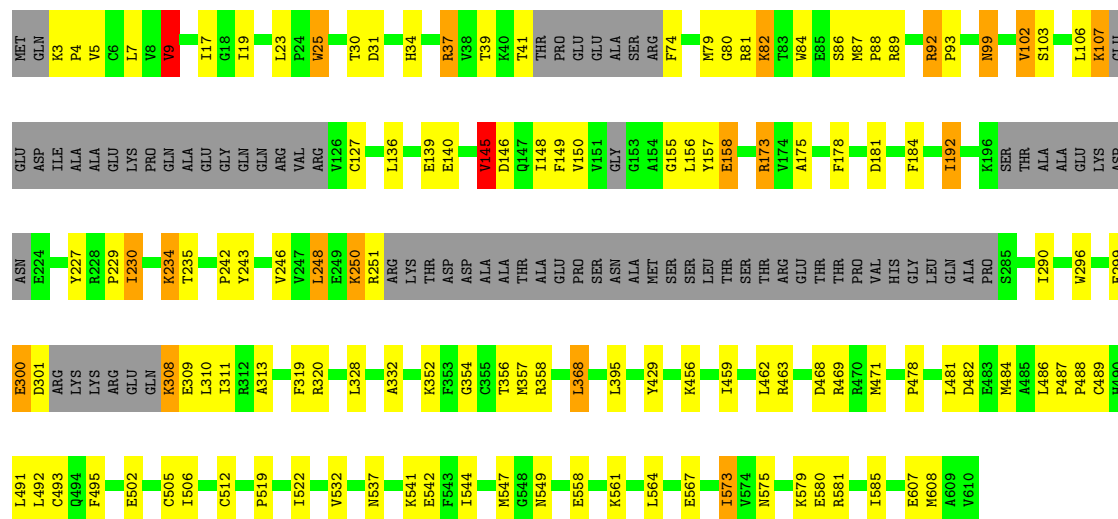
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain C:  69% 18% 10%



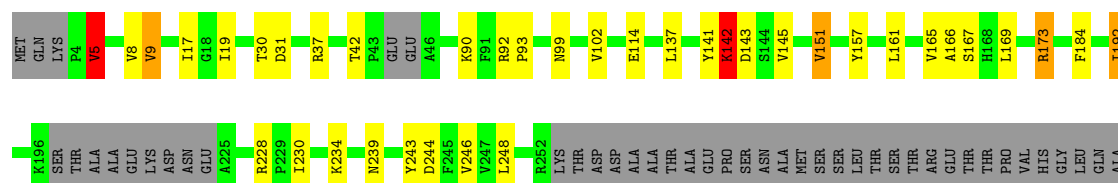
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

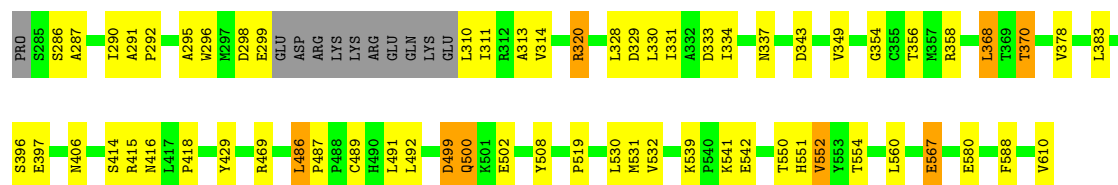
Chain D:  64% 19% 13%



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

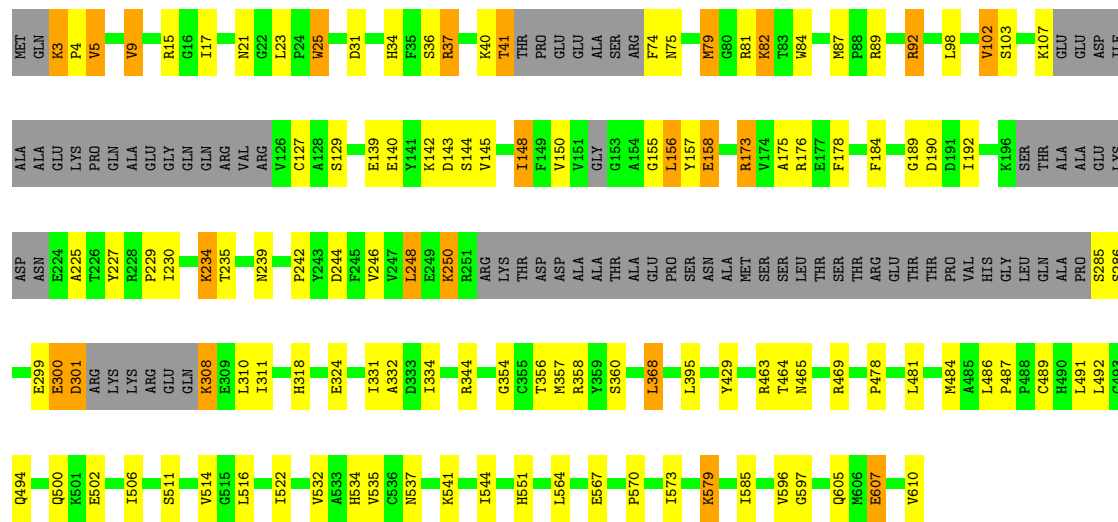
Chain E:  72% 16% 10%





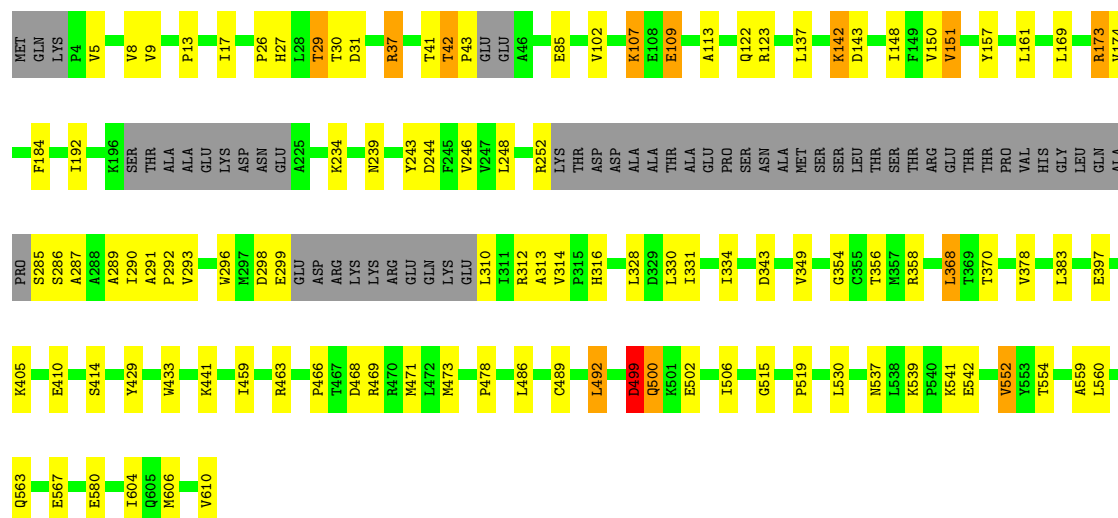
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain F: 65% 17% 13%



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

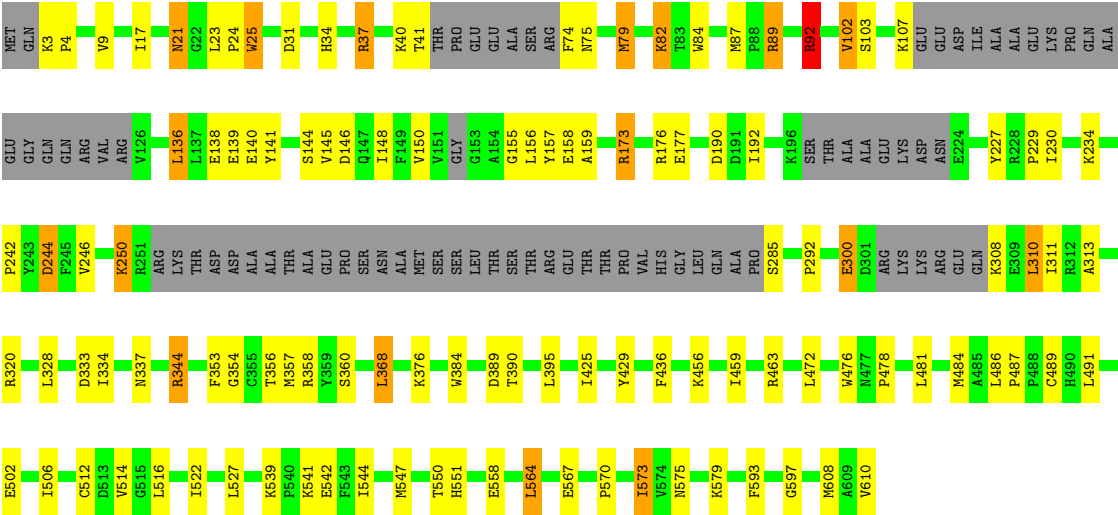
Chain G: 71% 17% 10%



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain H: 66% 17% 13%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.79Å 144.40Å 177.60Å 90.01° 89.93° 90.38°	Depositor
Resolution (Å)	48.40 – 2.20 48.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.40-2.20) 95.6 (48.40-2.20)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309, REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.183 , 0.233 0.184 , 0.235	Depositor DCC
$R_{free}$ test set	13380 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.417 for h,-k,-l 0.410 for -h,k,-l 0.447 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	35087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CB3, NDP, UMP, FOL

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	0.43	0/4196	0.84	8/5683 (0.1%)
1	B	0.42	0/4043	0.84	3/5473 (0.1%)
1	C	0.44	0/4196	0.85	4/5683 (0.1%)
1	D	0.43	0/4043	0.84	4/5473 (0.1%)
1	E	0.43	0/4196	0.82	3/5683 (0.1%)
1	F	0.42	0/4043	0.82	4/5473 (0.1%)
1	G	0.44	0/4196	0.80	0/5683
1	H	0.42	0/4043	0.83	2/5473 (0.0%)
All	All	0.43	0/32956	0.83	28/44624 (0.1%)

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	1

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ARG	CA-C-N	-7.25	111.37	120.79
1	B	92	ARG	C-N-CA	-7.25	111.37	120.79
1	C	230	ILE	N-CA-C	-6.43	106.98	113.47
1	A	9	VAL	CB-CA-C	-6.28	99.88	111.18
1	D	9	VAL	CB-CA-C	-5.96	99.75	110.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	609	ALA	Peptide

## 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	4096	0	4058	89	0
1	B	3948	0	3910	79	0
1	C	4096	0	4058	70	0
1	D	3948	0	3910	83	0
1	E	4096	0	4058	61	0
1	F	3948	0	3910	87	0
1	G	4096	0	4058	62	0
1	H	3948	0	3910	81	0
2	A	20	0	11	3	0
2	B	20	0	11	7	0
2	C	20	0	11	4	0
2	D	20	0	11	4	0
2	E	20	0	11	3	0
2	F	20	0	11	4	0
2	G	20	0	11	2	0
2	H	20	0	11	5	0
3	A	35	0	21	2	0
3	B	35	0	21	4	0
3	C	35	0	21	4	0
3	D	35	0	21	4	0
3	E	35	0	21	1	0
3	F	35	0	21	3	0
3	G	35	0	21	1	0
3	H	35	0	21	4	0
4	A	32	0	17	4	0
4	B	32	0	17	2	0
4	C	32	0	17	5	0
4	D	32	0	17	2	0
4	E	32	0	17	4	0
4	F	32	0	17	3	0
4	G	32	0	17	4	0
4	H	32	0	17	2	0
5	A	48	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	48	0	25	7	0
5	C	48	0	24	5	0
5	D	48	0	24	7	0
5	E	48	0	24	4	0
5	F	48	0	25	8	0
5	G	48	0	24	3	0
5	H	48	0	25	8	0
6	A	248	0	0	28	0
6	B	229	0	0	11	0
6	C	224	0	0	10	0
6	D	232	0	0	21	0
6	E	220	0	0	16	0
6	F	242	0	0	28	0
6	G	221	0	0	14	0
6	H	215	0	0	21	0
All	All	35087	0	32459	603	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 9.

The worst 5 of 603 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:F:481:LEU:HA	1:F:484:MET:HE2	1.52	0.91
1:B:481:LEU:HA	1:B:484:MET:HE2	1.52	0.90
1:G:287:ALA:HA	1:G:290:ILE:HD12	1.54	0.89
1:H:481:LEU:HA	1:H:484:MET:HE2	1.53	0.89
1:D:481:LEU:HA	1:D:484:MET:HE2	1.56	0.86

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/566 (89%)	487 (97%)	14 (3%)	1 (0%)	43	51
1	B	478/566 (84%)	456 (95%)	19 (4%)	3 (1%)	21	23
1	C	502/566 (89%)	488 (97%)	12 (2%)	2 (0%)	30	34
1	D	478/566 (84%)	449 (94%)	24 (5%)	5 (1%)	12	11
1	E	502/566 (89%)	489 (97%)	10 (2%)	3 (1%)	21	23
1	F	478/566 (84%)	454 (95%)	21 (4%)	3 (1%)	21	23
1	G	502/566 (89%)	488 (97%)	10 (2%)	4 (1%)	16	16
1	H	478/566 (84%)	456 (95%)	18 (4%)	4 (1%)	16	16
All	All	3920/4528 (87%)	3767 (96%)	128 (3%)	25 (1%)	21	23

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	TYR
1	B	429	TYR
1	C	286	SER
1	D	429	TYR
1	E	429	TYR

### 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	444/491 (90%)	404 (91%)	40 (9%)	9	9
1	B	431/491 (88%)	395 (92%)	36 (8%)	10	11
1	C	444/491 (90%)	402 (90%)	42 (10%)	8	8
1	D	431/491 (88%)	389 (90%)	42 (10%)	8	8
1	E	444/491 (90%)	408 (92%)	36 (8%)	11	12
1	F	431/491 (88%)	390 (90%)	41 (10%)	8	8
1	G	444/491 (90%)	402 (90%)	42 (10%)	8	8
1	H	431/491 (88%)	393 (91%)	38 (9%)	9	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3500/3928 (89%)	3183 (91%)	317 (9%)	<b>9</b> <b>9</b>

5 of 317 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	564	LEU
1	H	92	ARG
1	G	29	THR
1	G	368	LEU
1	H	300	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	435	HIS
1	H	444	HIS
1	H	537	ASN
1	G	575	ASN
1	D	534	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	CB3	H	702	-	37,37,37	1.87	8 (21%)	50,51,51	1.32	6 (12%)
2	UMP	H	701	-	21,21,21	1.24	4 (19%)	30,31,31	5.28	15 (50%)
3	CB3	C	702	-	37,37,37	1.86	7 (18%)	50,51,51	1.27	5 (10%)
4	FOL	B	703	-	34,34,34	1.88	6 (17%)	43,47,47	1.30	7 (16%)
4	FOL	E	703	-	34,34,34	1.92	8 (23%)	43,47,47	2.33	12 (27%)
2	UMP	B	701	-	21,21,21	1.26	4 (19%)	30,31,31	5.29	15 (50%)
2	UMP	A	701	-	21,21,21	1.30	4 (19%)	30,31,31	5.26	16 (53%)
2	UMP	E	701	-	21,21,21	1.29	4 (19%)	30,31,31	5.31	16 (53%)
5	NDP	F	704	-	51,52,52	2.24	17 (33%)	71,80,80	4.07	26 (36%)
2	UMP	C	701	-	21,21,21	1.30	4 (19%)	30,31,31	5.31	15 (50%)
4	FOL	F	703	-	34,34,34	1.85	6 (17%)	43,47,47	1.55	6 (13%)
5	NDP	D	704	-	51,52,52	2.38	19 (37%)	71,80,80	3.70	27 (38%)
5	NDP	G	704	-	51,52,52	2.40	18 (35%)	71,80,80	3.79	28 (39%)
5	NDP	E	704	-	51,52,52	2.36	18 (35%)	71,80,80	3.75	30 (42%)
4	FOL	C	703	-	34,34,34	1.92	8 (23%)	43,47,47	2.42	11 (25%)
5	NDP	A	704	-	51,52,52	2.37	15 (29%)	71,80,80	3.76	27 (38%)
5	NDP	C	704	-	51,52,52	2.38	16 (31%)	71,80,80	3.79	28 (39%)
3	CB3	A	702	-	37,37,37	1.95	7 (18%)	50,51,51	1.64	8 (16%)
2	UMP	F	701	-	21,21,21	1.23	3 (14%)	30,31,31	5.28	15 (50%)
5	NDP	H	704	-	51,52,52	2.27	18 (35%)	71,80,80	3.84	26 (36%)
5	NDP	B	704	-	51,52,52	2.22	17 (33%)	71,80,80	3.93	26 (36%)
4	FOL	D	703	-	34,34,34	1.94	7 (20%)	43,47,47	1.52	5 (11%)
3	CB3	B	702	-	37,37,37	1.85	7 (18%)	50,51,51	1.45	7 (14%)
3	CB3	D	702	-	37,37,37	1.76	7 (18%)	50,51,51	1.55	10 (20%)
4	FOL	G	703	-	34,34,34	1.90	7 (20%)	43,47,47	2.31	11 (25%)
3	CB3	F	702	-	37,37,37	1.78	6 (16%)	50,51,51	1.46	8 (16%)
2	UMP	G	701	-	21,21,21	1.29	4 (19%)	30,31,31	5.25	16 (53%)
4	FOL	A	703	-	34,34,34	1.87	7 (20%)	43,47,47	1.55	7 (16%)
4	FOL	H	703	-	34,34,34	1.87	6 (17%)	43,47,47	1.53	6 (13%)
3	CB3	G	702	-	37,37,37	2.03	8 (21%)	50,51,51	1.83	11 (22%)
2	UMP	D	701	-	21,21,21	1.24	4 (19%)	30,31,31	5.27	16 (53%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CB3	E	702	-	37,37,37	1.89	8 (21%)	50,51,51	1.32	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	H	702	-	-	3/27/28/28	0/3/3/3
2	UMP	H	701	-	-	4/10/22/22	0/2/2/2
3	CB3	C	702	-	-	7/27/28/28	0/3/3/3
4	FOL	B	703	-	-	6/22/22/22	0/3/3/3
4	FOL	E	703	-	-	2/22/22/22	0/3/3/3
2	UMP	B	701	-	-	2/10/22/22	0/2/2/2
2	UMP	A	701	-	-	6/10/22/22	0/2/2/2
2	UMP	E	701	-	-	5/10/22/22	0/2/2/2
5	NDP	F	704	-	-	7/34/77/77	0/5/5/5
2	UMP	C	701	-	-	5/10/22/22	0/2/2/2
4	FOL	F	703	-	-	2/22/22/22	0/3/3/3
5	NDP	D	704	-	-	10/34/77/77	0/5/5/5
5	NDP	G	704	-	-	8/34/77/77	0/5/5/5
5	NDP	E	704	-	-	10/34/77/77	0/5/5/5
4	FOL	C	703	-	-	1/22/22/22	0/3/3/3
5	NDP	A	704	-	-	9/34/77/77	0/5/5/5
5	NDP	C	704	-	-	10/34/77/77	0/5/5/5
3	CB3	A	702	-	-	4/27/28/28	0/3/3/3
2	UMP	F	701	-	-	4/10/22/22	0/2/2/2
5	NDP	H	704	-	-	6/34/77/77	0/5/5/5
5	NDP	B	704	-	-	7/34/77/77	0/5/5/5
4	FOL	D	703	-	-	2/22/22/22	0/3/3/3
3	CB3	B	702	-	-	5/27/28/28	0/3/3/3
3	CB3	D	702	-	-	3/27/28/28	0/3/3/3
4	FOL	G	703	-	-	2/22/22/22	0/3/3/3
3	CB3	F	702	-	-	3/27/28/28	0/3/3/3
2	UMP	G	701	-	-	6/10/22/22	0/2/2/2
4	FOL	A	703	-	-	0/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FOL	H	703	-	-	2/22/22/22	0/3/3/3
3	CB3	G	702	-	-	5/27/28/28	0/3/3/3
2	UMP	D	701	-	-	3/10/22/22	0/2/2/2
3	CB3	E	702	-	-	9/27/28/28	0/3/3/3

The worst 5 of 282 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	704	NDP	C4N-C3N	-5.93	1.38	1.50
5	F	704	NDP	C4N-C3N	-5.92	1.38	1.50
3	A	702	CB3	C9-C6	-5.88	1.40	1.51
5	G	704	NDP	C4N-C3N	-5.78	1.39	1.50
5	C	704	NDP	C4N-C3N	-5.77	1.39	1.50

The worst 5 of 468 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	UMP	O4'-C1'-C2'	-21.17	66.69	106.25
2	F	701	UMP	O4'-C1'-C2'	-21.16	66.71	106.25
2	C	701	UMP	O4'-C1'-C2'	-21.14	66.74	106.25
2	H	701	UMP	O4'-C1'-C2'	-21.13	66.76	106.25
2	B	701	UMP	O4'-C1'-C2'	-21.11	66.80	106.25

There are no chirality outliers.

5 of 158 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	UMP	C5'-O5'-P-OP2
2	A	701	UMP	C5'-O5'-P-OP3
2	B	701	UMP	C5'-O5'-P-OP3
2	C	701	UMP	C5'-O5'-P-OP1
2	C	701	UMP	C5'-O5'-P-OP2

There are no ring outliers.

32 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	702	CB3	4	0
2	H	701	UMP	5	0
3	C	702	CB3	4	0

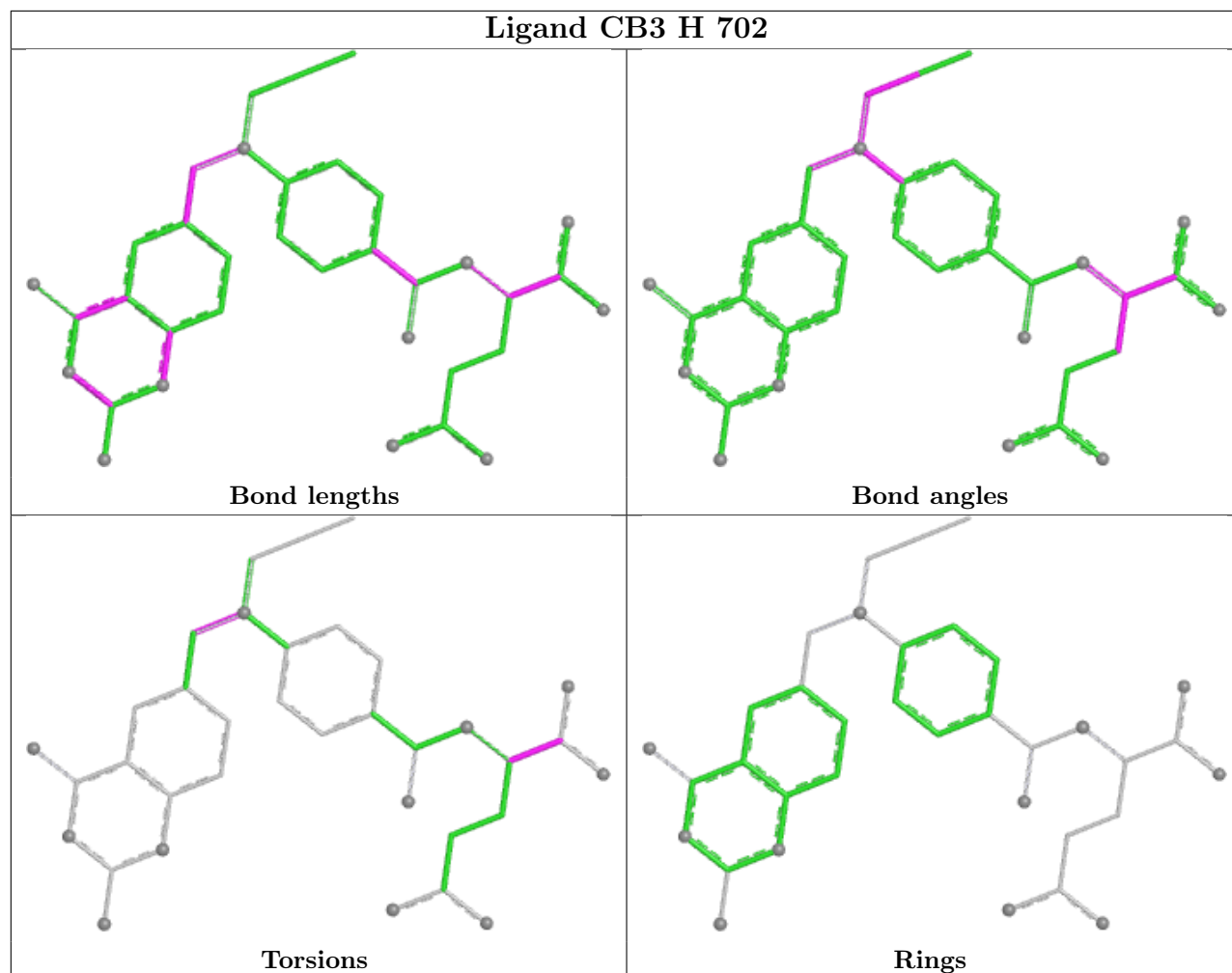
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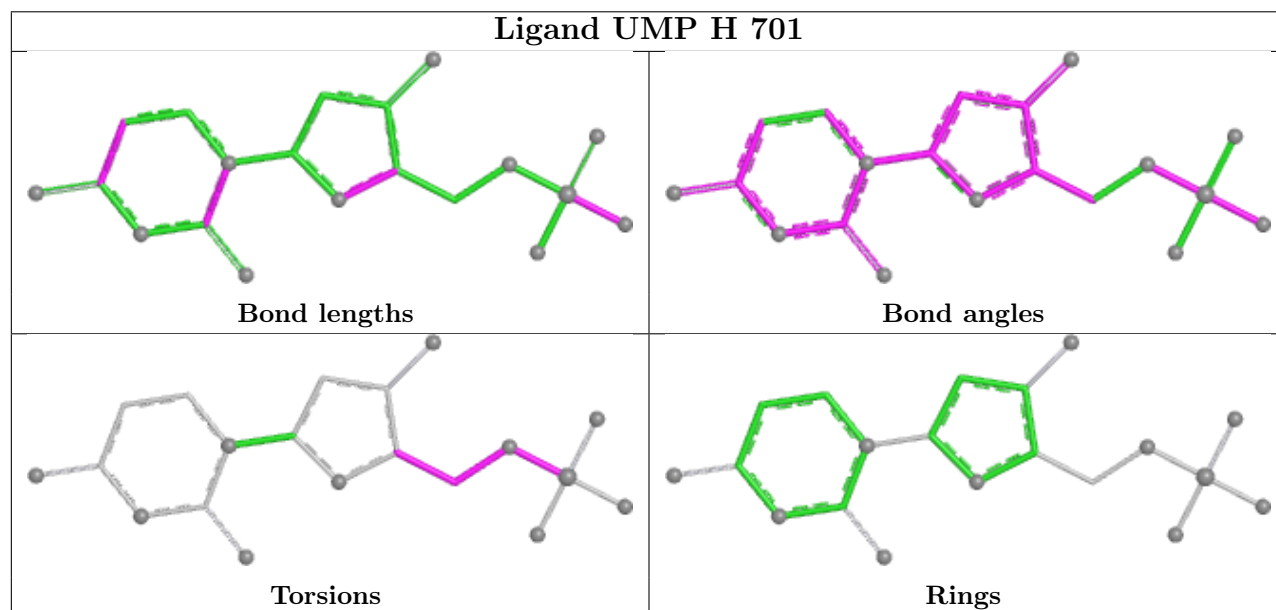
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	703	FOL	2	0
4	E	703	FOL	4	0
2	B	701	UMP	7	0
2	A	701	UMP	3	0
2	E	701	UMP	3	0
5	F	704	NDP	8	0
2	C	701	UMP	4	0
4	F	703	FOL	3	0
5	D	704	NDP	7	0
5	G	704	NDP	3	0
5	E	704	NDP	4	0
4	C	703	FOL	5	0
5	A	704	NDP	3	0
5	C	704	NDP	5	0
3	A	702	CB3	2	0
2	F	701	UMP	4	0
5	H	704	NDP	8	0
5	B	704	NDP	7	0
4	D	703	FOL	2	0
3	B	702	CB3	4	0
3	D	702	CB3	4	0
4	G	703	FOL	4	0
3	F	702	CB3	3	0
2	G	701	UMP	2	0
4	A	703	FOL	4	0
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3	G	702	CB3	1	0
2	D	701	UMP	4	0
3	E	702	CB3	1	0

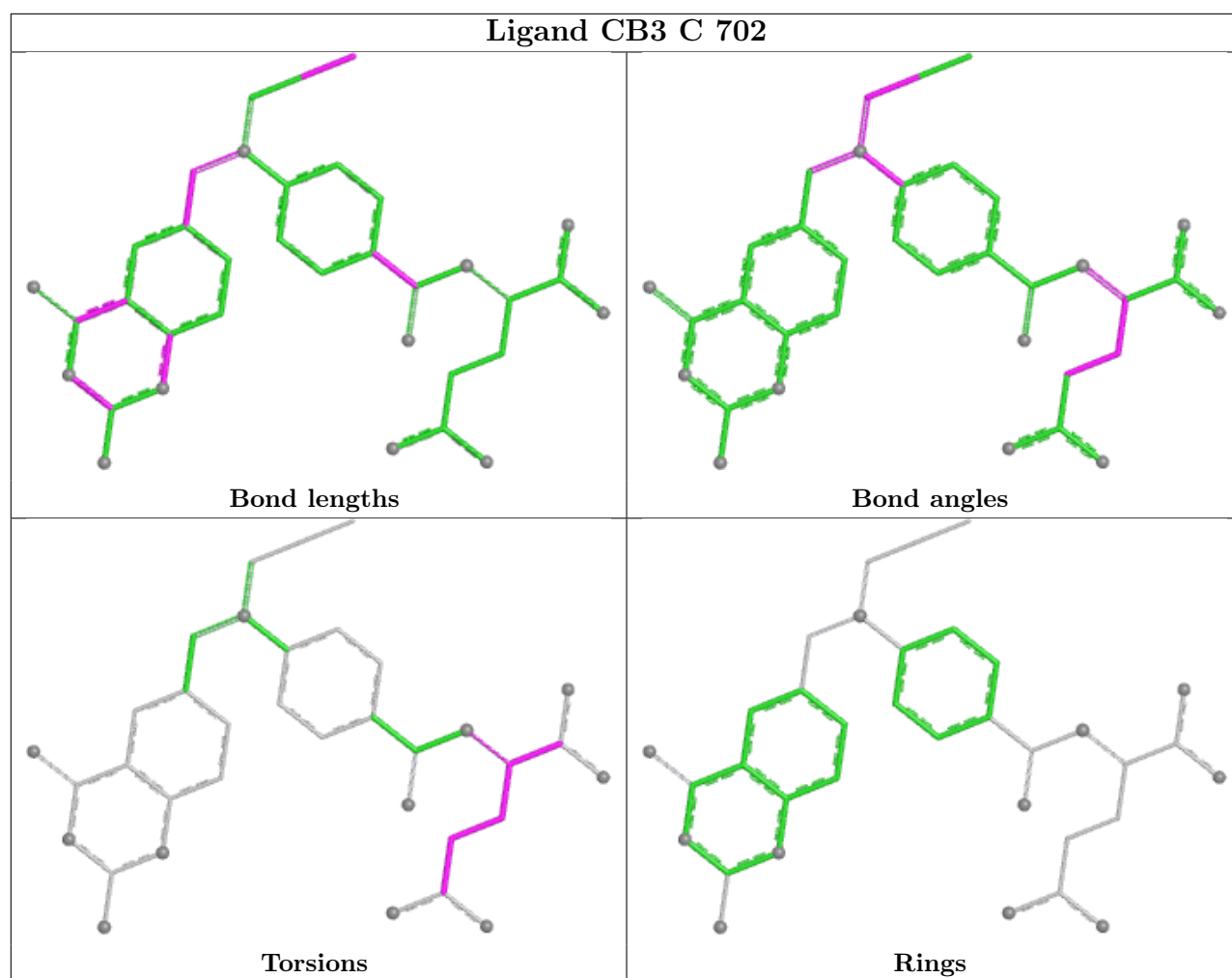
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

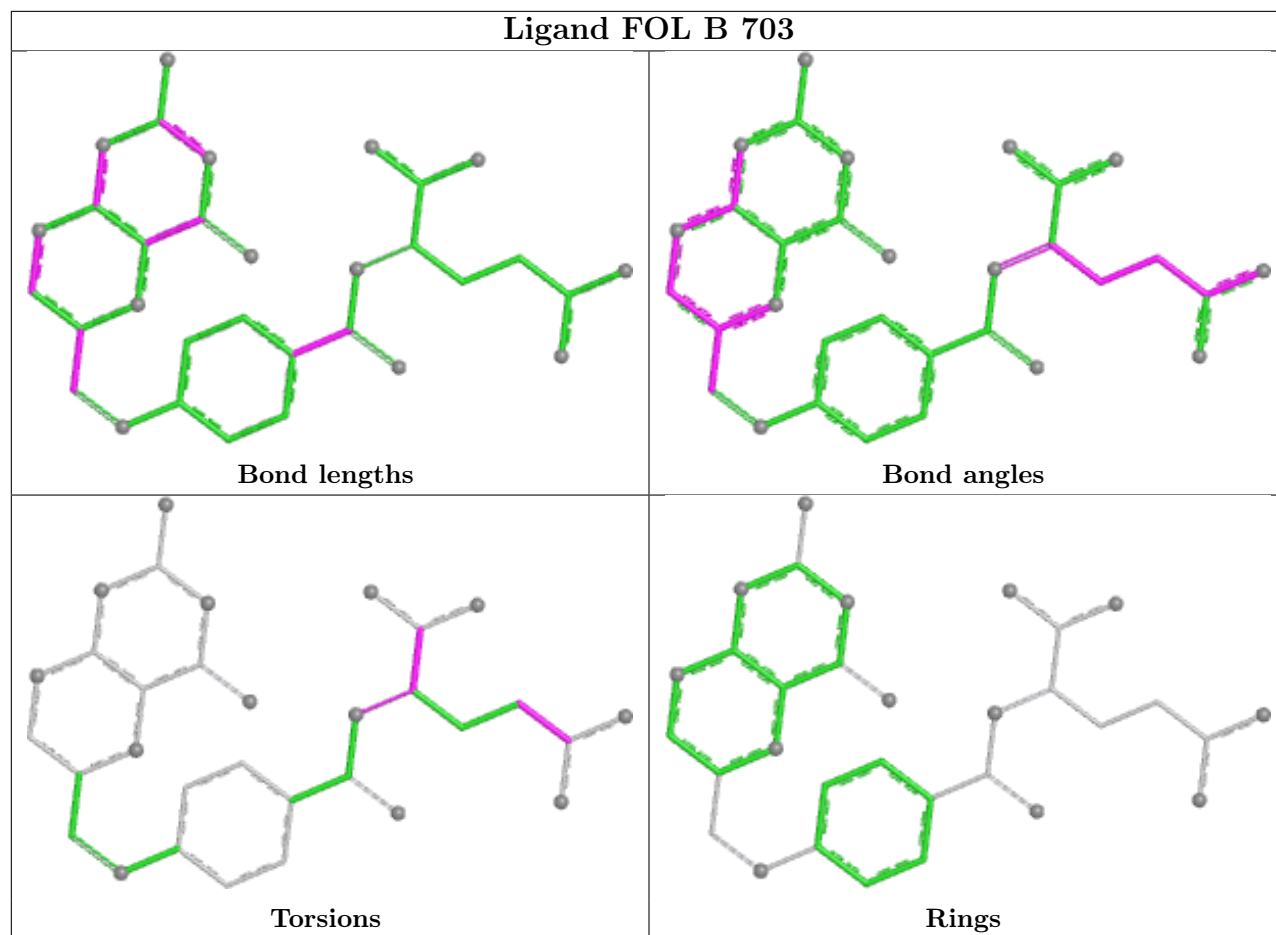
## Ligand CB3 H 702



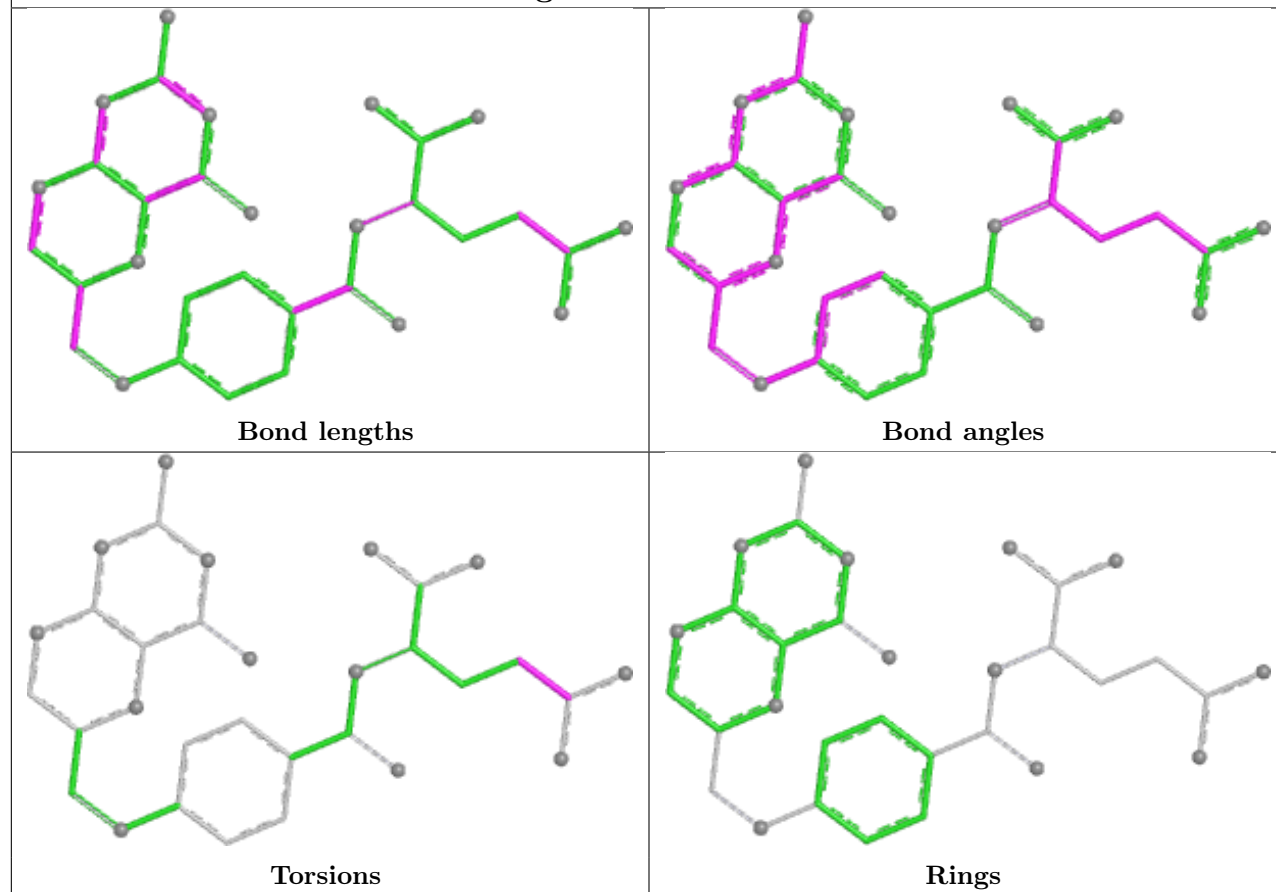
## Ligand UMP H 701



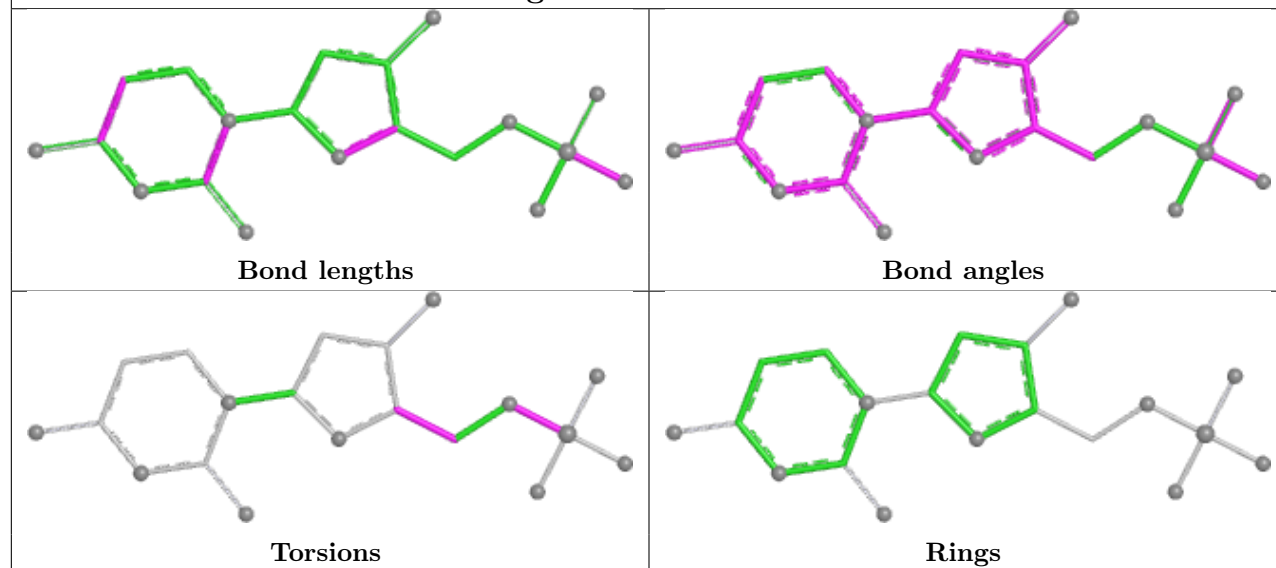


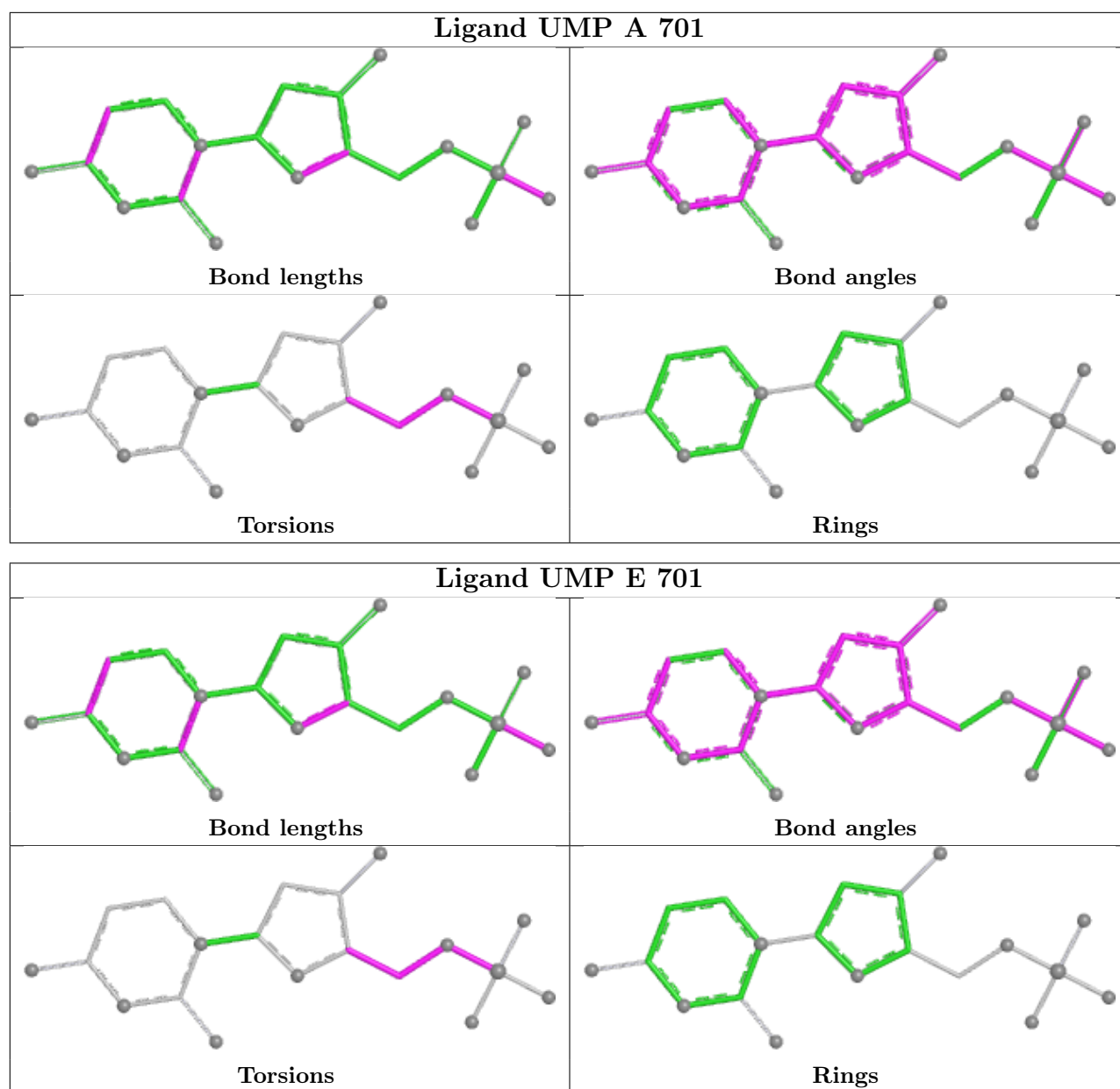


## Ligand FOL E 703

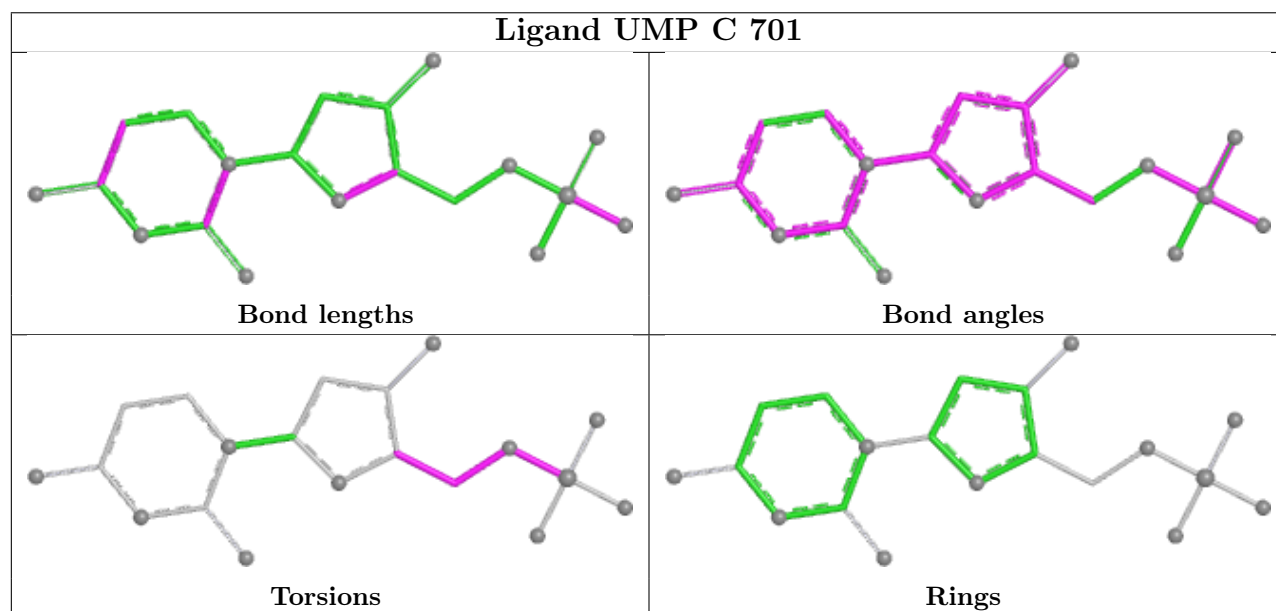
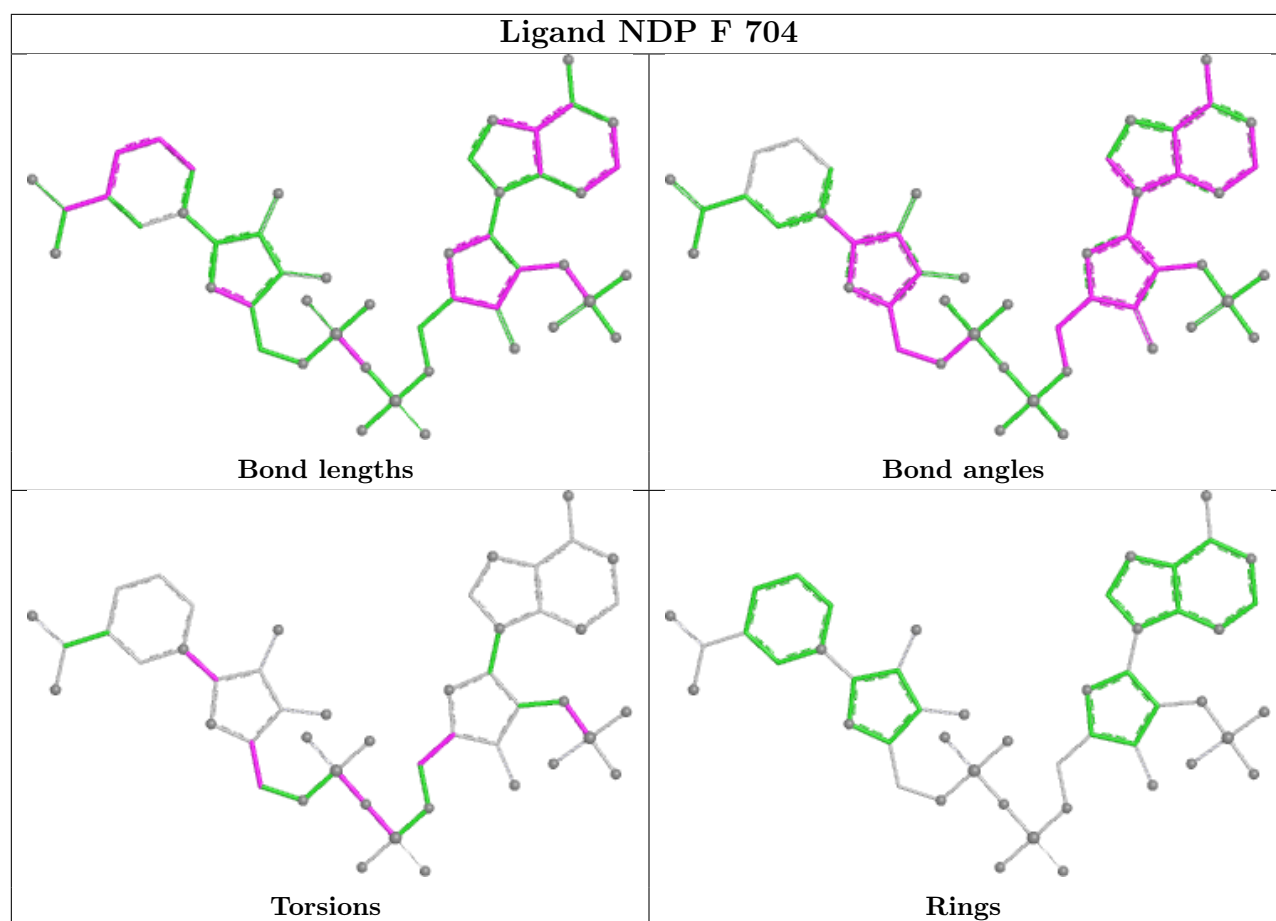


## Ligand UMP B 701

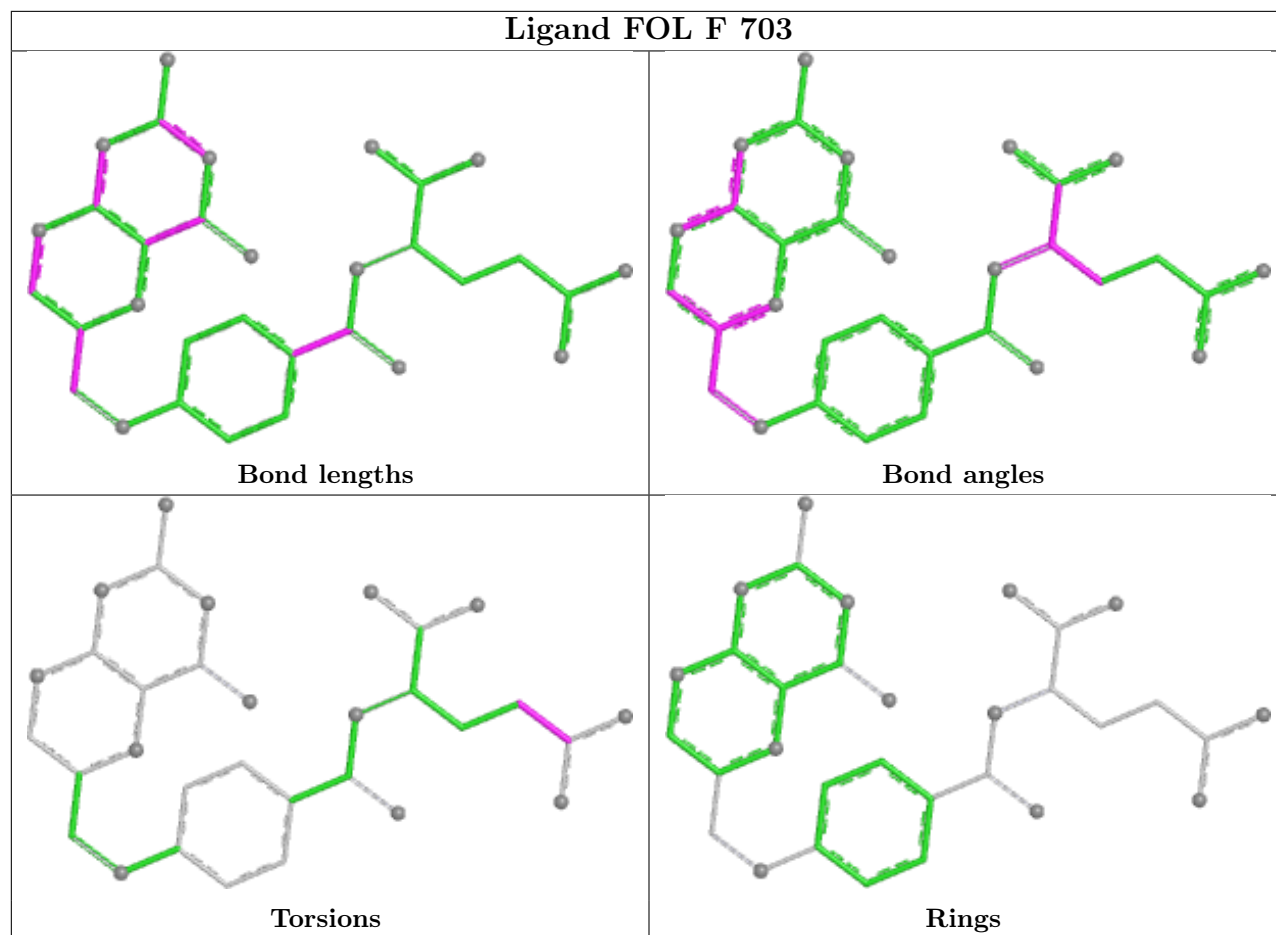


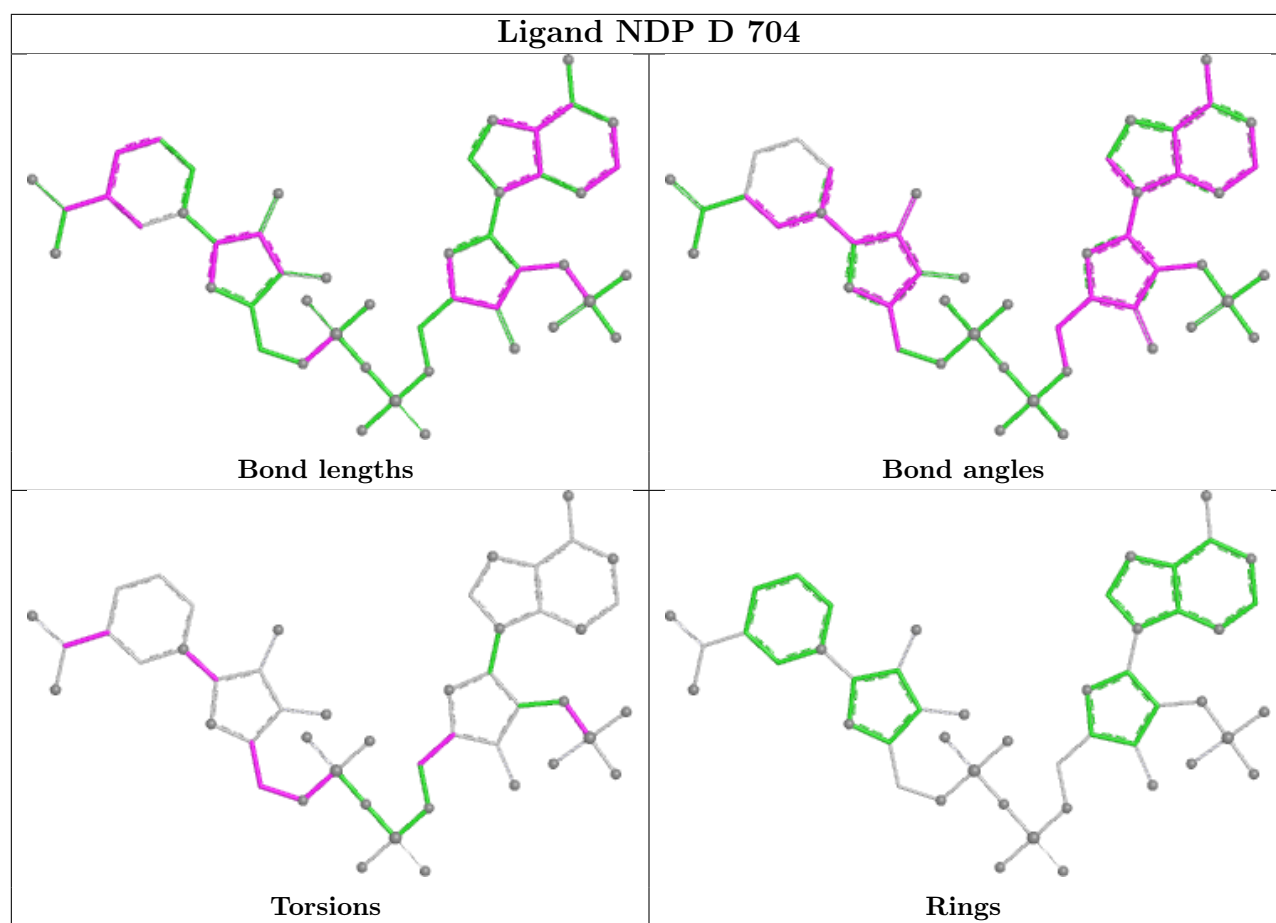


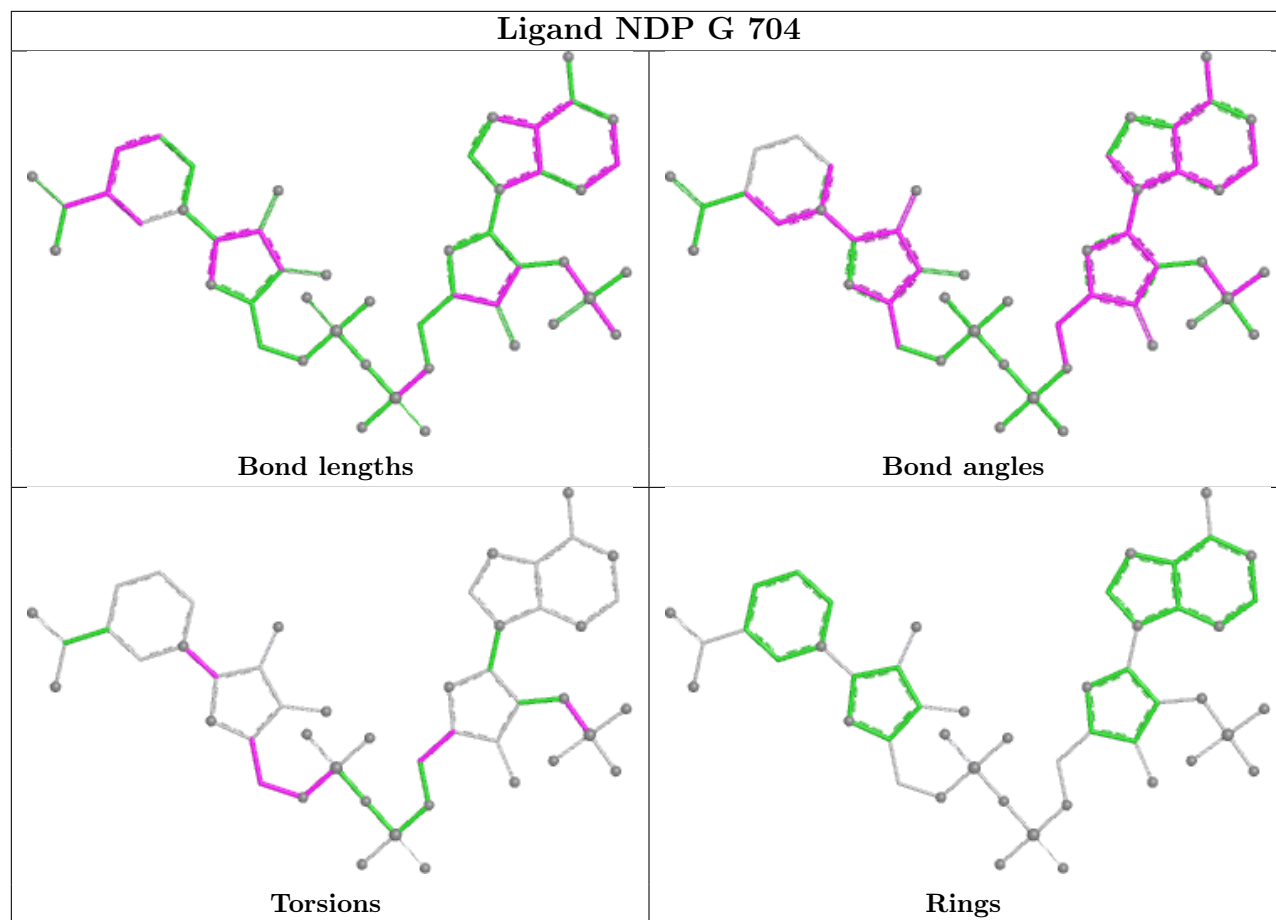


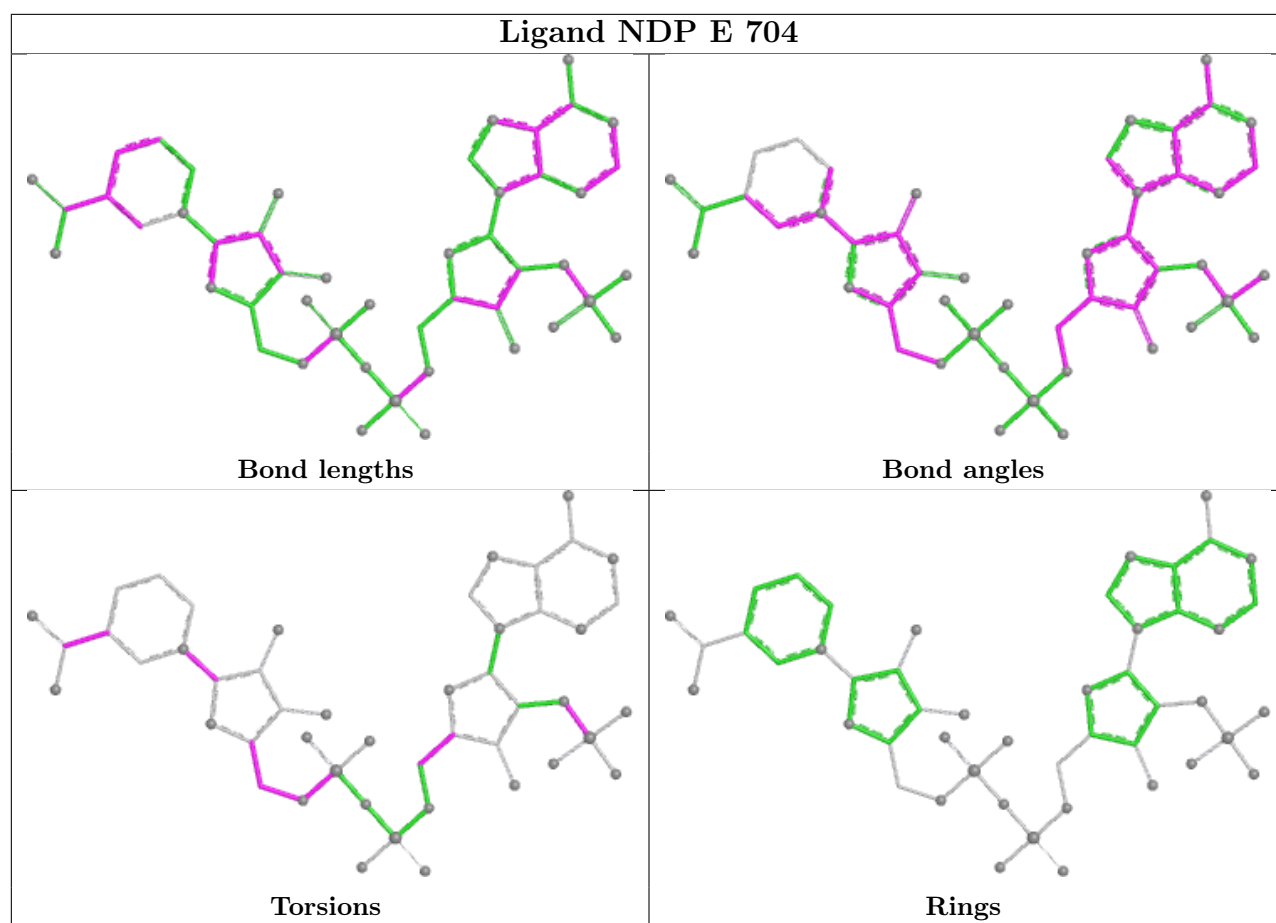


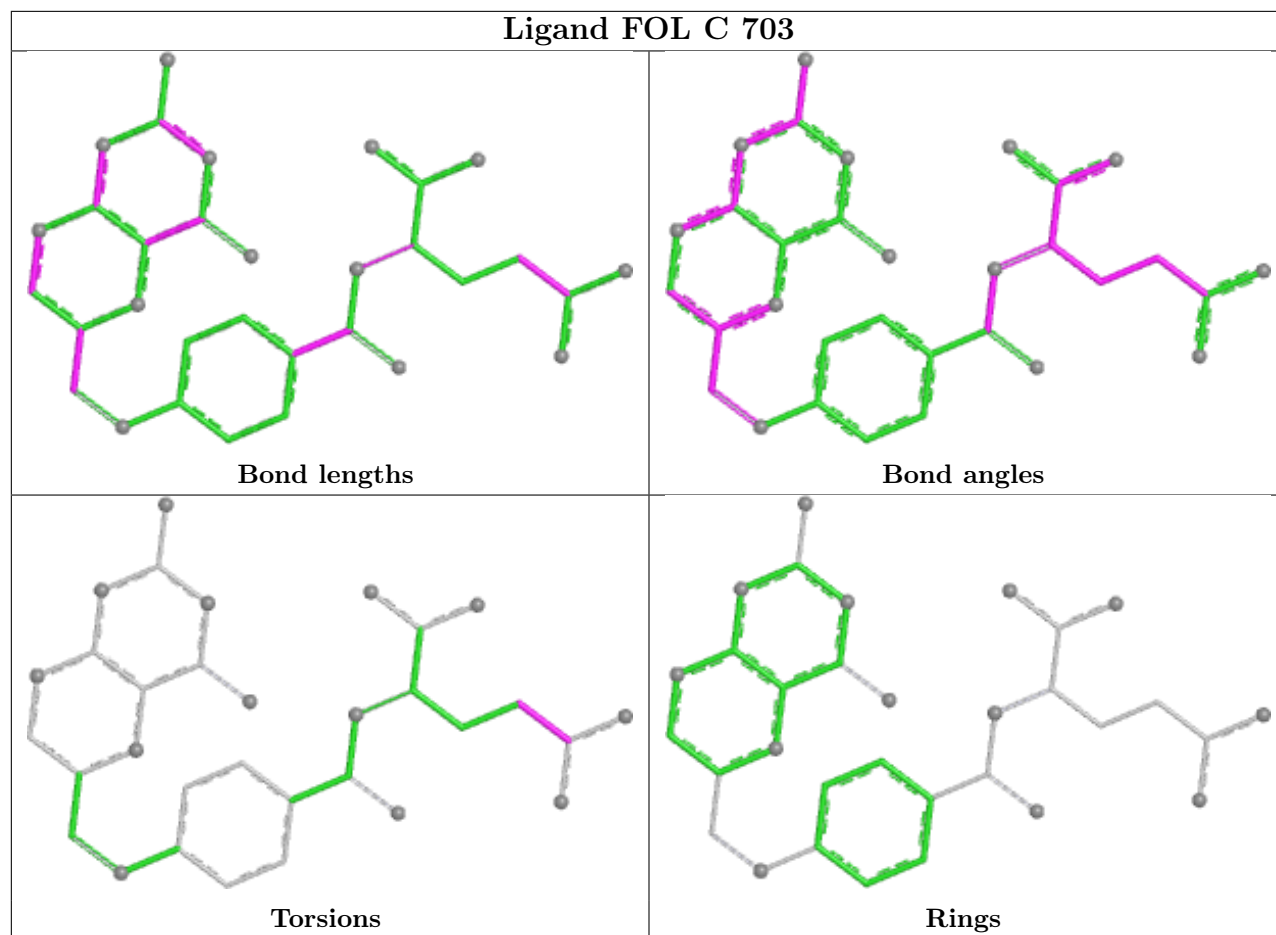
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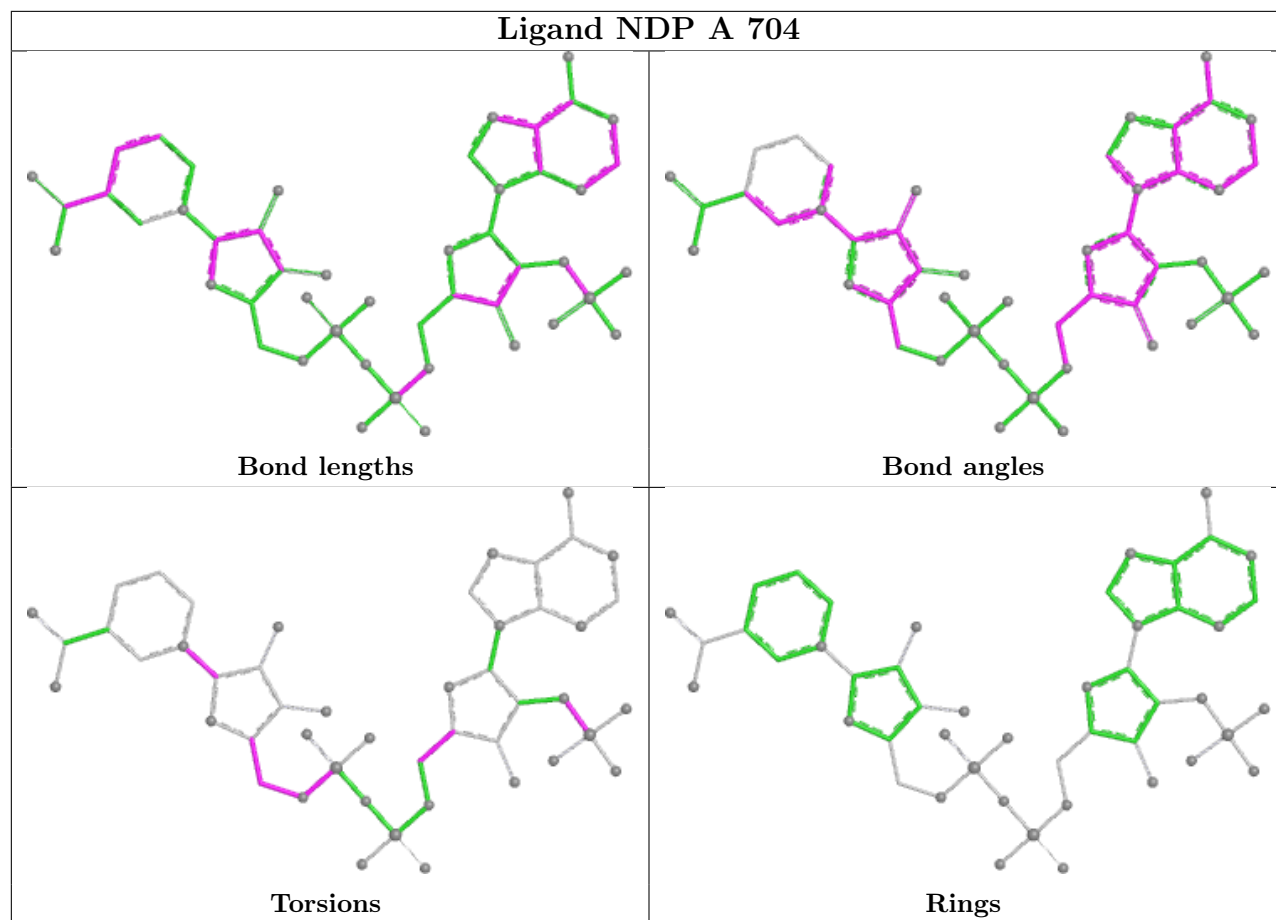


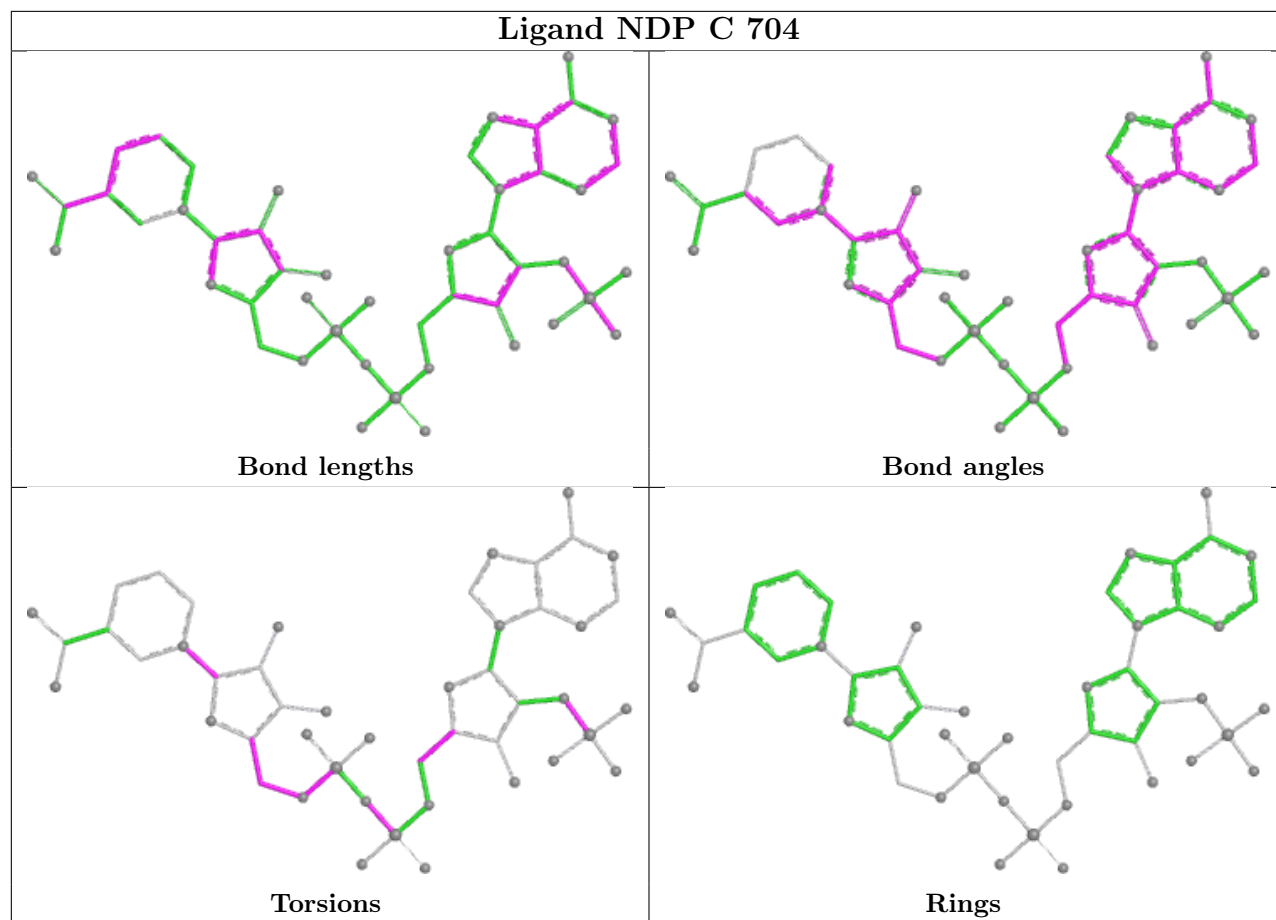






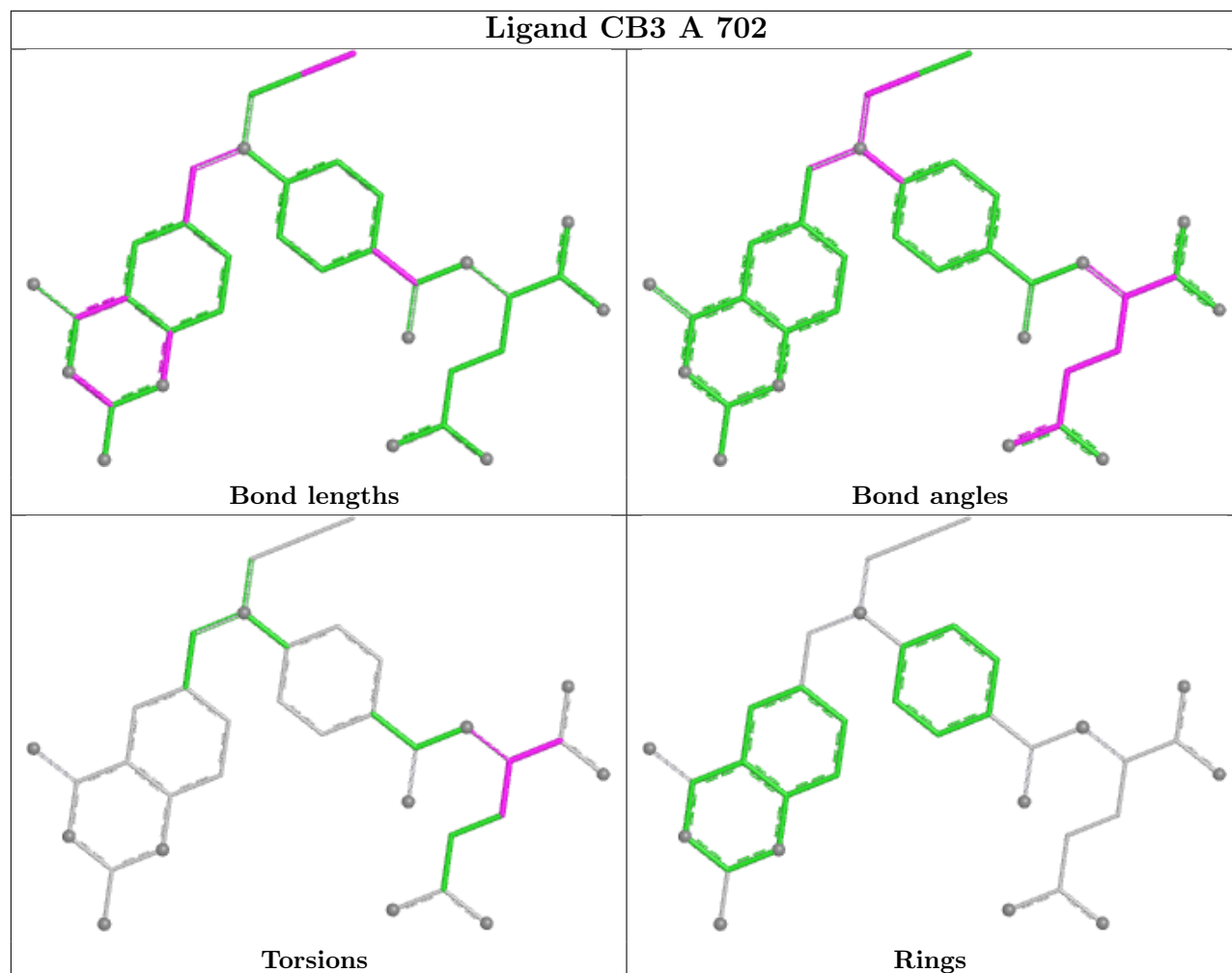




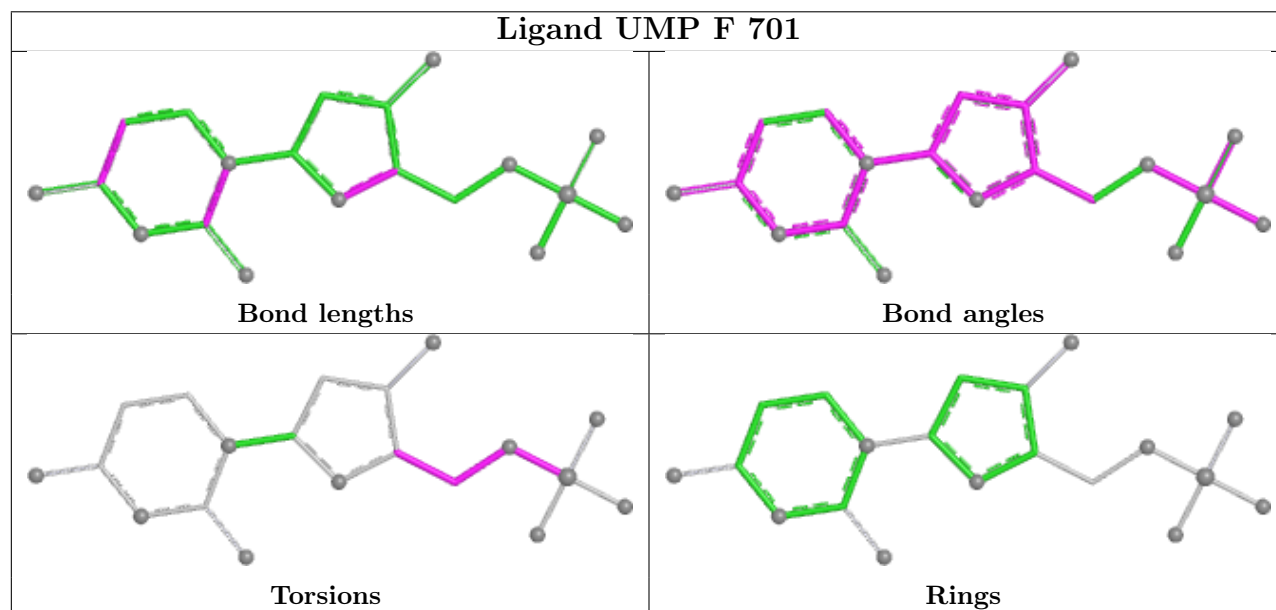


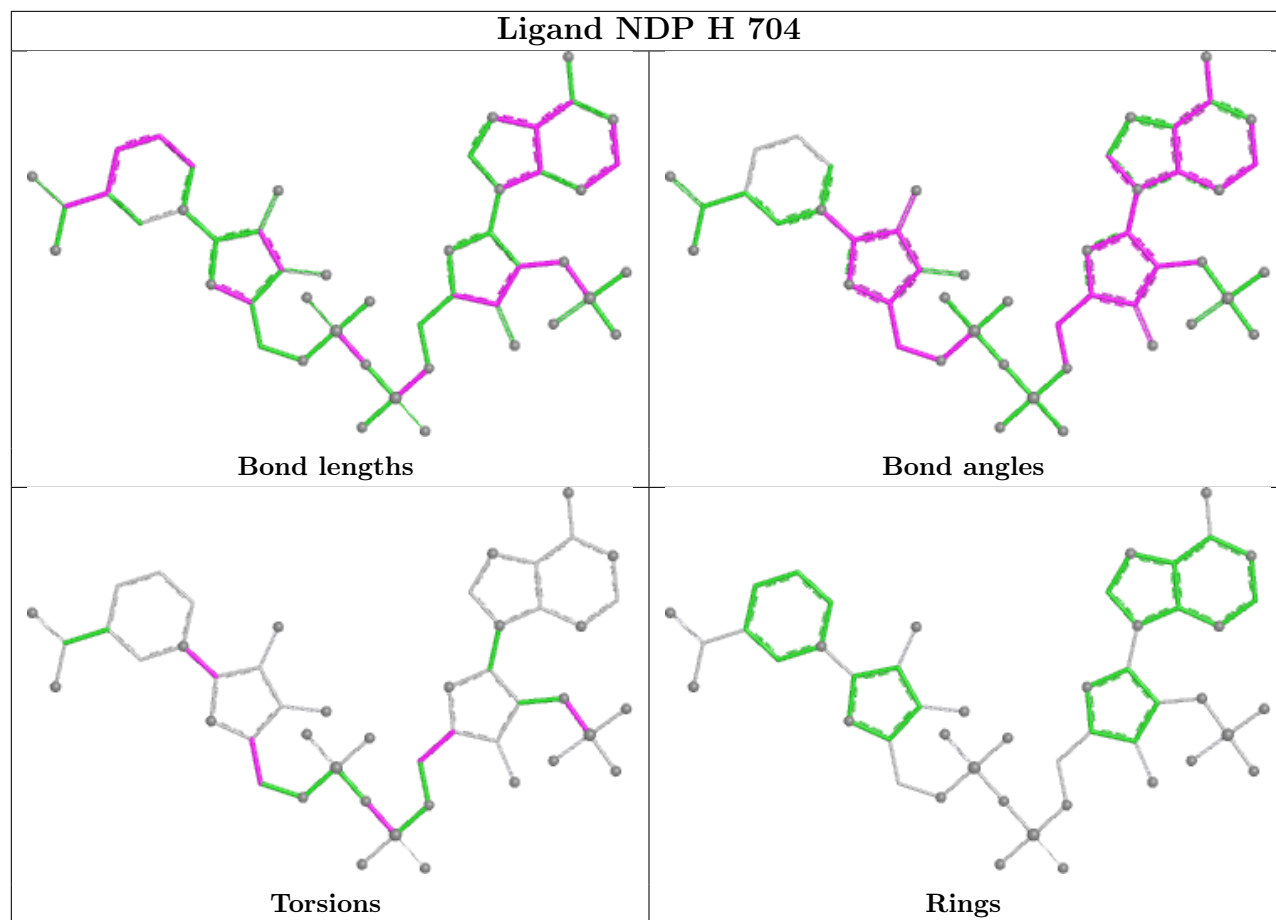


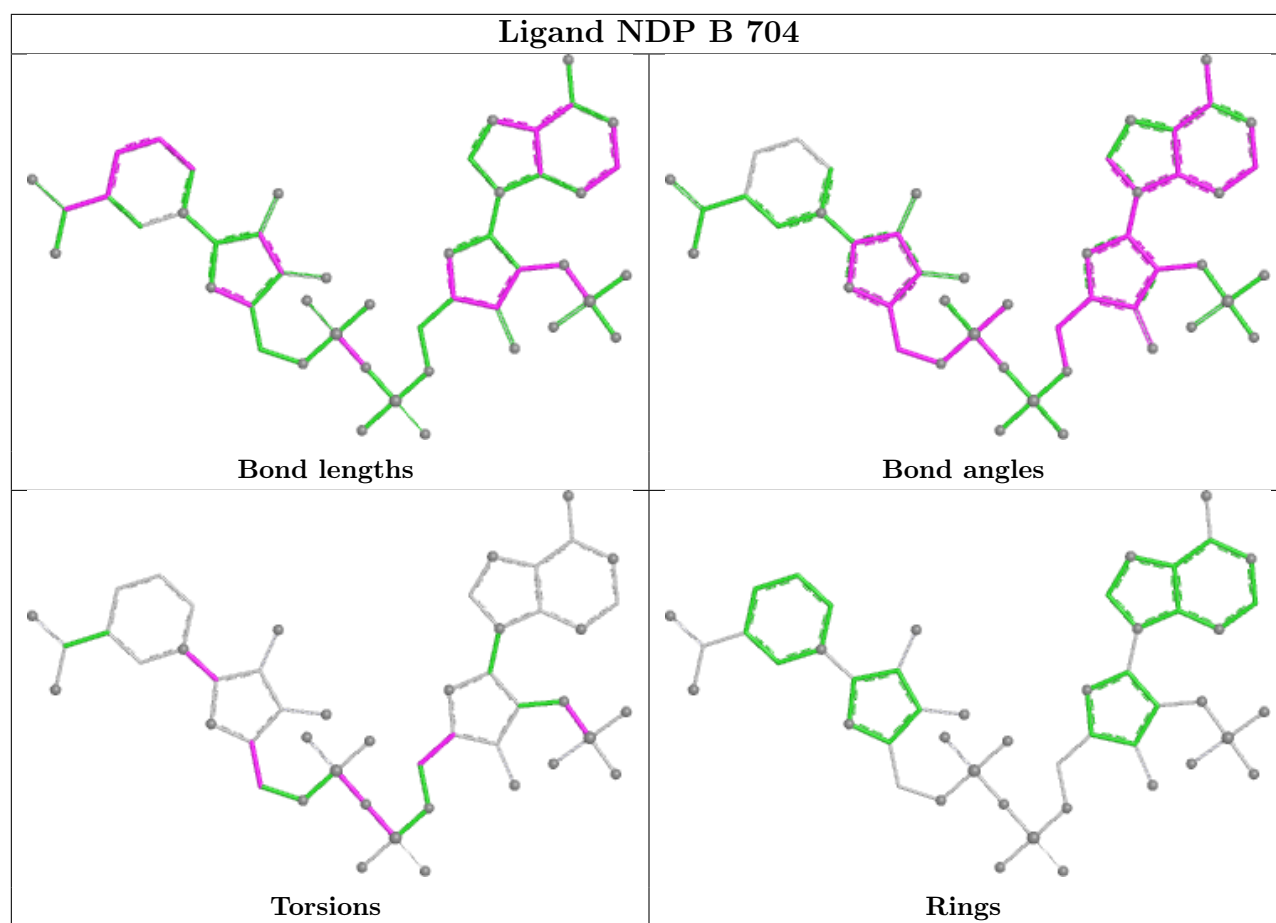
## Ligand CB3 A 702

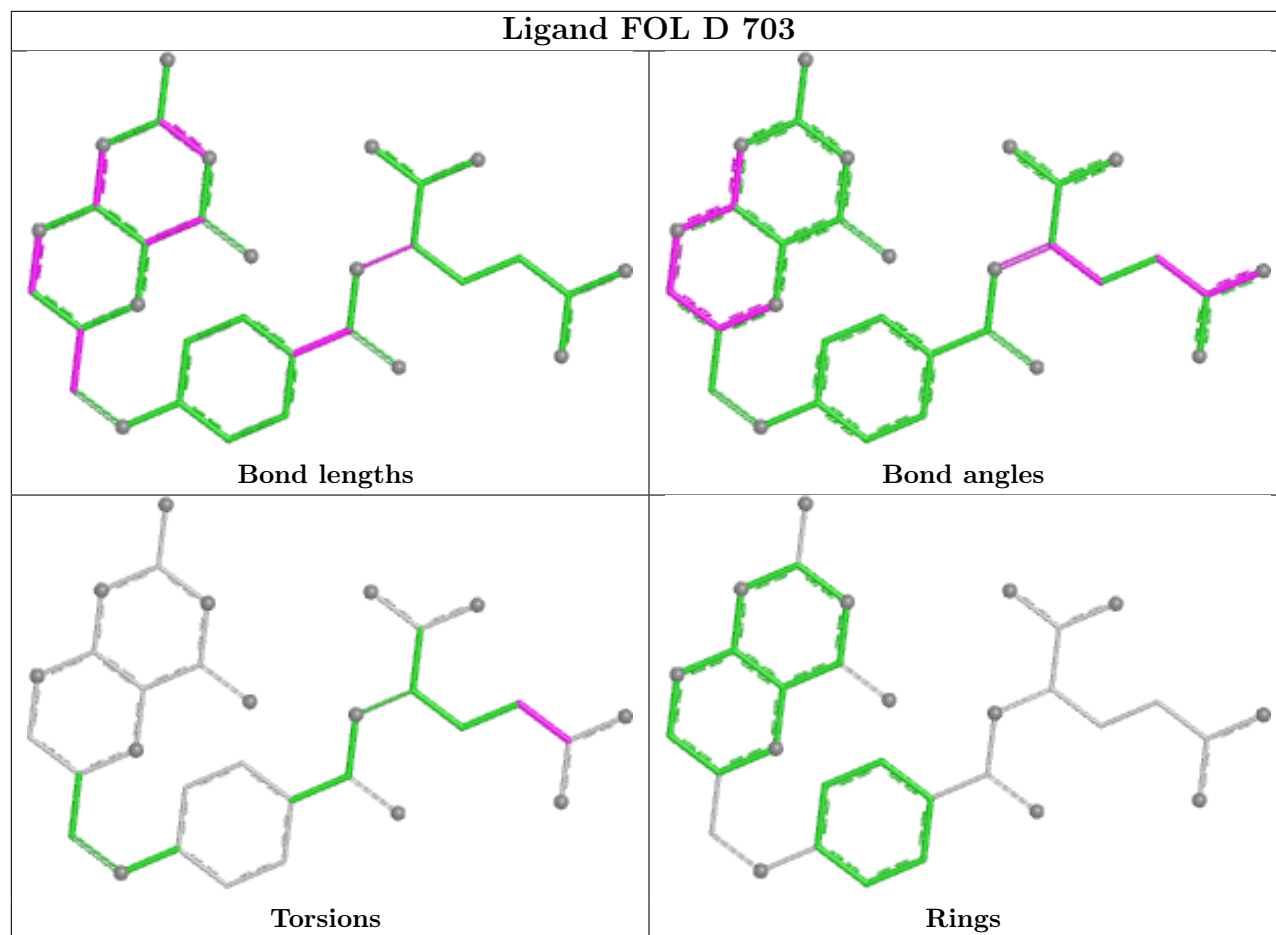


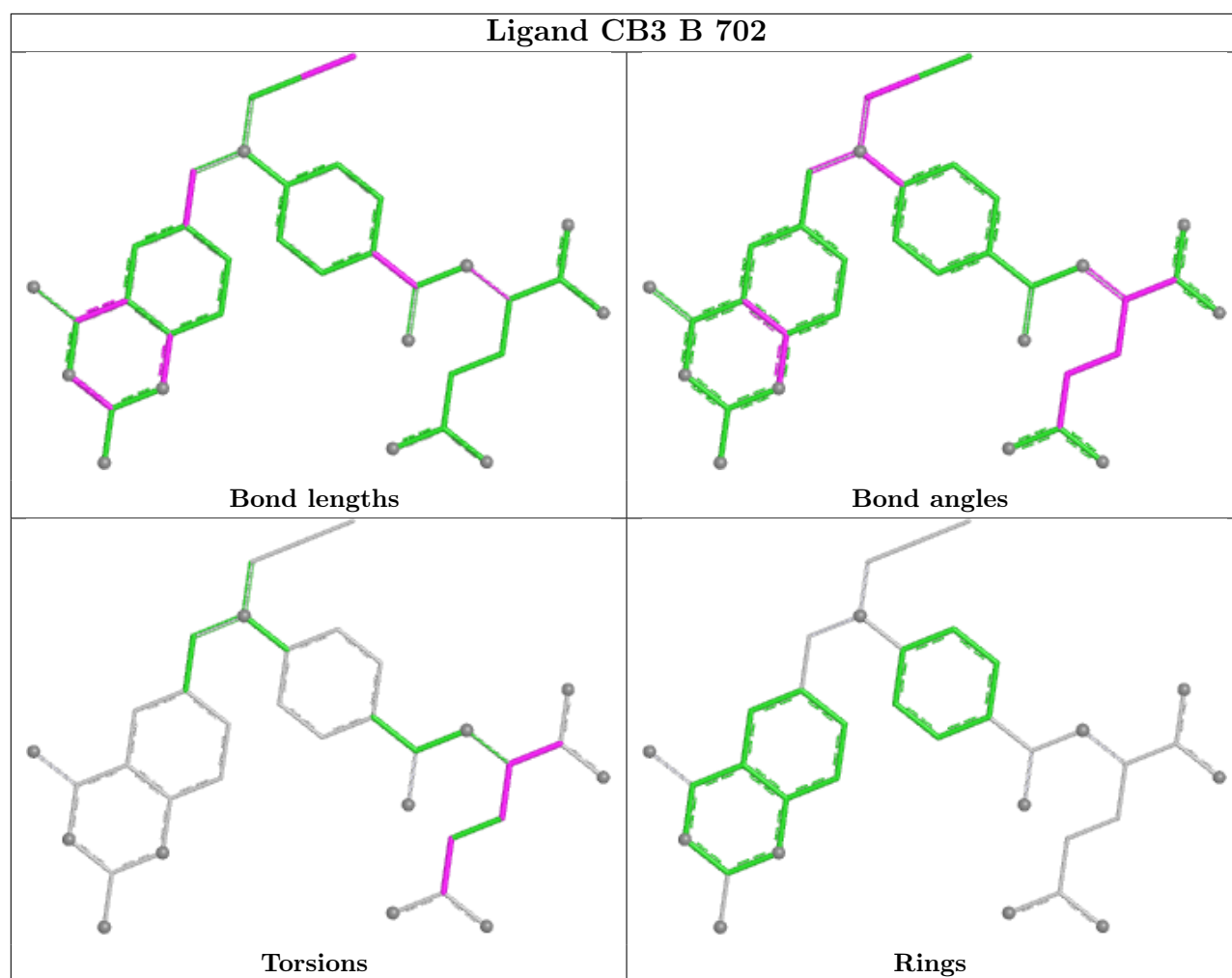
## Ligand UMP F 701

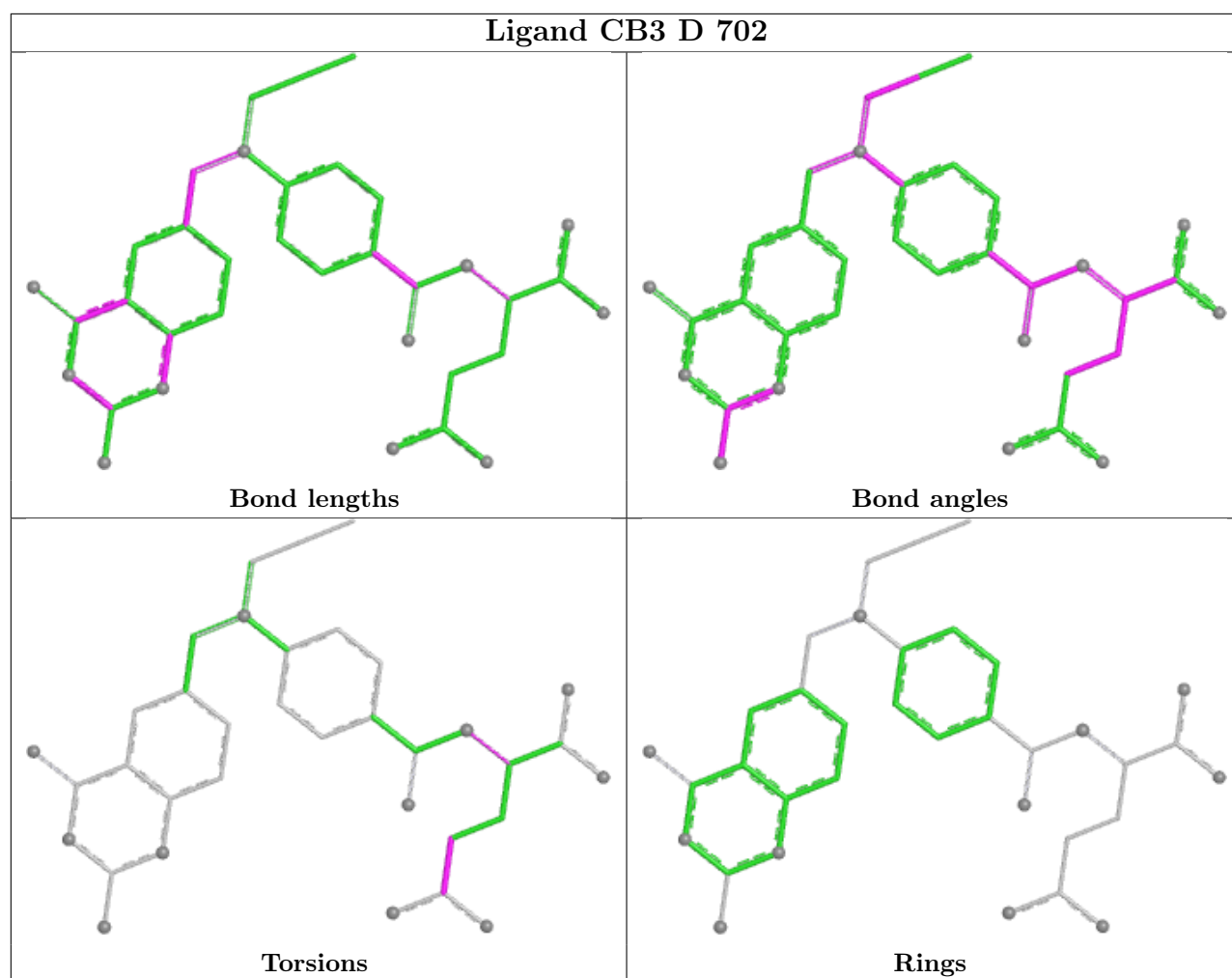


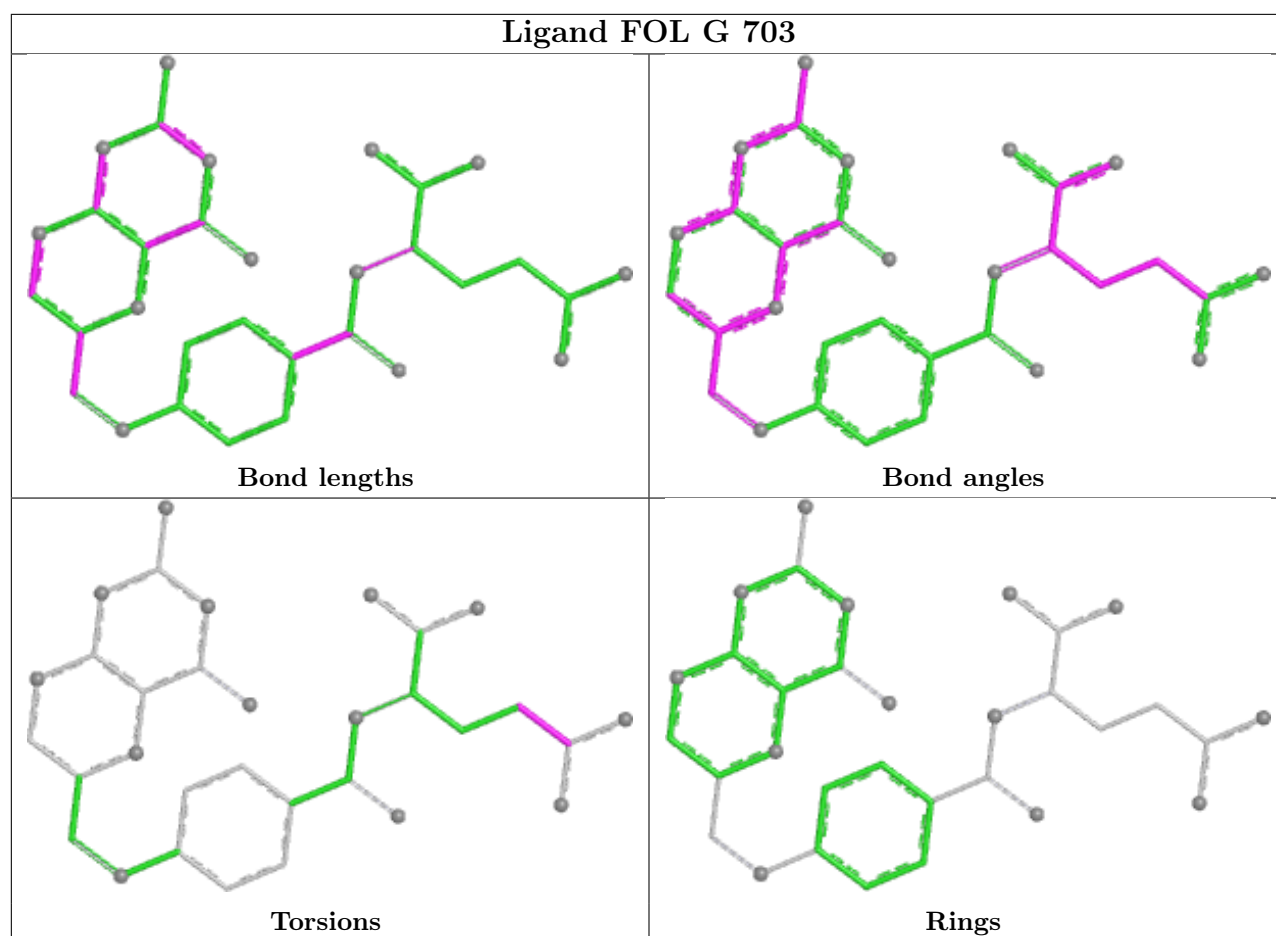




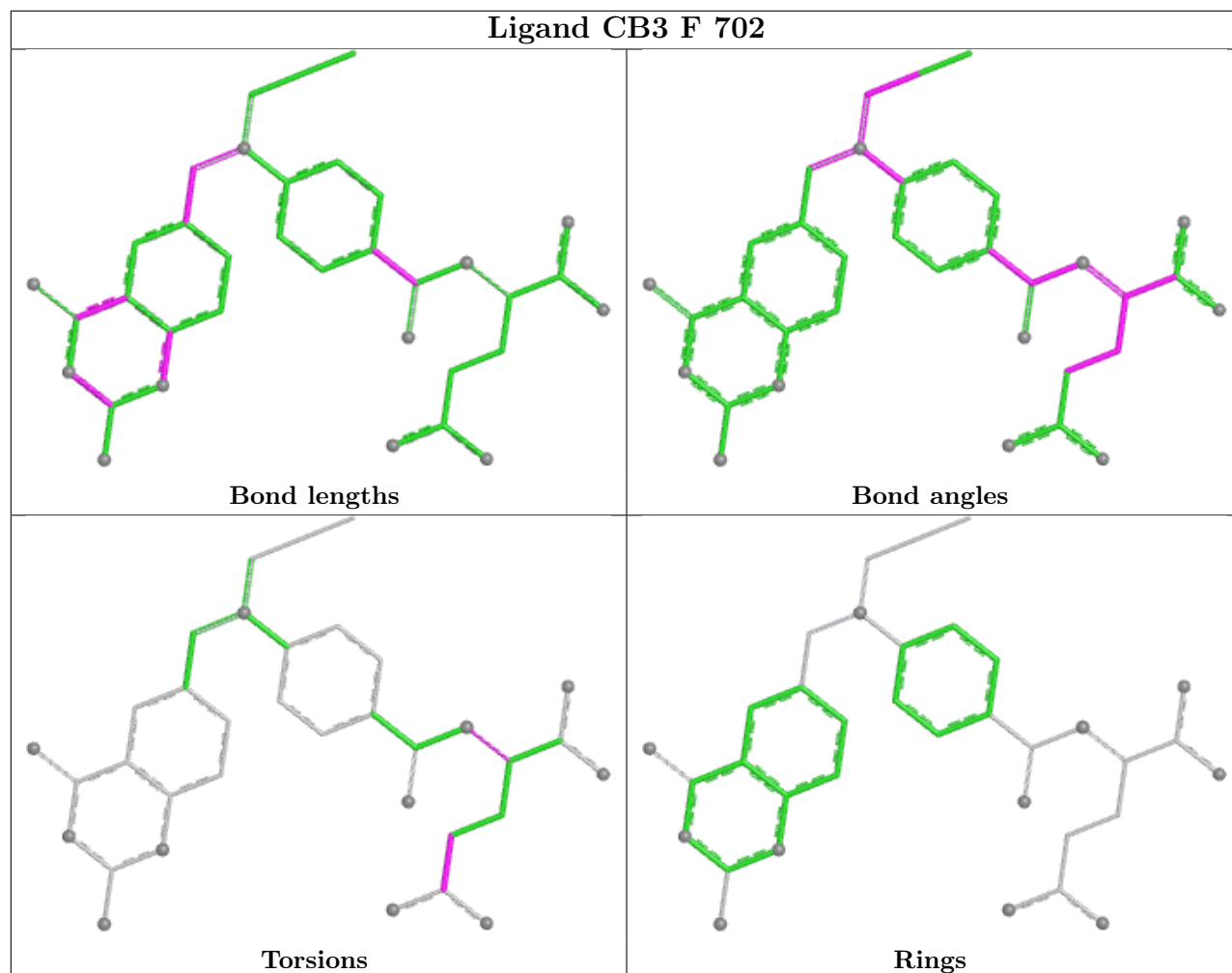




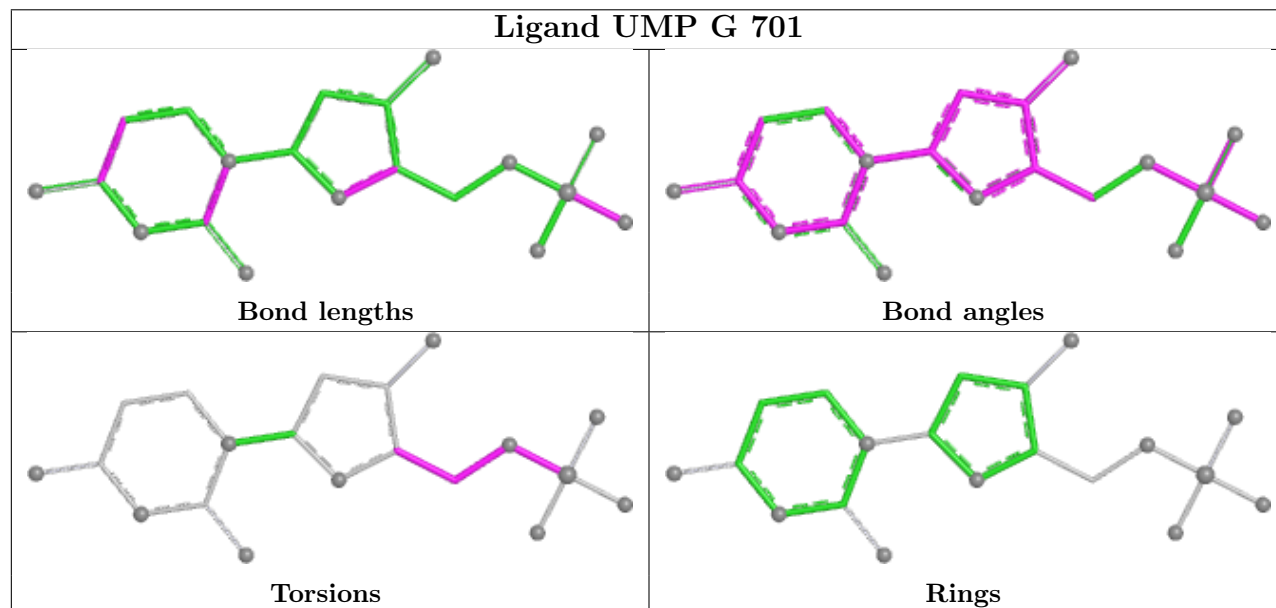




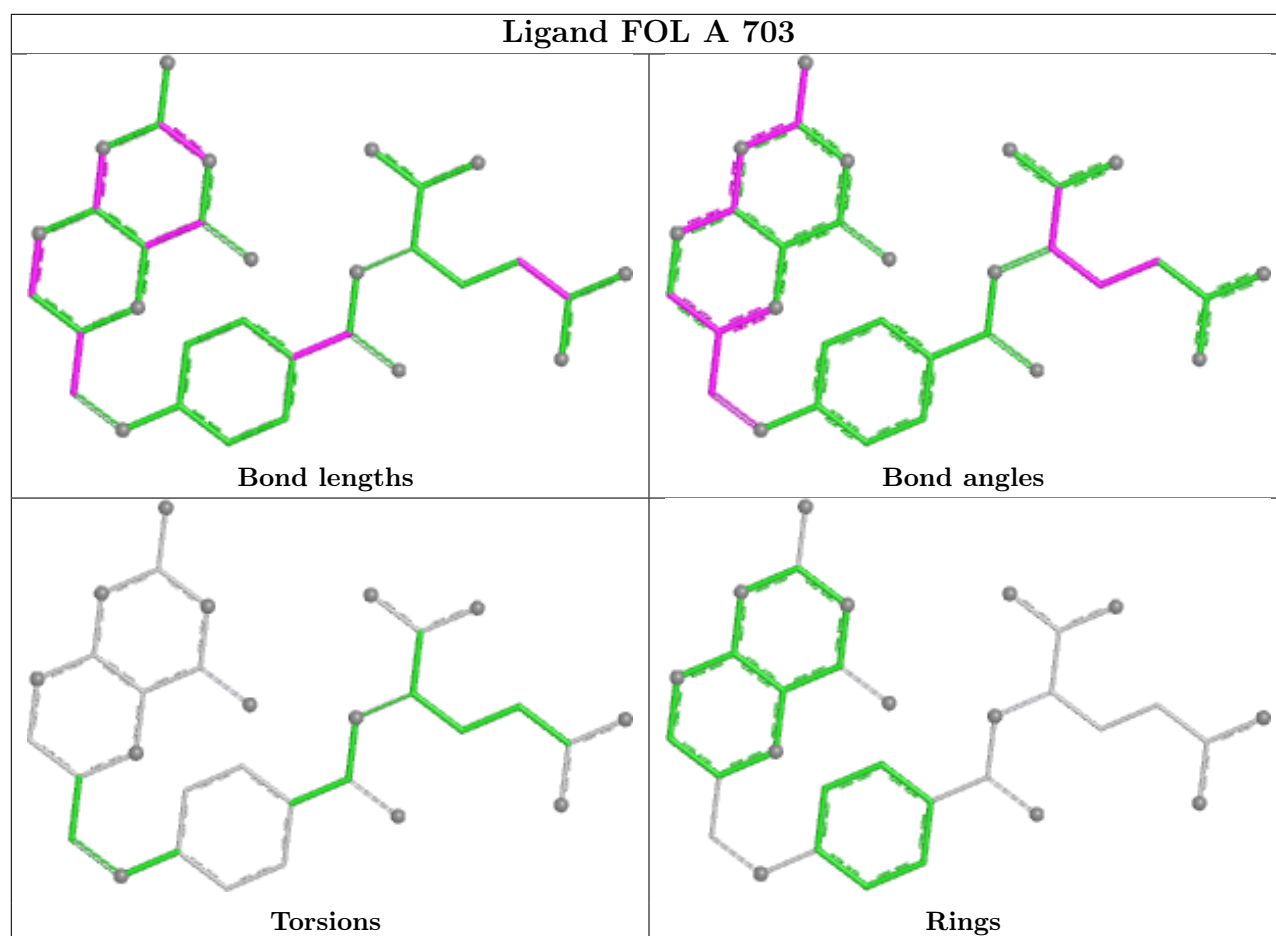
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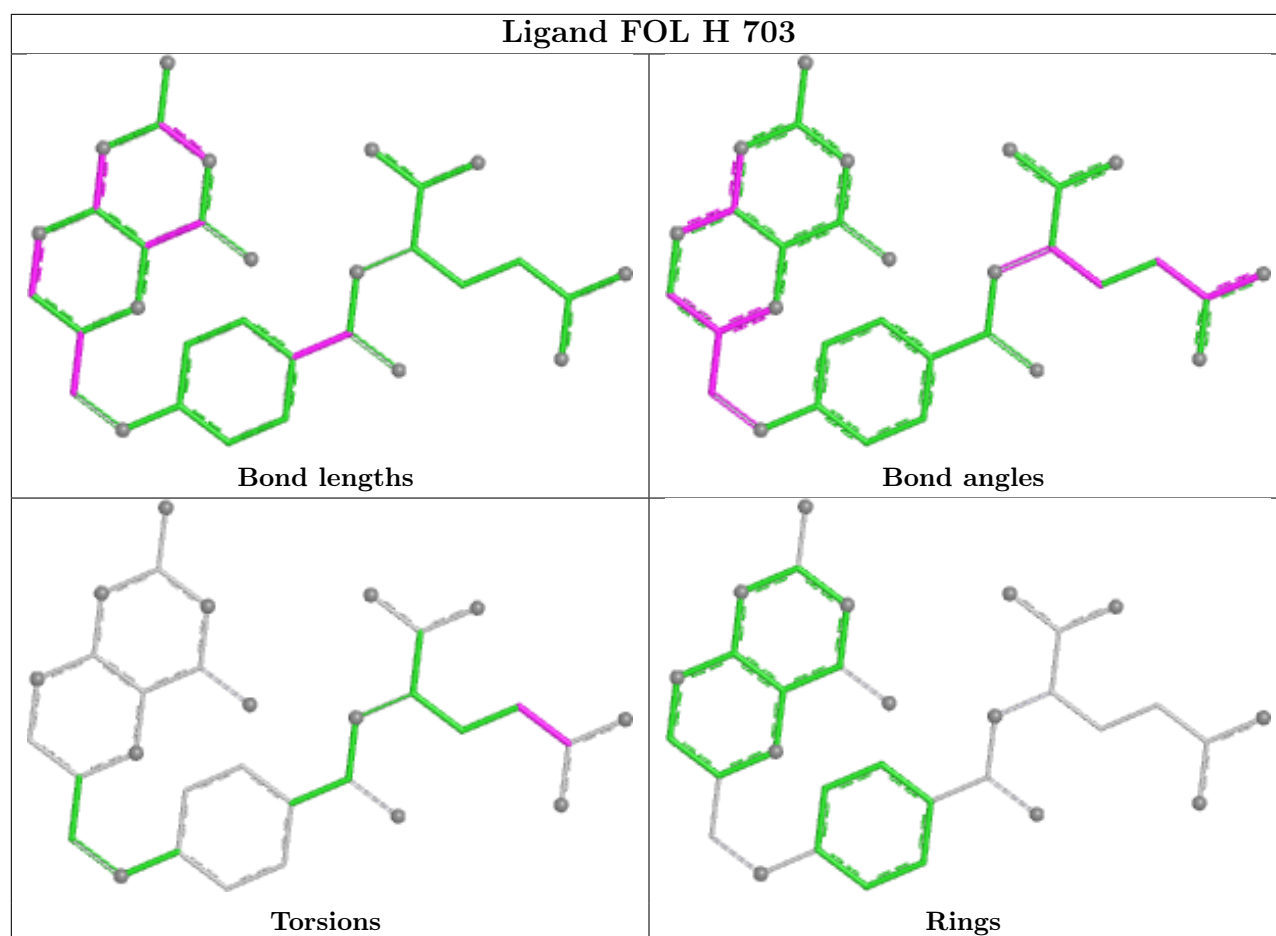


## Ligand UMP G 701

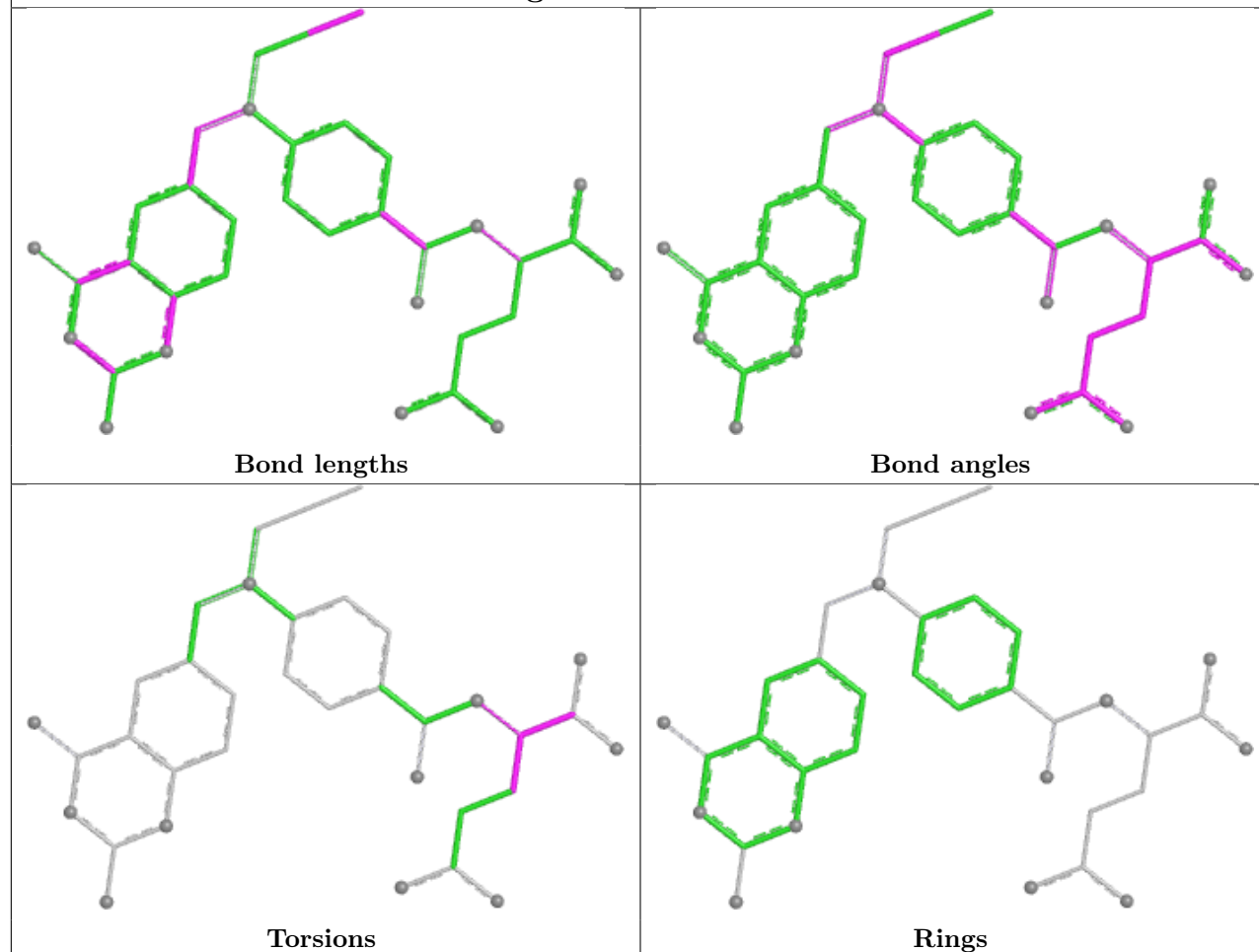




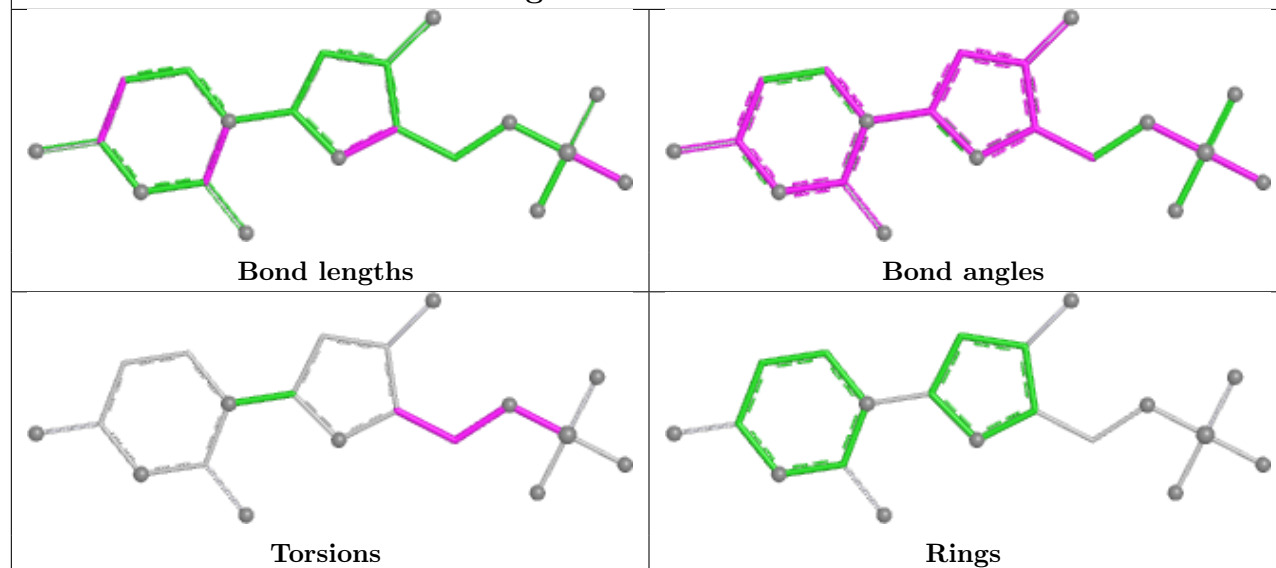


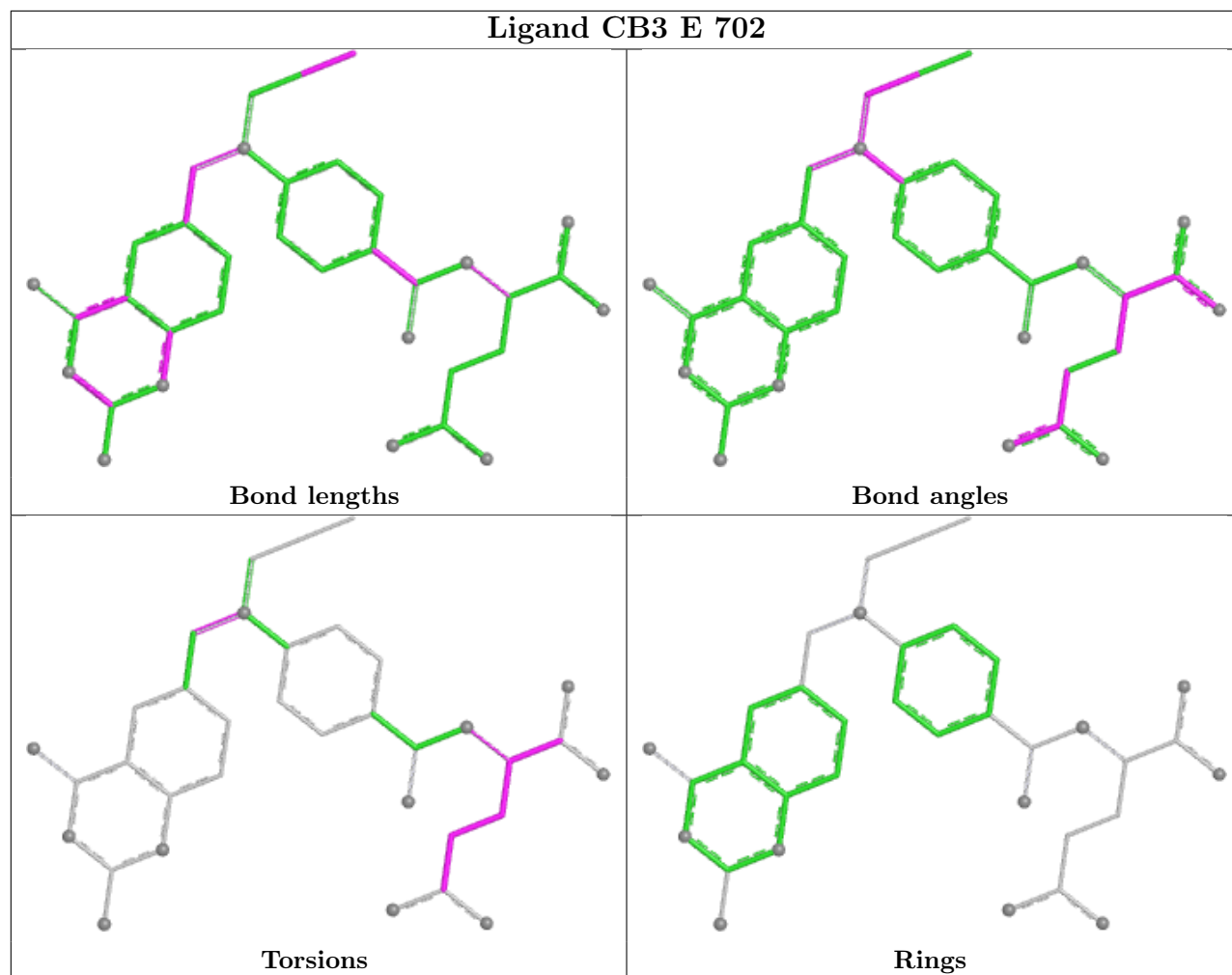


## Ligand CB3 G 702



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	510/566 (90%)	-1.09	0 100 100	20, 39, 75, 107	2 (0%)
1	B	491/566 (86%)	-1.03	0 100 100	22, 40, 90, 113	1 (0%)
1	C	510/566 (90%)	-1.08	0 100 100	19, 39, 73, 105	2 (0%)
1	D	491/566 (86%)	-1.03	0 100 100	21, 40, 89, 112	1 (0%)
1	E	510/566 (90%)	-1.10	0 100 100	21, 39, 74, 109	2 (0%)
1	F	491/566 (86%)	-1.03	0 100 100	22, 41, 87, 114	1 (0%)
1	G	510/566 (90%)	-1.09	0 100 100	20, 39, 74, 107	2 (0%)
1	H	491/566 (86%)	-1.03	0 100 100	22, 40, 86, 118	1 (0%)
All	All	4004/4528 (88%)	-1.06	0 100 100	19, 39, 83, 118	12 (0%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

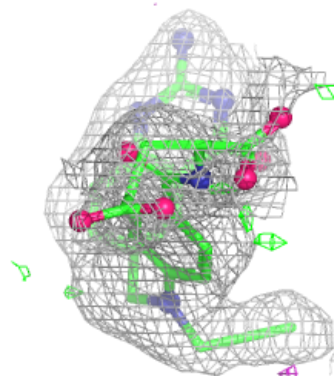
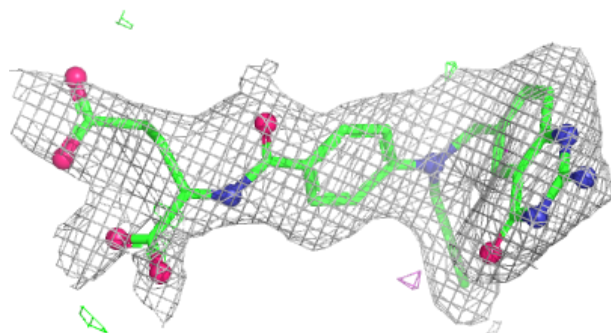
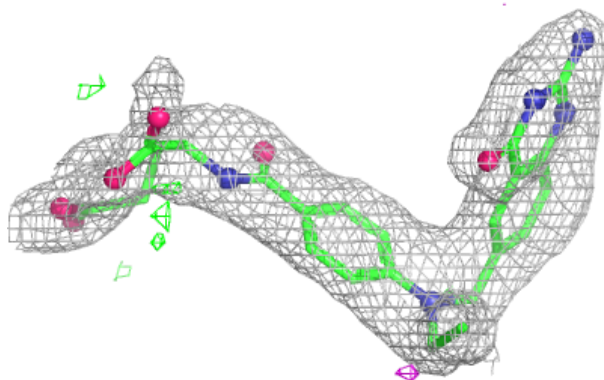
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CB3	E	702	35/35	0.98	0.06	30,44,86,91	0
4	FOL	B	703	32/32	0.98	0.06	38,71,99,107	0
4	FOL	F	703	32/32	0.98	0.06	33,70,96,101	0
2	UMP	E	701	20/20	0.99	0.03	27,39,50,58	0
2	UMP	F	701	20/20	0.99	0.03	27,35,42,52	0
2	UMP	G	701	20/20	0.99	0.04	29,37,51,65	0
2	UMP	H	701	20/20	0.99	0.03	25,34,44,54	0
3	CB3	A	702	35/35	0.99	0.05	27,41,88,93	0
3	CB3	B	702	35/35	0.99	0.05	26,36,82,106	0
3	CB3	C	702	35/35	0.99	0.04	30,41,86,93	0
3	CB3	D	702	35/35	0.99	0.05	26,35,101,111	0
2	UMP	A	701	20/20	0.99	0.04	28,36,50,57	0
3	CB3	F	702	35/35	0.99	0.05	21,34,103,108	0
3	CB3	G	702	35/35	0.99	0.05	32,40,86,90	0
3	CB3	H	702	35/35	0.99	0.05	22,33,84,109	0
4	FOL	A	703	32/32	0.99	0.04	28,52,83,88	0
2	UMP	C	701	20/20	0.99	0.04	31,38,50,54	0
4	FOL	C	703	32/32	0.99	0.04	33,53,75,84	0
4	FOL	D	703	32/32	0.99	0.05	34,71,93,102	0
4	FOL	E	703	32/32	0.99	0.04	30,57,81,94	0
2	UMP	D	701	20/20	0.99	0.03	27,36,43,52	0
4	FOL	G	703	32/32	0.99	0.05	32,57,85,109	0
4	FOL	H	703	32/32	0.99	0.05	37,71,89,102	0
5	NDP	A	704	48/48	0.99	0.03	25,42,56,64	0
5	NDP	B	704	48/48	0.99	0.04	35,65,114,126	0
5	NDP	C	704	48/48	0.99	0.03	24,41,53,62	0
5	NDP	D	704	48/48	0.99	0.04	38,66,111,114	0
5	NDP	E	704	48/48	0.99	0.03	24,41,58,61	0
5	NDP	F	704	48/48	0.99	0.04	38,61,107,116	0
5	NDP	G	704	48/48	0.99	0.03	23,41,53,67	0
5	NDP	H	704	48/48	0.99	0.04	31,62,108,114	0
2	UMP	B	701	20/20	1.00	0.03	28,33,41,54	0

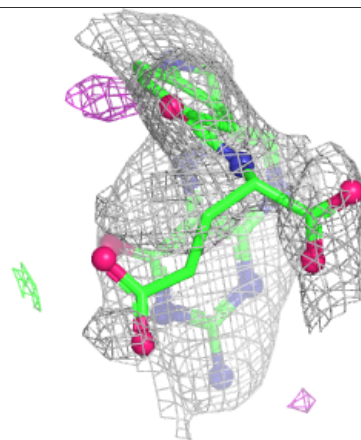
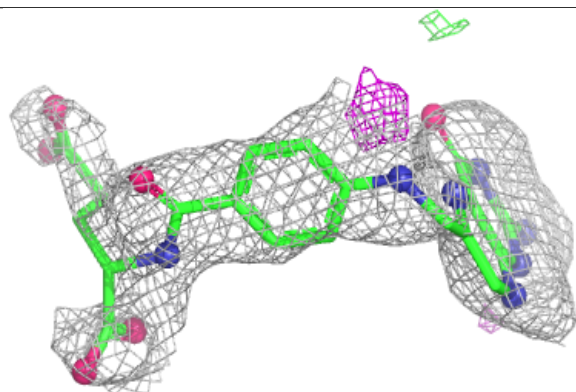
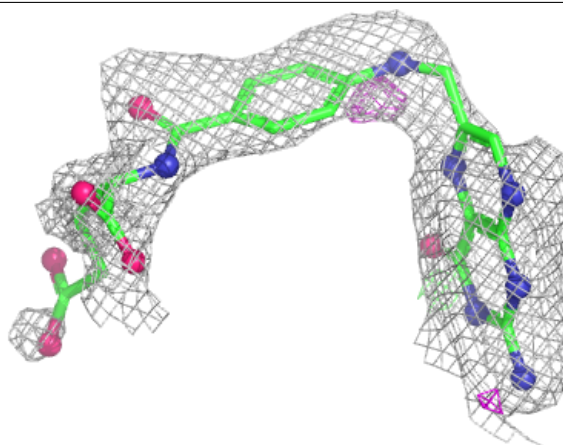
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CB3 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 FOL B 703:**

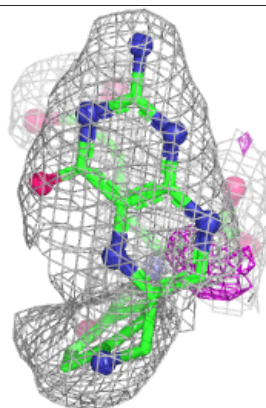
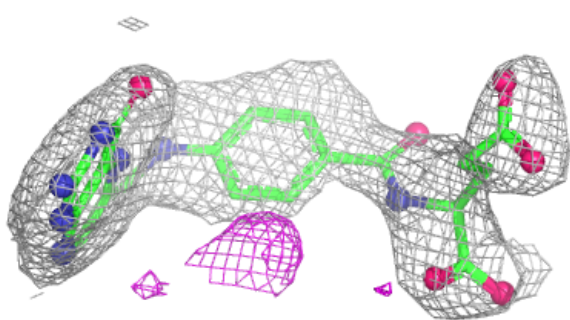
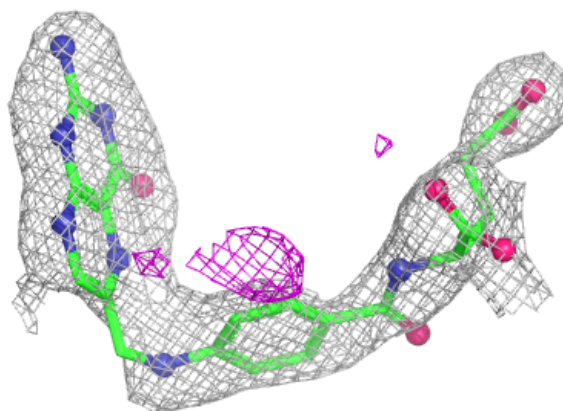
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



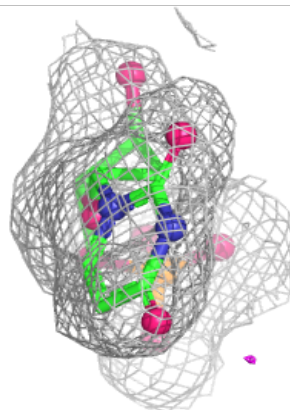
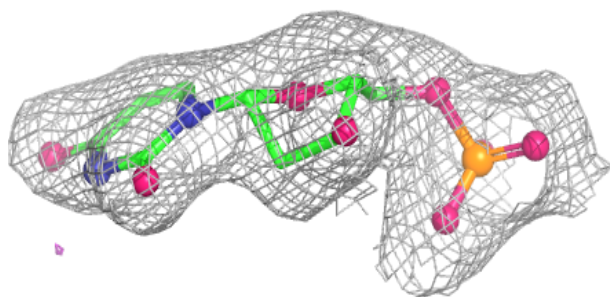
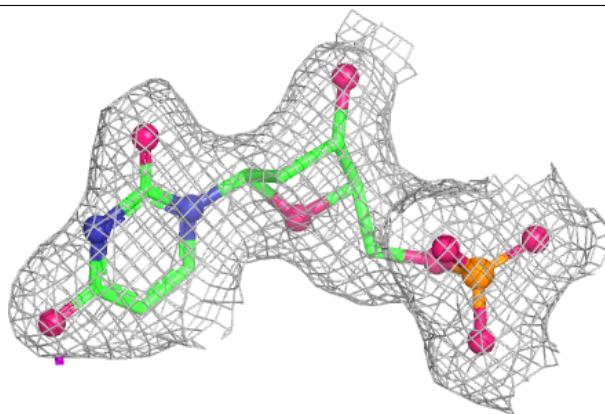


**Electron density around FOL F 703:**

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

**Electron density around UMP E 701:**

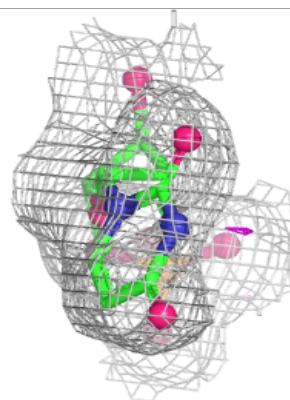
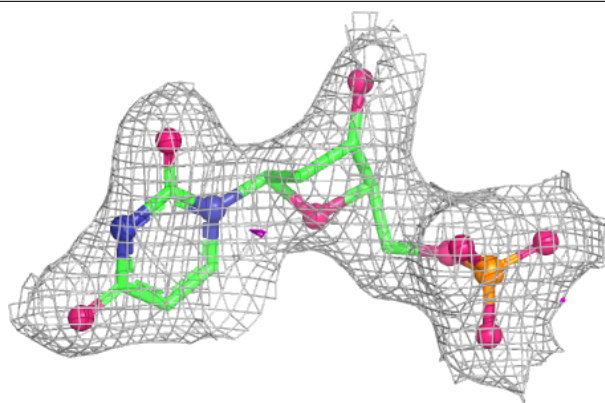
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



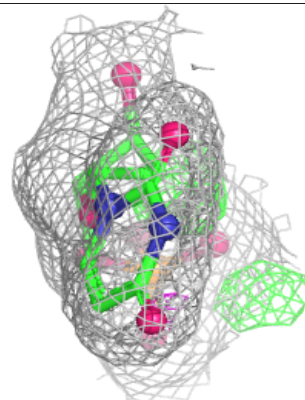
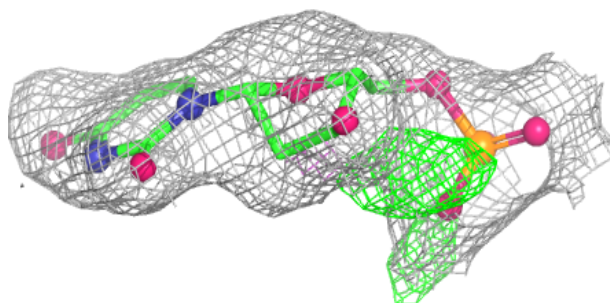
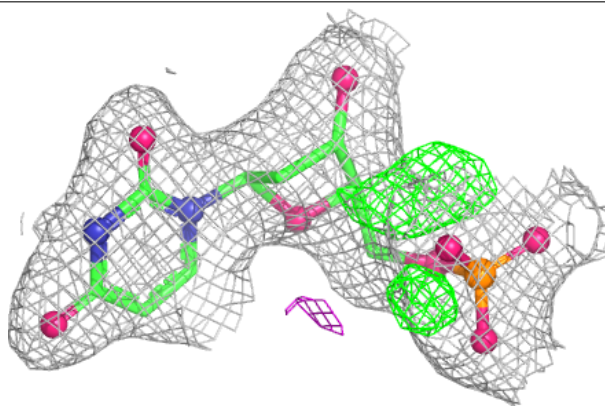


**Electron density around UMP F 701:**

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

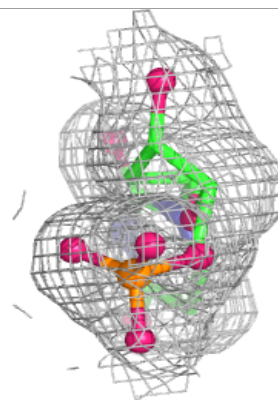
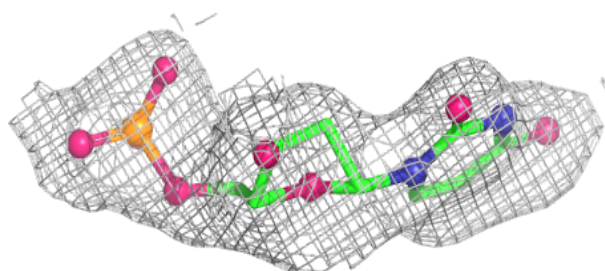
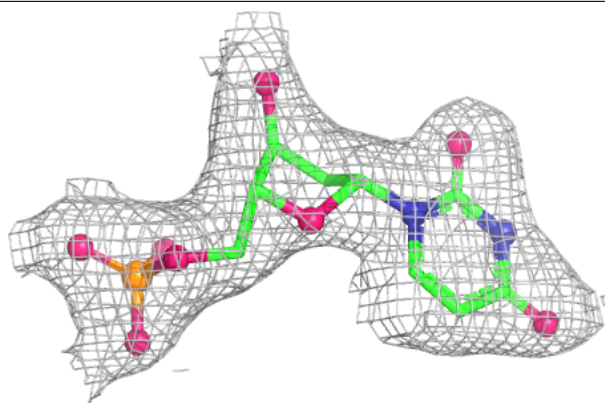
**Electron density around UMP G 701:**

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

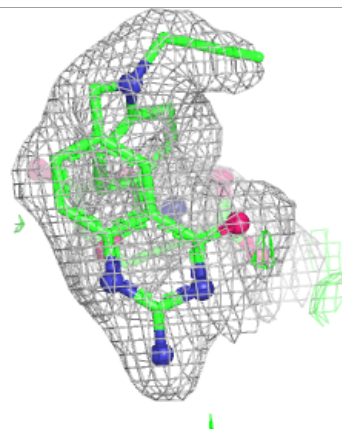
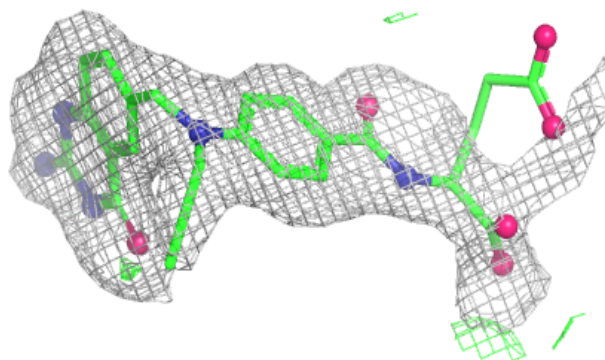
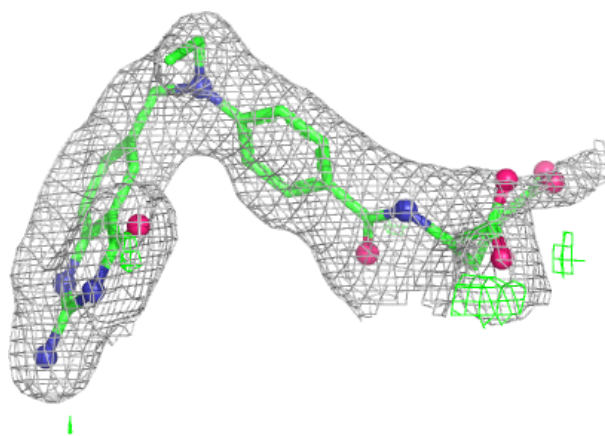


**Electron density around UMP H 701:**

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

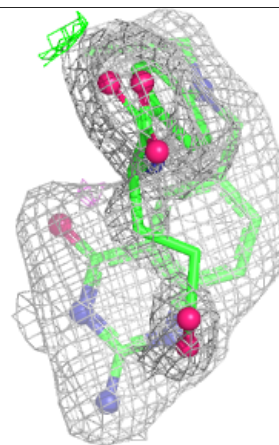
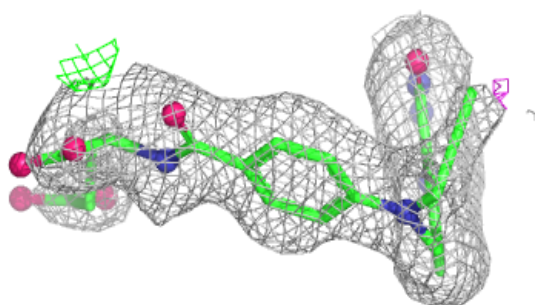
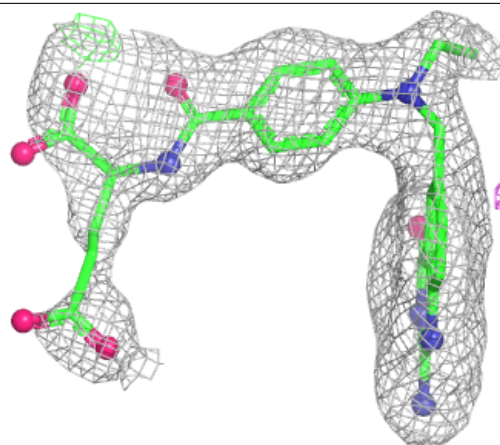
**Electron density around CB3 A 702:**

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

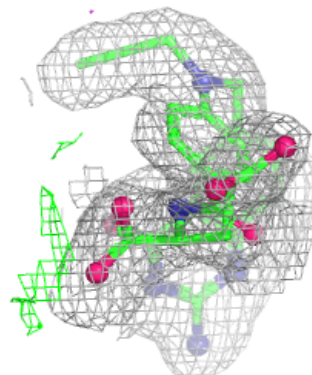
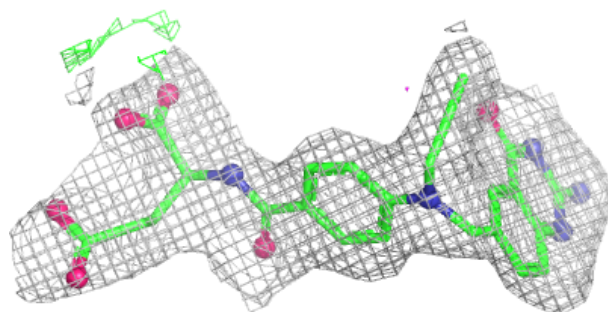
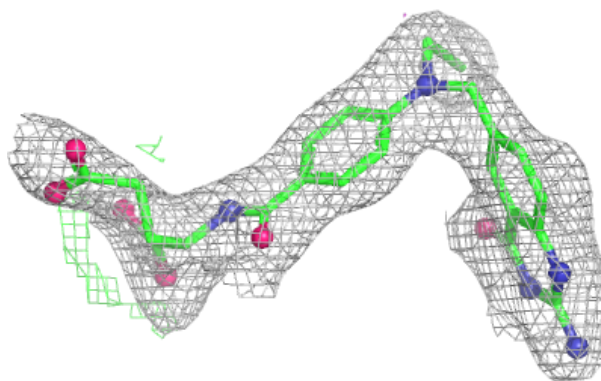


**Electron density around CB3 B 702:**

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

**Electron density around CB3 C 702:**

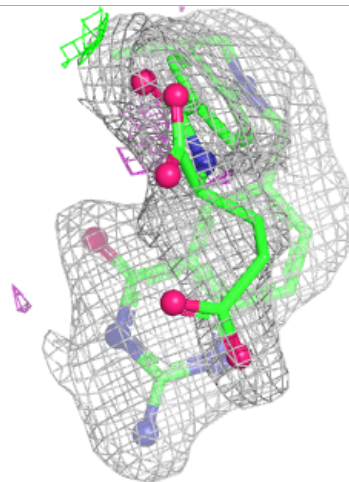
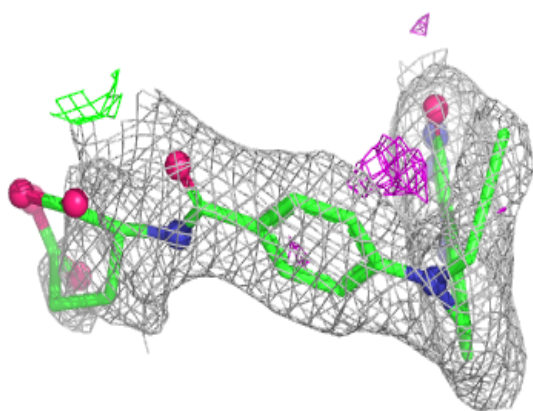
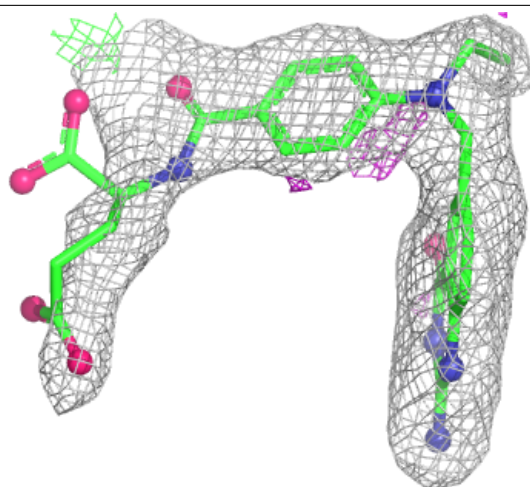
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





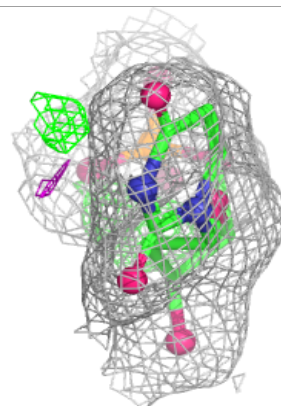
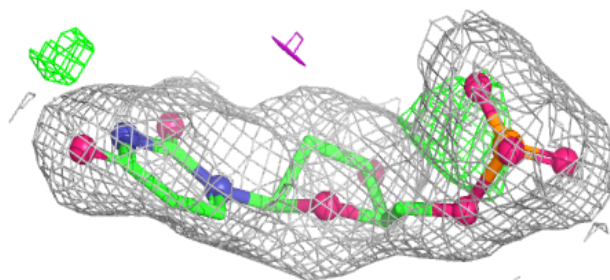
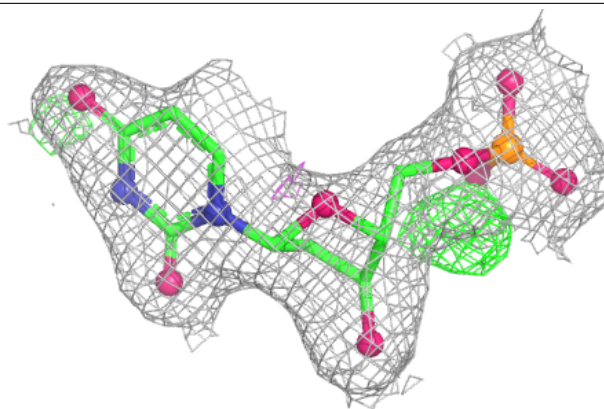
**Electron density around CB3 D 702:**

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



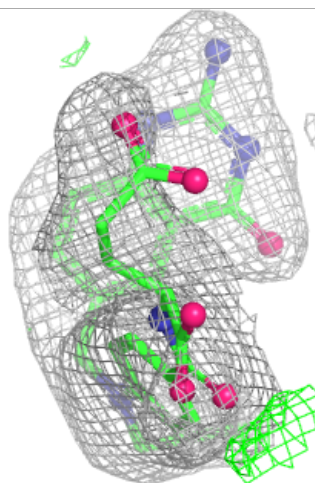
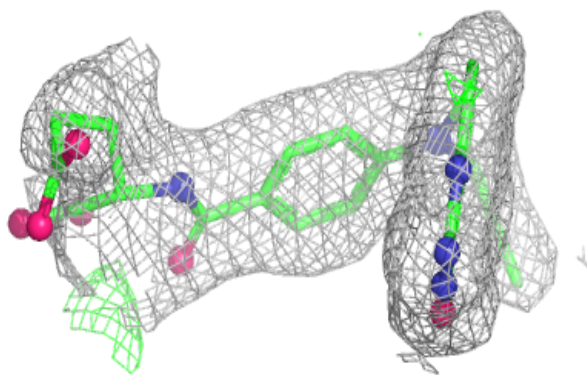
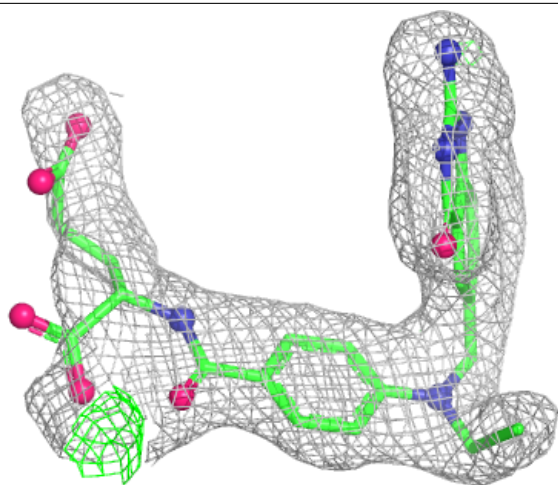
**Electron density around UMP A 701:**

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



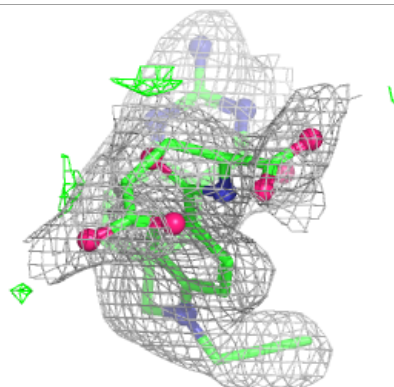
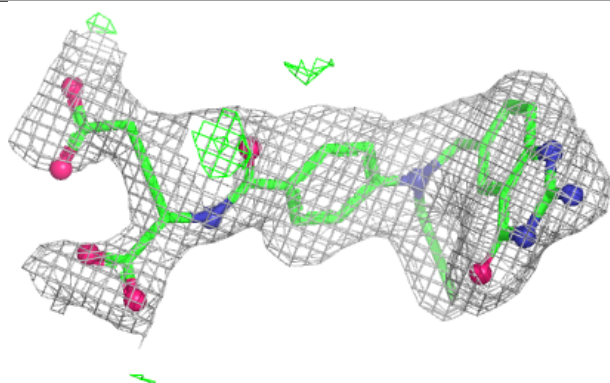
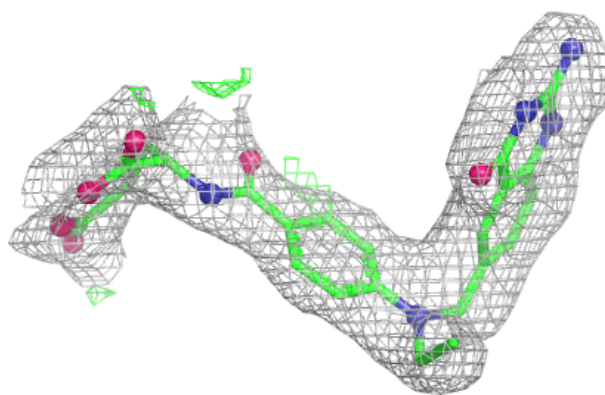
**Electron density around CB3 F 702:**

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



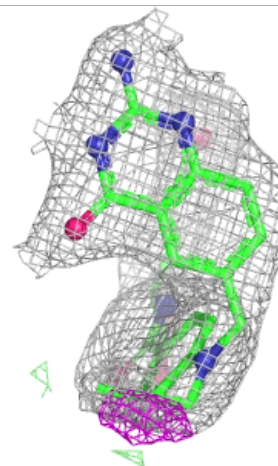
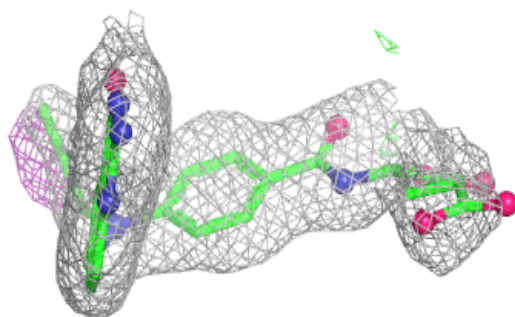
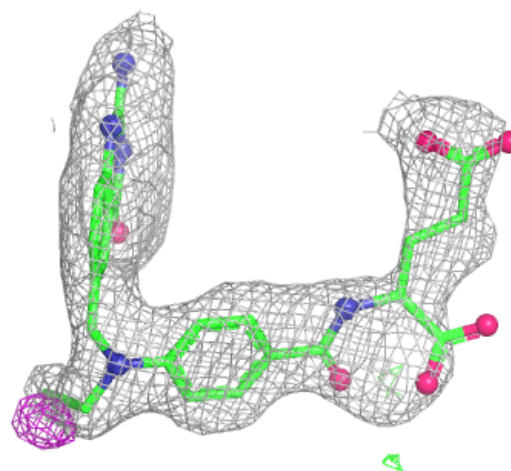
**Electron density around CB3 G 702:**

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



**Electron density around CB3 H 702:**

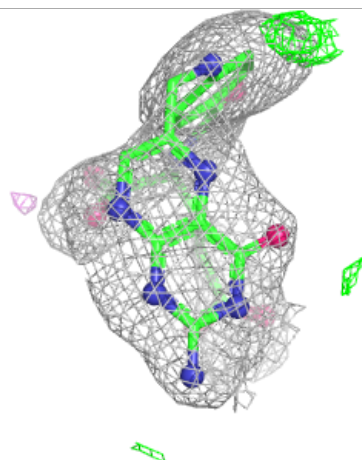
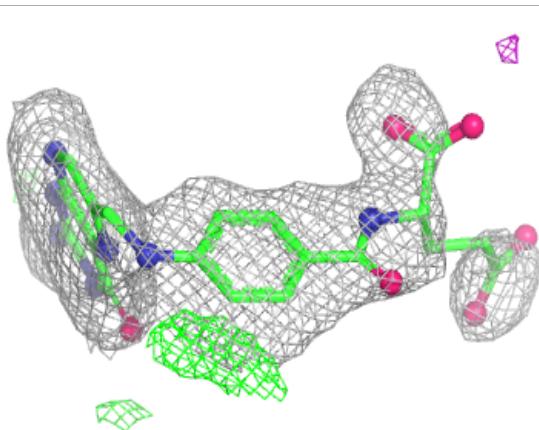
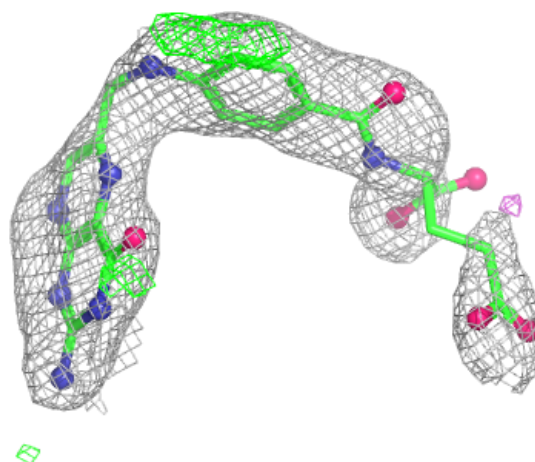
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





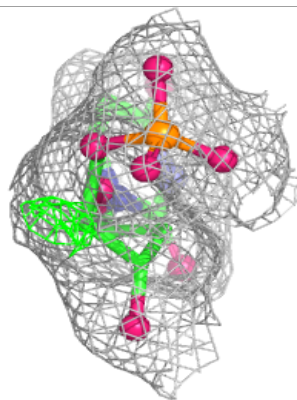
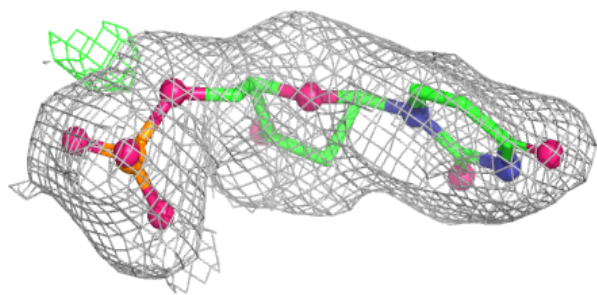
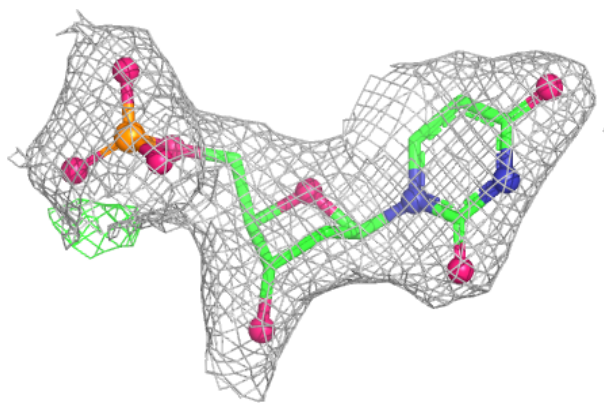
**Electron density around FOL A 703:**

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



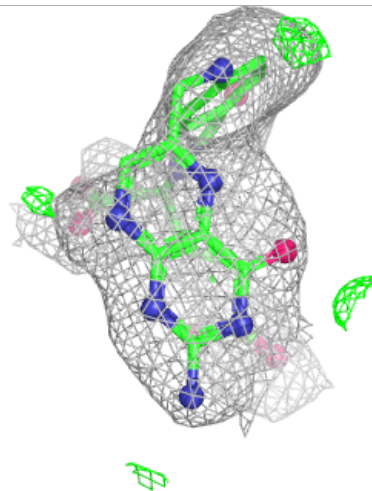
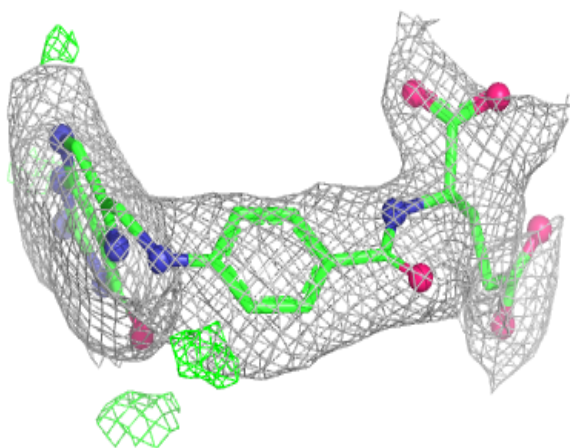
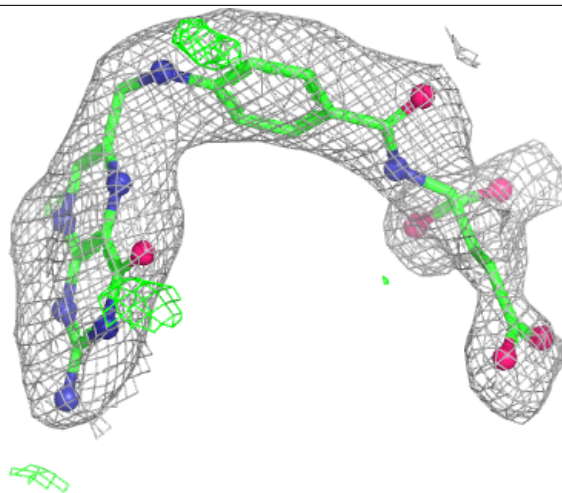
**Electron density around UMP C 701:**

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



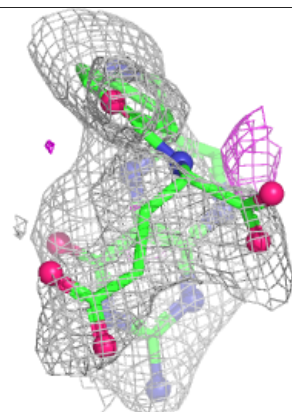
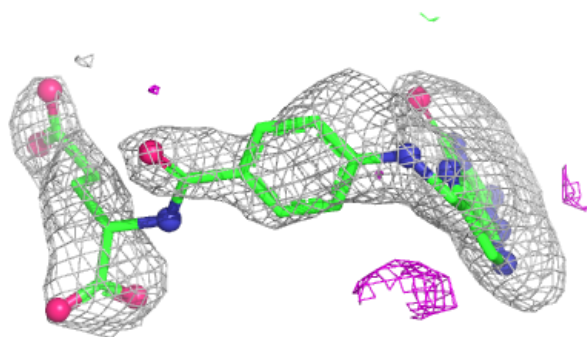
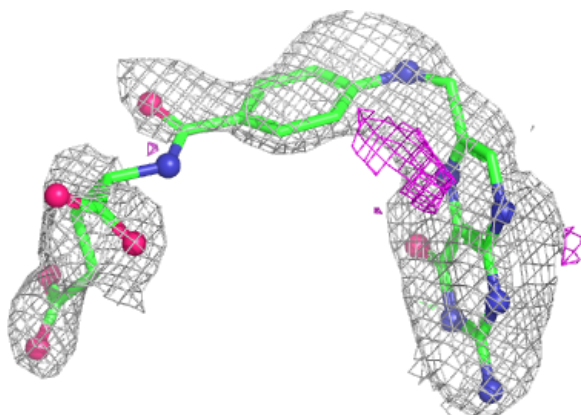
**Electron density around FOL C 703:**

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

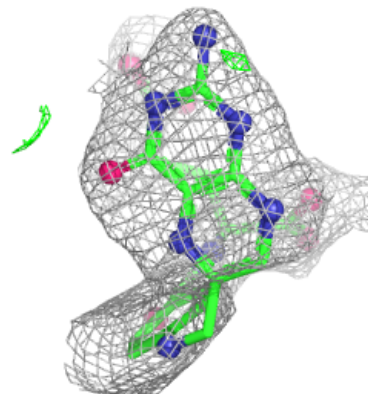
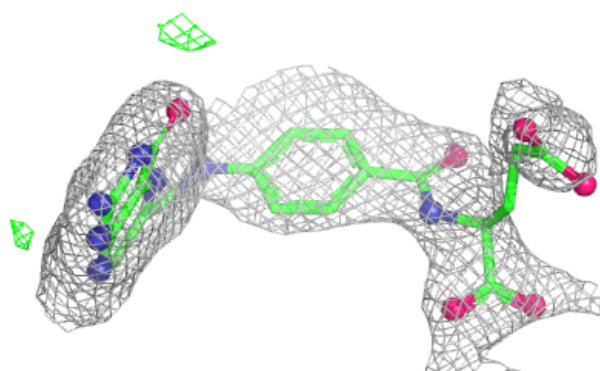
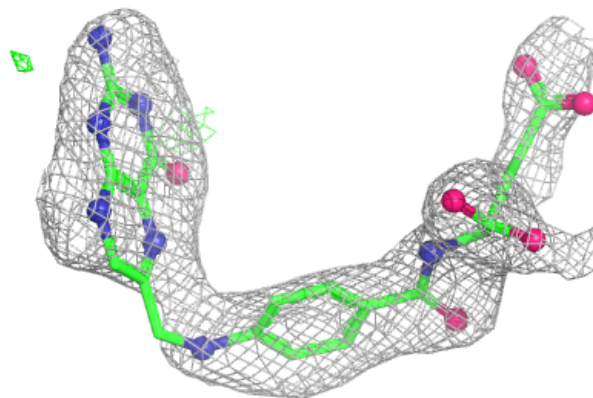


**Electron density around FOL D 703:**

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

**Electron density around FOL E 703:**

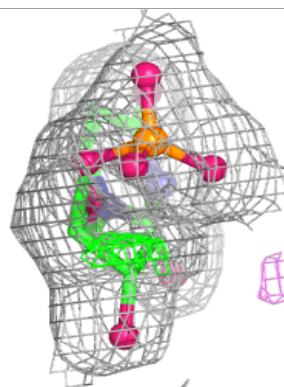
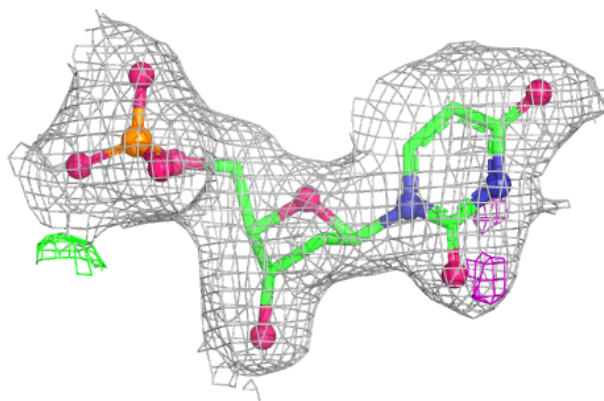
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



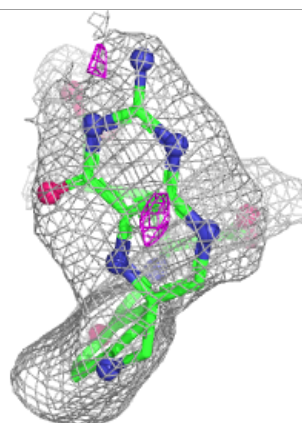
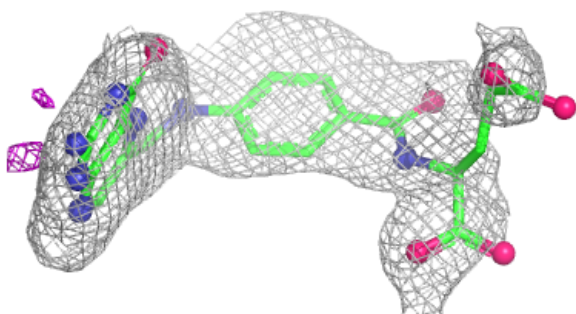
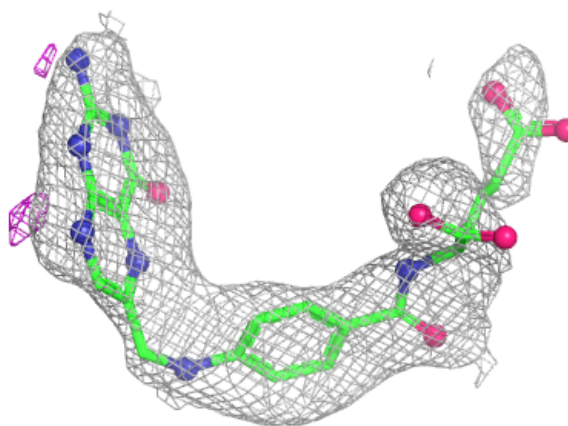


**Electron density around UMP D 701:**

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

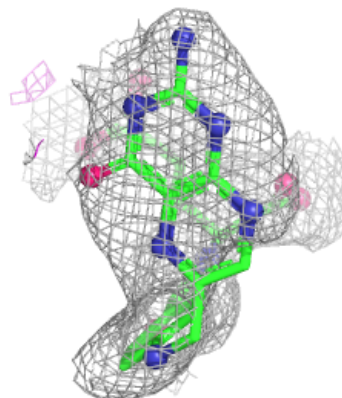
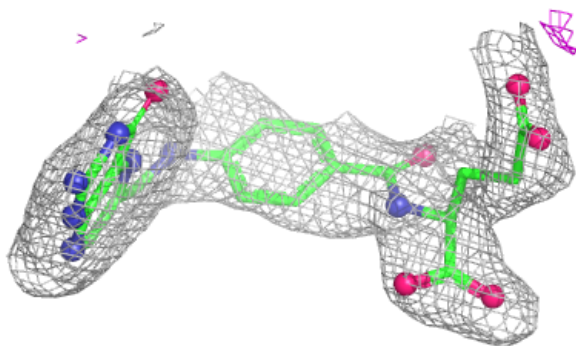
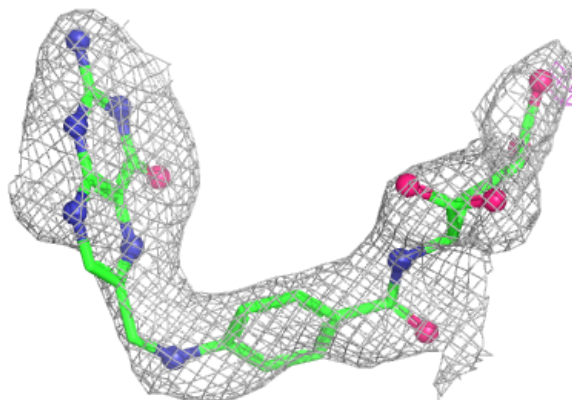
**Electron density around FOL G 703:**

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

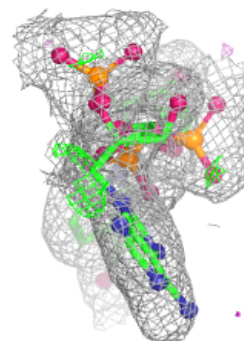
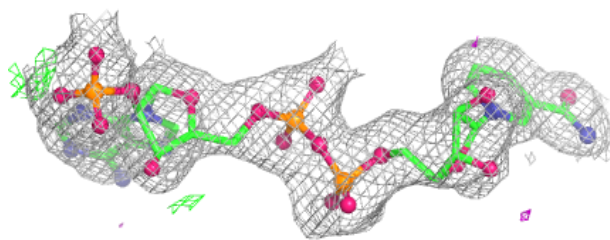
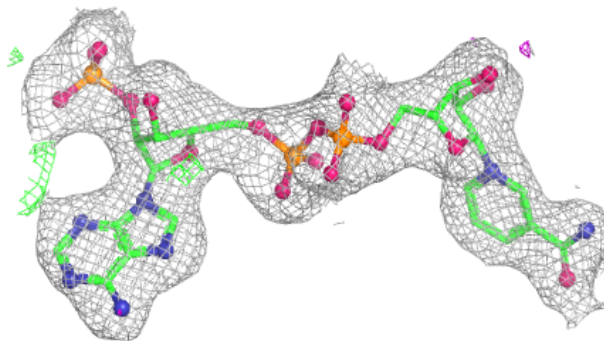


**Electron density around FOL H 703:**

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

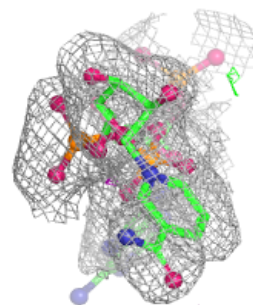
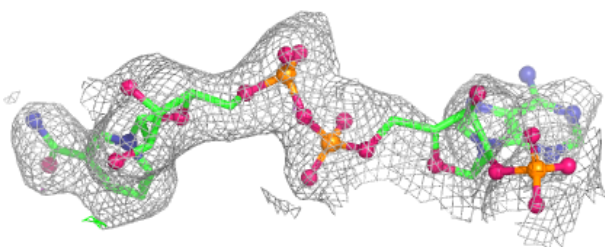
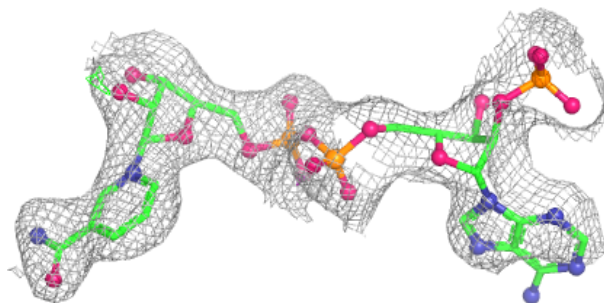
**Electron density around NDP A 704:**

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

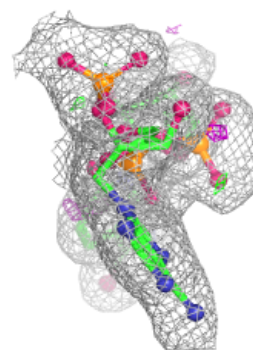
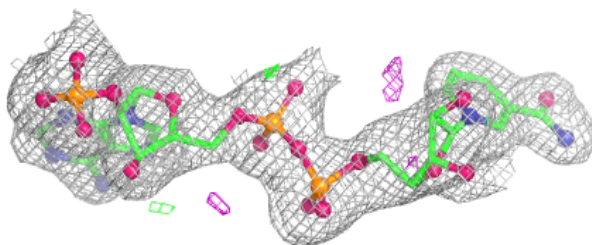
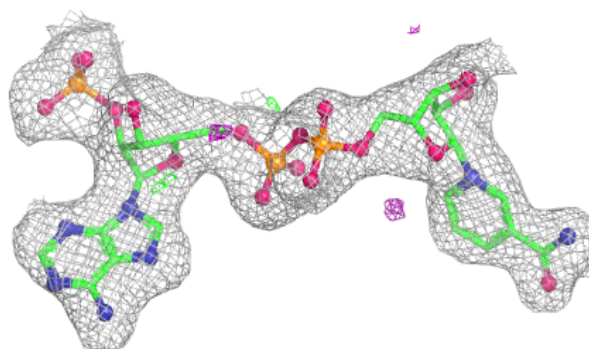


**Electron density around NDP B 704:**

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

**Electron density around NDP C 704:**

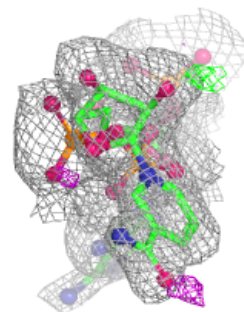
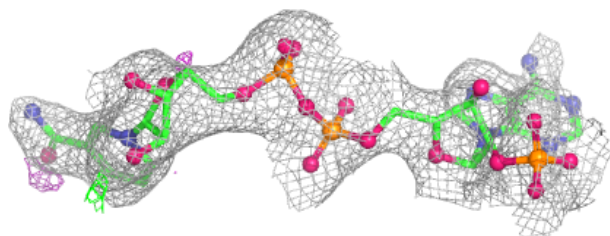
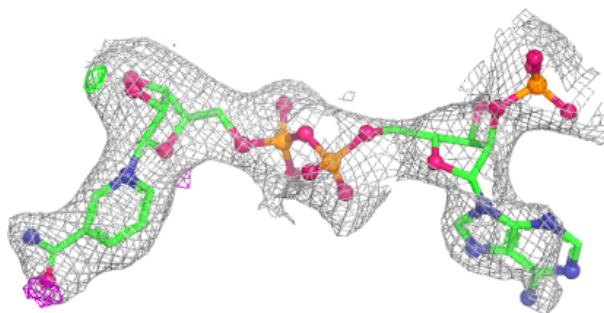
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



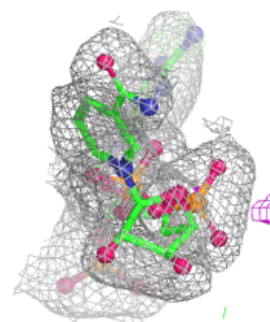
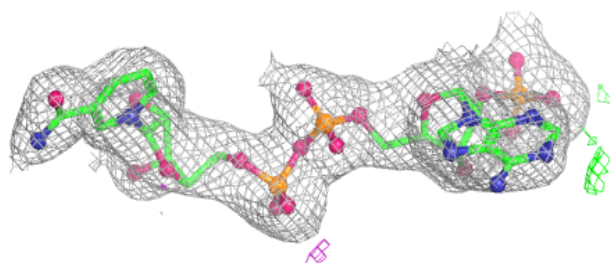
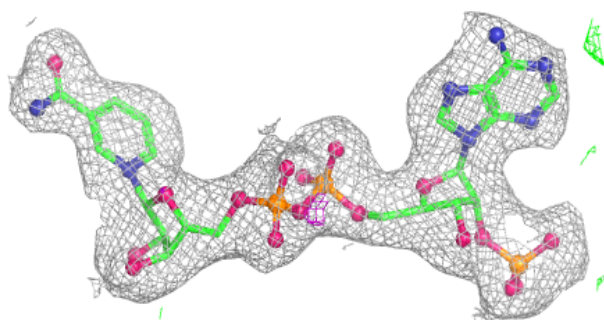


**Electron density around NDP D 704:**

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

**Electron density around NDP E 704:**

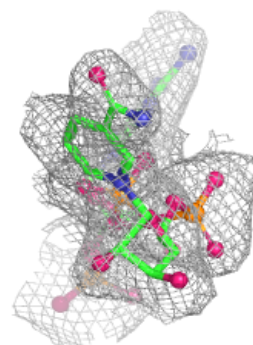
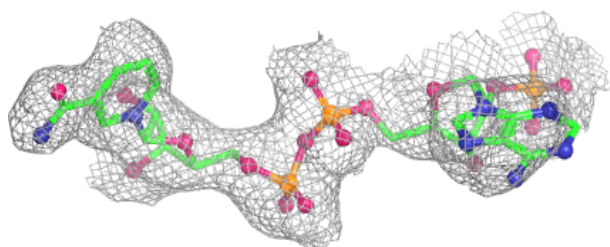
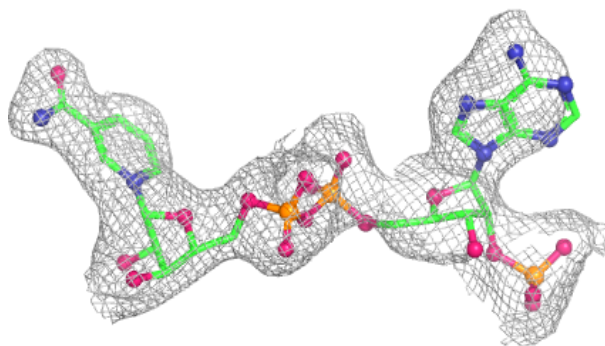
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



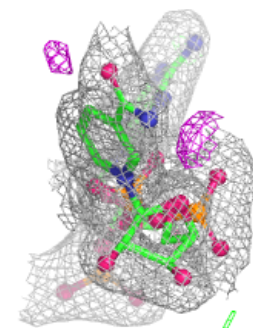
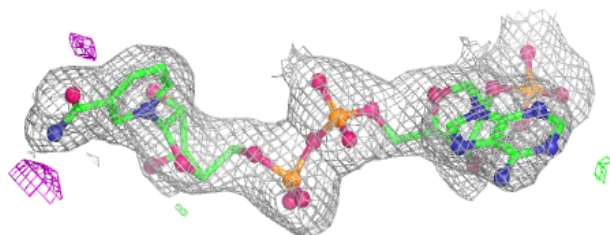
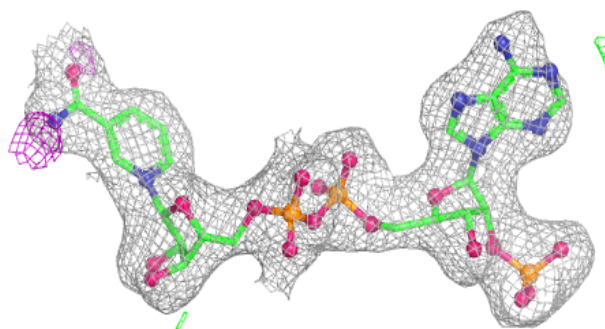


**Electron density around NDP F 704:**

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

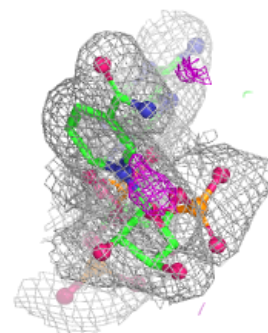
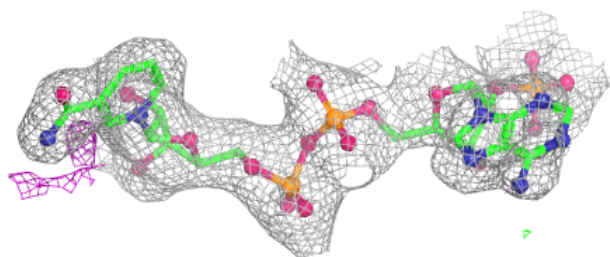
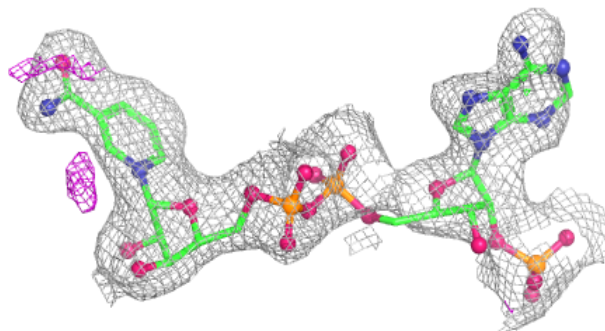
**Electron density around NDP G 704:**

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

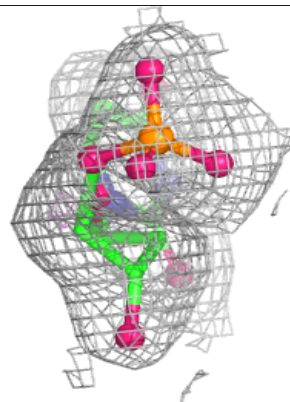
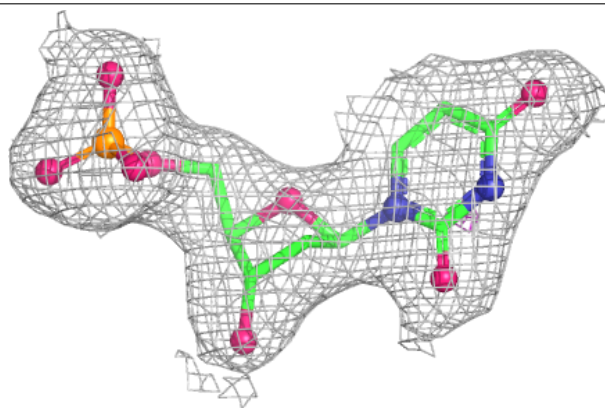


**Electron density around NDP H 704:**

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

**Electron density around UMP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.