



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 12:24 PM UTC

PDB ID : 4KYA / pdb_00004kya
Title : Crystal structure of non-classical TS inhibitor 3 in complex with Toxoplasma gondii TS-DHFR
Authors : Sharma, H.; Anderson, K.S.
Deposited on : 2013-05-28
Resolution : 3.26 Å(reported)

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

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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

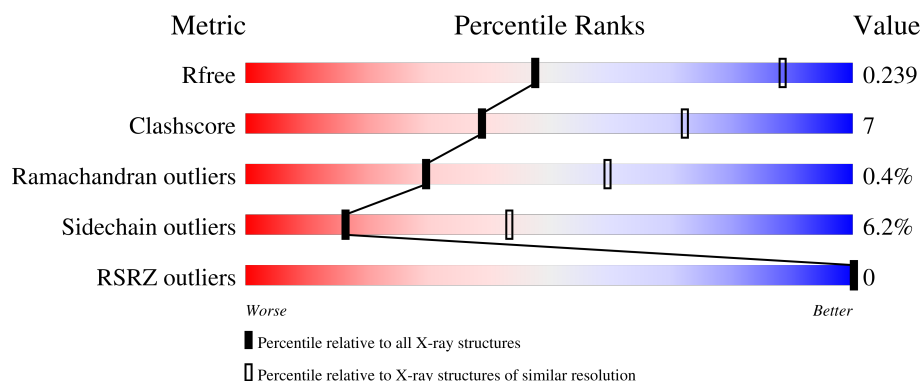
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	566	
1	B	566	
1	C	566	
1	D	566	
1	E	566	

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Mol	Chain	Length	Quality of chain
1	F	566	 68% 17% • 13%
1	G	566	 72% 17% • 10%
1	H	566	 69% 16% • 13%

2 Entry composition

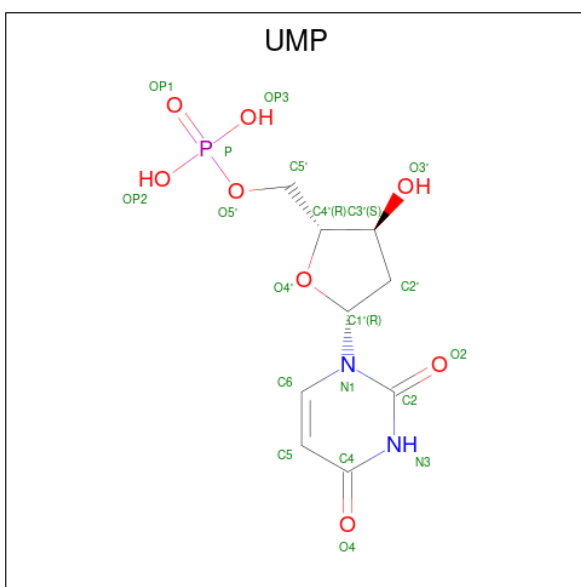
There are 5 unique types of molecules in this entry. The entry contains 33184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

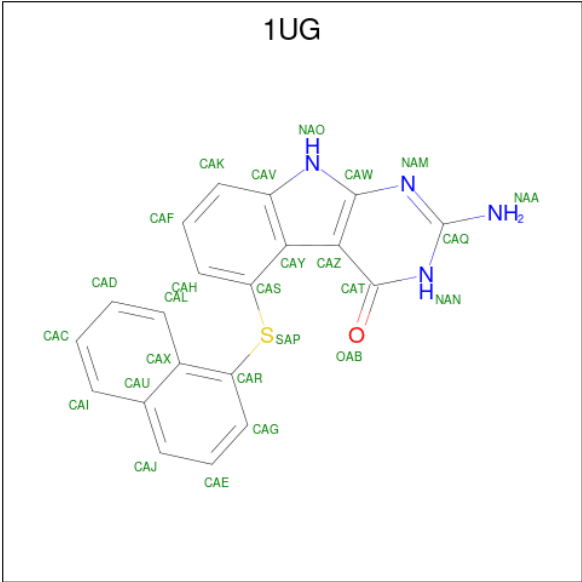
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	B	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	C	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	D	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	E	510	Total	C	N	O	S	0	2	0
	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

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



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 2-Amino-5-(1-naphthylsulfanyl)-3,9-dihydro-4H-pyrimido[4,5-b]indol-4-one (CCD ID: 1UG) (formula: C₂₀H₁₄N₄OS).

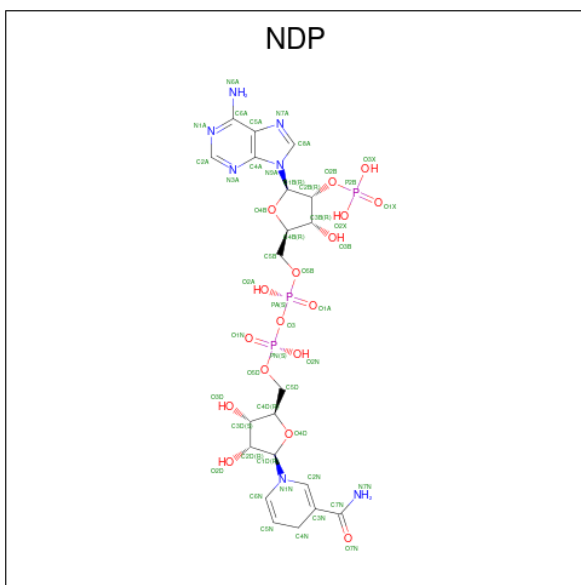


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	B	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	C	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	D	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	E	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	F	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	G	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	H	1	Total	C	N	O	S	0	0
			26	20	4	1	1		

- Molecule 4 is FOLIC ACID (CCD ID: FOL) (formula: C₁₉H₁₉N₇O₆).



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

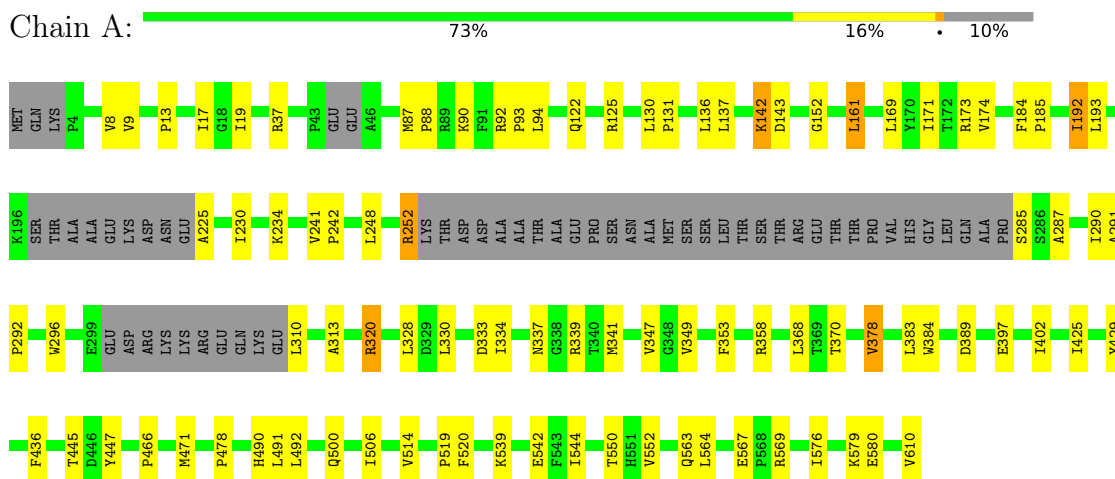


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	H	1	Total 48	C 21	N 7	O 17	P 3	0	0

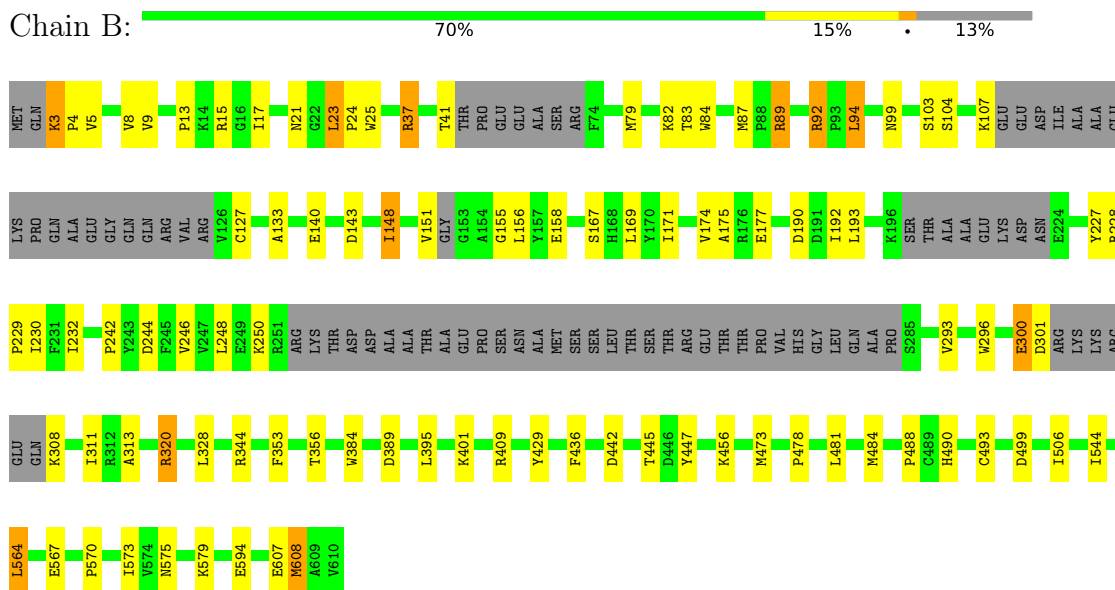
3 Residue-property plots

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



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E381	THR	L161	MET
L382	THR	L169	GLN
L383	PRO	L169	LYS
L384	VAL	Y170	P4
L385	HIS	I171	V5
L386	GLY	T172	V8
D389	LEU	R173	V9
	GLN	V174	V9
	ALA	A175	A10
E397	PRO	R176	A10
R409	S285	F184	I17
	S286		
I425	A287	I192	T30
Y429	I290	L193	R37
	A291		
	P292		
R434	W296	K196	P43
H435		SER	GLU
F436	E299	THR	GLU
	GLU	ALA	A46
T445	ASP	ALA	G80
D446	ARG	LYS	R81
Y447	LYS	ASP	
P466	LYS	ASN	P88
	LYS	GLU	R89
	ARG	A225	K90
M471	GLU		
	GLN	I230	L94
P478	LYS		
H490	GLU	K234	R97
	L310		L98
Q500	A313	P242	N99
		Y243	
I506	R320	L248	S103
V514	L328	E252	Q122
P519	D329	R125	
F520	L330	THR	
	I334	ASP	L130
V535		ALA	P131
	R339	ALA	
K539	V349	ALA	L136
E542		THR	L137
F543	F353	GLU	E140
I544	G354	PRO	Y141
		SER	K142
T550		ASN	D143
	R358	ALA	S144
H551		MET	
V552	L368	SER	I148
	T369	SER	
Q563	T370	LEU	V151
L564		THR	G152
	W375	SER	
E567		THR	L156
	V378	ARG	Y157
		GLU	

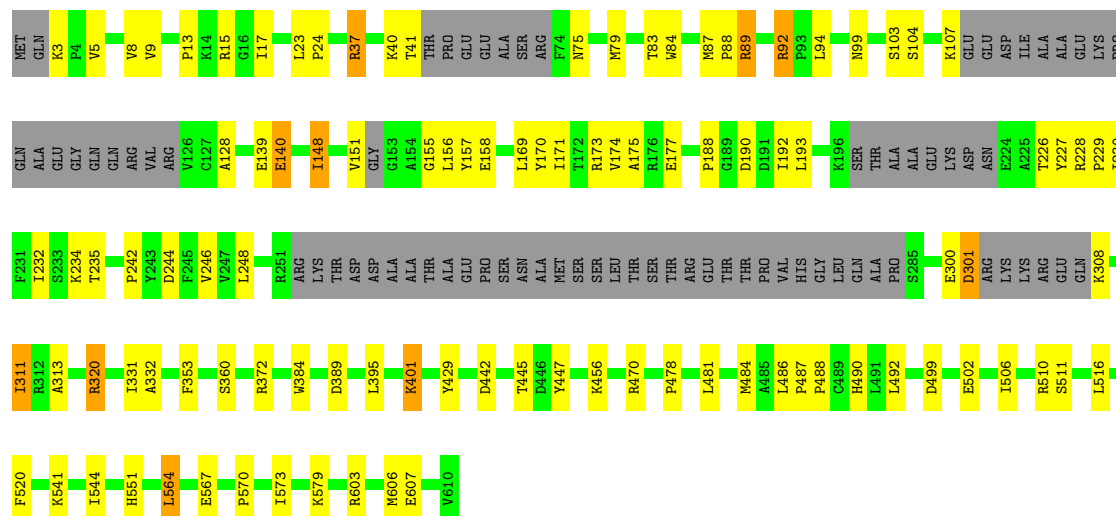
- | | | | | |
|------|------|------|------|------|
| M531 | GLU | Y227 | GLN | MET |
| | | R228 | ALA | |
| I544 | K308 | P229 | GLU | K3 |
| | E309 | I230 | GLY | P4 |
| L560 | I310 | F231 | GLN | Y5 |
| L564 | I311 | I232 | GLN | |
| | R312 | S233 | ARG | W8 |
| | A313 | K234 | VAL | N9 |
| | | T235 | ARG | |
| | R320 | | V126 | P13 |
| | | P242 | C127 | |
| | L328 | Y243 | | I17 |
| | | D244 | A133 | |
| | I331 | F245 | | M21 |
| | A332 | V246 | L136 | G22 |
| | D333 | V247 | | L23 |
| | | L248 | E139 | P24 |
| | N337 | | E140 | V25 |
| | | R251 | | |
| | F353 | ARG | D143 | R37 |
| | G354 | LVS | S144 | |
| | S360 | ASP | | K40 |
| | L395 | ASP | I148 | T41 |
| | | ALA | V151 | THR |
| | R409 | THR | GLY | PRO |
| | | | G153 | GLU |
| | Y429 | GLU | A154 | ALA |
| | | PRO | G155 | SER |
| | F436 | SER | L156 | ARG |
| | | ASN | Y157 | F74 |
| | D442 | ALA | E158 | N75 |
| | | MET | L169 | M79 |
| | T445 | SER | Y170 | |
| | D446 | SER | I171 | W84 |
| | Y447 | LEU | I172 | |
| | | THR | R173 | M87 |
| | K456 | SER | V174 | P88 |
| | | THR | A175 | R89 |
| | P478 | ARG | R176 | |
| | | GLU | E177 | R92 |
| | L481 | THR | | P93 |
| | | THR | P188 | L94 |
| | M484 | PRO | | |
| | | VAL | D191 | N99 |
| | P487 | HIS | I192 | |
| | P488 | GLY | | S103 |
| | C489 | LEU | K196 | S104 |
| | H490 | GLN | SER | |
| | | ALA | THR | K107 |
| | D499 | PRO | ALA | GLU |
| | Q500 | | ALA | GLU |
| | | S285 | | ASP |
| | I506 | E300 | | ILE |
| | R510 | D301 | ASP | ALA |
| | | ARG | ASN | ALA |
| | | LVS | E224 | GLU |
| | L516 | LYS | A225 | LYS |
| | | ASP | T226 | PRO |

- | | | | | | | | | | | | | |
|------|------|------|------|------|-----|-----|-----|-----|-----|------|------|------|
| HIS | GLY | LEU | GLN | ALA | PRO | S285 | A289 | L280 | A291 | P282 | V283 | L284 | A285 | W286 | E289 | ASP | ARG | LYS | LYS | ARG | GLU | GLN | GLY | GLN | GLY | GLU | L310 | A313 | R320 | E324 | L330 | I334 | D343 | V349 | G354 | R358 | L368 | T369 | T370 | V378 | L383 | W384 | D389 | P397 | | | | | | | |
| F184 | P185 | I192 | L193 | K196 | SER | THR | ALA | ALA | GLU | ASP | ASN | GLU | A225 | I230 | F231 | I232 | S233 | K234 | P242 | Y243 | D244 | F245 | V246 | V247 | L248 | R252 | LYS | THR | ASP | ASP | ALA | ALA | THR | ALA | GLU | PRO | SER | ASN | ALA | MET | SER | LEU | THR | SER | THR | ARG | GLU | THR | P373 | V174 | P175 |
| GLN | LYS | P4 | V5 | V8 | V9 | P13 | I17 | T30 | R37 | F43 | GLU | GLU | A46 | G60 | M67 | P88 | R89 | X90 | F91 | R92 | F93 | L94 | Q122 | R125 | L130 | P131 | L136 | L137 | K142 | D143 | S144 | I148 | G152 | L156 | L161 | L169 | R173 | V174 | A175 | | | | | | | | | | | | |



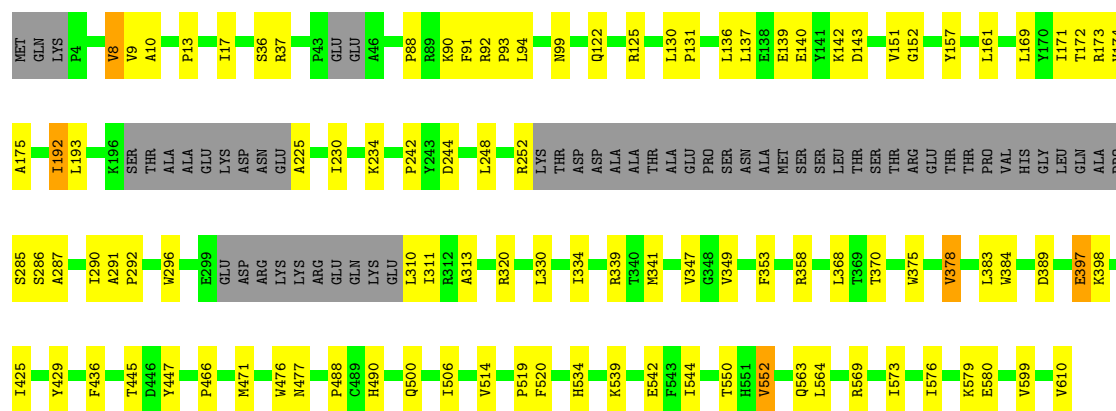
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain F: 68% 17% 13%



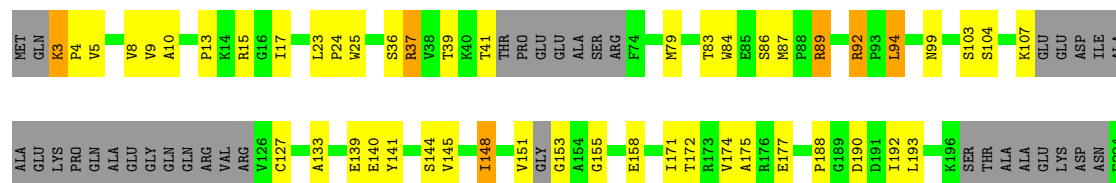
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

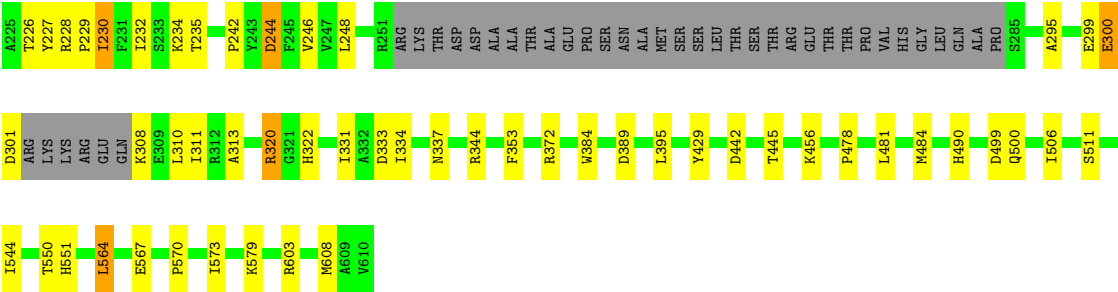
Chain G: 72% 17% 10%



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain H: 69% 16% 13%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.53Å 145.08Å 176.61Å 90.07° 89.96° 90.07°	Depositor
Resolution (Å)	46.66 – 3.26 46.66 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.66-3.26) 98.5 (46.66-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.9_1692, REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.241 0.182 , 0.239	Depositor DCC
R_{free} test set	4073 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 3.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l 0.448 for -h,k,-l 0.448 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33184	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, NDP, FOL, 1UG

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	0.30	0/4196	0.74	0/5683
1	B	0.29	0/4043	0.75	4/5473 (0.1%)
1	C	0.30	0/4196	0.73	0/5683
1	D	0.29	0/4043	0.74	2/5473 (0.0%)
1	E	0.30	0/4196	0.73	0/5683
1	F	0.30	0/4043	0.75	2/5473 (0.0%)
1	G	0.30	0/4196	0.74	2/5683 (0.0%)
1	H	0.30	0/4043	0.75	2/5473 (0.0%)
All	All	0.30	0/32956	0.74	12/44624 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	477	ASN	CA-C-N	5.54	125.89	119.47
1	G	477	ASN	C-N-CA	5.54	125.89	119.47
1	B	23	LEU	CA-C-N	5.48	124.83	118.85
1	B	23	LEU	C-N-CA	5.48	124.83	118.85
1	D	92	ARG	CA-C-N	-5.47	113.00	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4096	0	4058	49	0
1	B	3948	0	3910	53	0
1	C	4096	0	4058	59	0
1	D	3948	0	3910	63	0
1	E	4096	0	4058	55	0
1	F	3948	0	3910	61	0
1	G	4096	0	4058	59	0
1	H	3948	0	3910	53	0
2	A	20	0	11	0	0
2	B	20	0	11	0	0
2	C	20	0	11	0	0
2	D	20	0	11	0	0
2	E	20	0	11	0	0
2	F	20	0	11	0	0
2	G	20	0	11	0	0
2	H	20	0	11	0	0
3	A	26	0	14	2	0
3	B	26	0	14	2	0
3	C	26	0	14	4	0
3	D	26	0	14	2	0
3	E	26	0	14	5	0
3	F	26	0	14	4	0
3	G	26	0	14	3	0
3	H	26	0	14	2	0
4	A	32	0	17	1	0
4	B	32	0	17	4	0
4	C	32	0	17	1	0
4	D	32	0	17	4	0
4	E	32	0	17	1	0
4	F	32	0	17	4	0
4	G	32	0	17	5	0
4	H	32	0	17	4	0
5	A	48	0	26	3	0
5	B	48	0	26	4	0
5	C	48	0	26	3	0
5	D	48	0	26	4	0
5	E	48	0	26	3	0
5	F	48	0	26	5	0
5	G	48	0	26	3	0
5	H	48	0	26	4	0
All	All	33184	0	32416	447	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 7.

The worst 5 of 447 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:608:MET:HE2	3:H:702:1UG:H6	1.60	0.82
1:H:481:LEU:HA	1:H:484:MET:HE2	1.64	0.79
1:E:313:ALA:O	1:E:320:ARG:NH2	2.14	0.79
1:F:481:LEU:HA	1:F:484:MET:HE2	1.65	0.78
1:D:481:LEU:HA	1:D:484:MET:HE2	1.66	0.77

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	502/566 (89%)	482 (96%)	19 (4%)	1 (0%)	43	70
1	B	478/566 (84%)	447 (94%)	29 (6%)	2 (0%)	30	59
1	C	502/566 (89%)	485 (97%)	15 (3%)	2 (0%)	30	59
1	D	478/566 (84%)	448 (94%)	27 (6%)	3 (1%)	21	51
1	E	502/566 (89%)	486 (97%)	15 (3%)	1 (0%)	43	70
1	F	478/566 (84%)	448 (94%)	28 (6%)	2 (0%)	30	59
1	G	502/566 (89%)	485 (97%)	15 (3%)	2 (0%)	30	59
1	H	478/566 (84%)	449 (94%)	25 (5%)	4 (1%)	16	44
All	All	3920/4528 (87%)	3730 (95%)	173 (4%)	17 (0%)	30	59

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	429	TYR
1	H	429	TYR
1	E	429	TYR

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Mol	Chain	Res	Type
1	F	429	TYR
1	H	144	SER

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%)	418 (94%)	26 (6%)	18	45
1	B	431/491 (88%)	404 (94%)	27 (6%)	16	43
1	C	444/491 (90%)	418 (94%)	26 (6%)	18	45
1	D	431/491 (88%)	404 (94%)	27 (6%)	16	43
1	E	444/491 (90%)	415 (94%)	29 (6%)	15	42
1	F	431/491 (88%)	405 (94%)	26 (6%)	17	44
1	G	444/491 (90%)	418 (94%)	26 (6%)	18	45
1	H	431/491 (88%)	402 (93%)	29 (7%)	15	41
All	All	3500/3928 (89%)	3284 (94%)	216 (6%)	16	43

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	161	LEU
1	F	190	ASP
1	H	190	ASP
1	E	252	ARG
1	E	539	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	432	GLN
1	F	168	HIS
1	H	500	GLN

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Mol	Chain	Res	Type
1	E	435	HIS
1	E	575	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
2	UMP	E	701	-	21,21,21	1.60	3 (14%)	30,31,31	2.10	11 (36%)
2	UMP	D	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.07	12 (40%)
3	1UG	D	702	-	30,30,30	2.04	10 (33%)	38,44,44	2.29	16 (42%)
5	NDP	C	704	-	51,52,52	1.34	5 (9%)	71,80,80	1.60	12 (16%)
5	NDP	B	704	-	51,52,52	1.37	6 (11%)	71,80,80	1.58	9 (12%)
2	UMP	C	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.09	11 (36%)
3	1UG	A	702	-	30,30,30	2.12	11 (36%)	38,44,44	2.22	15 (39%)
2	UMP	B	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.06	12 (40%)
5	NDP	H	704	-	51,52,52	1.37	6 (11%)	71,80,80	1.56	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FOL	F	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.75	9 (20%)
5	NDP	A	704	-	51,52,52	1.35	6 (11%)	71,80,80	1.60	11 (15%)
2	UMP	A	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.09	11 (36%)
4	FOL	G	703	-	34,34,34	1.21	3 (8%)	43,47,47	1.80	9 (20%)
5	NDP	D	704	-	51,52,52	1.39	6 (11%)	71,80,80	1.57	6 (8%)
4	FOL	A	703	-	34,34,34	1.20	3 (8%)	43,47,47	1.83	10 (23%)
4	FOL	D	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.74	9 (20%)
4	FOL	B	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.76	9 (20%)
3	1UG	H	702	-	30,30,30	2.02	10 (33%)	38,44,44	2.32	16 (42%)
2	UMP	F	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.04	12 (40%)
3	1UG	E	702	-	30,30,30	2.04	10 (33%)	38,44,44	2.12	14 (36%)
3	1UG	C	702	-	30,30,30	2.08	10 (33%)	38,44,44	2.10	14 (36%)
3	1UG	F	702	-	30,30,30	2.06	10 (33%)	38,44,44	2.13	15 (39%)
4	FOL	H	703	-	34,34,34	1.18	3 (8%)	43,47,47	1.77	10 (23%)
5	NDP	G	704	-	51,52,52	1.34	5 (9%)	71,80,80	1.59	10 (14%)
2	UMP	G	701	-	21,21,21	1.60	3 (14%)	30,31,31	2.09	11 (36%)
3	1UG	G	702	-	30,30,30	2.06	10 (33%)	38,44,44	2.09	14 (36%)
3	1UG	B	702	-	30,30,30	2.02	10 (33%)	38,44,44	2.28	16 (42%)
2	UMP	H	701	-	21,21,21	1.59	3 (14%)	30,31,31	2.06	12 (40%)
4	FOL	E	703	-	34,34,34	1.20	4 (11%)	43,47,47	1.83	10 (23%)
4	FOL	C	703	-	34,34,34	1.19	4 (11%)	43,47,47	1.85	10 (23%)
5	NDP	E	704	-	51,52,52	1.36	6 (11%)	71,80,80	1.60	11 (15%)
5	NDP	F	704	-	51,52,52	1.38	7 (13%)	71,80,80	1.57	7 (9%)

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
2	UMP	E	701	-	-	4/10/22/22	0/2/2/2
2	UMP	D	701	-	-	4/10/22/22	0/2/2/2
3	1UG	D	702	-	-	1/4/4/4	0/5/5/5
5	NDP	C	704	-	-	3/34/77/77	0/5/5/5
5	NDP	B	704	-	-	7/34/77/77	0/5/5/5
2	UMP	C	701	-	-	3/10/22/22	0/2/2/2

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

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	1UG	CAS-SAP	5.27	1.86	1.78
3	D	702	1UG	CAS-SAP	5.24	1.86	1.78
3	H	702	1UG	CAS-SAP	5.16	1.85	1.78
3	B	702	1UG	CAS-SAP	5.14	1.85	1.78
3	C	702	1UG	CAS-SAP	5.12	1.85	1.78

The worst 5 of 362 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	704	NDP	C5A-C4A-N3A	-5.82	118.70	126.72
5	F	704	NDP	C5A-C4A-N3A	-5.77	118.77	126.72
5	D	704	NDP	C5A-C4A-N3A	-5.76	118.78	126.72
5	B	704	NDP	C5A-C4A-N3A	-5.75	118.79	126.72
5	A	704	NDP	C5A-C4A-N3A	-5.74	118.81	126.72

There are no chirality outliers.

5 of 94 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	C	701	UMP	C5'-O5'-P-OP2
2	C	701	UMP	C5'-O5'-P-OP3
2	E	701	UMP	C5'-O5'-P-OP2

There are no ring outliers.

24 monomers are involved in 65 short contacts:

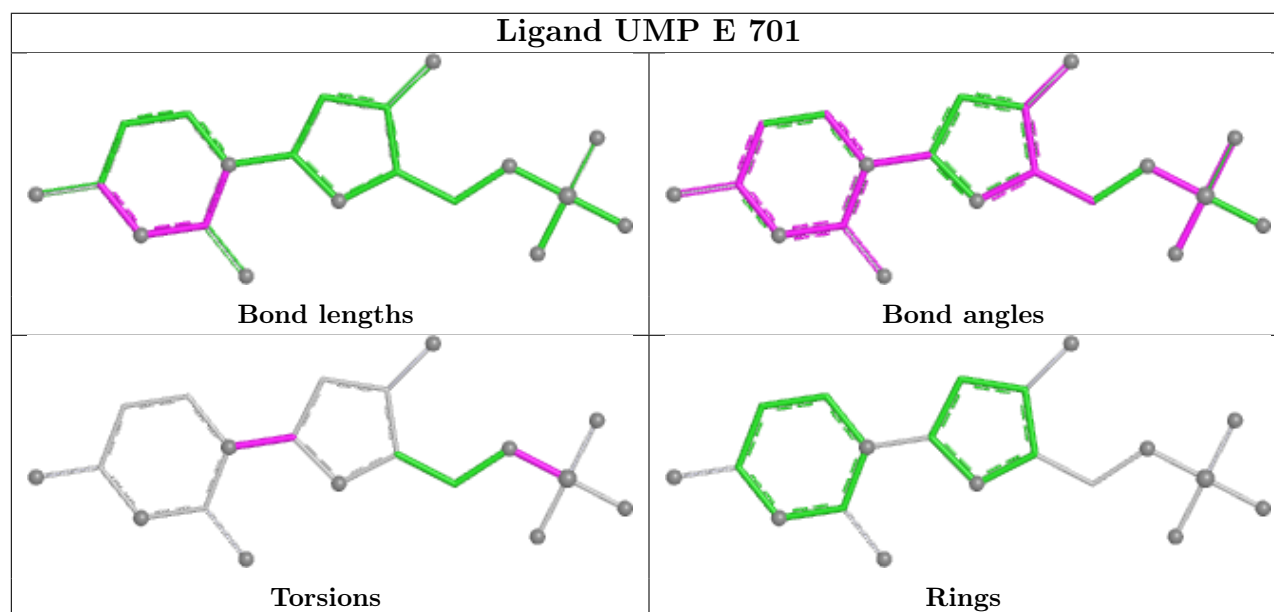
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	702	1UG	2	0
5	C	704	NDP	3	0
5	B	704	NDP	4	0
3	A	702	1UG	2	0
5	H	704	NDP	4	0
4	F	703	FOL	4	0
5	A	704	NDP	3	0
4	G	703	FOL	5	0
5	D	704	NDP	4	0
4	A	703	FOL	1	0
4	D	703	FOL	4	0
4	B	703	FOL	4	0
3	H	702	1UG	2	0
3	E	702	1UG	5	0
3	C	702	1UG	4	0
3	F	702	1UG	4	0
4	H	703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

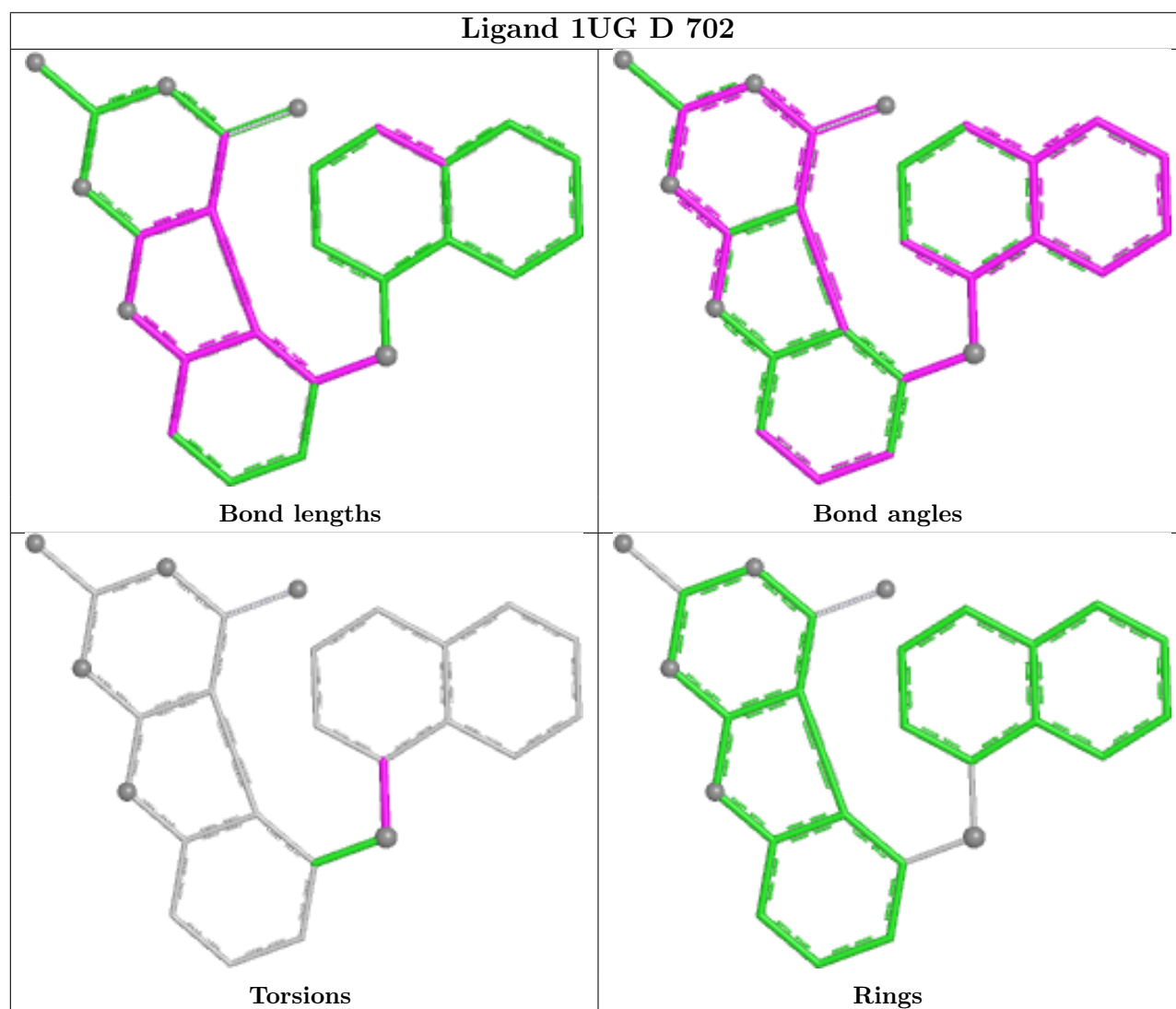
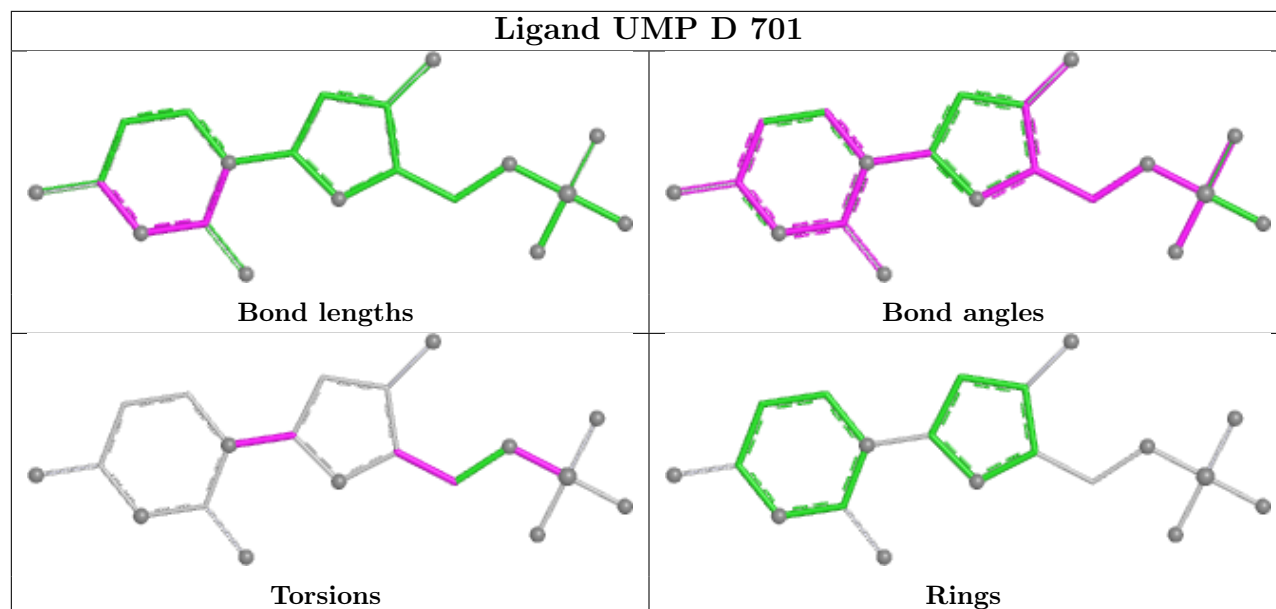
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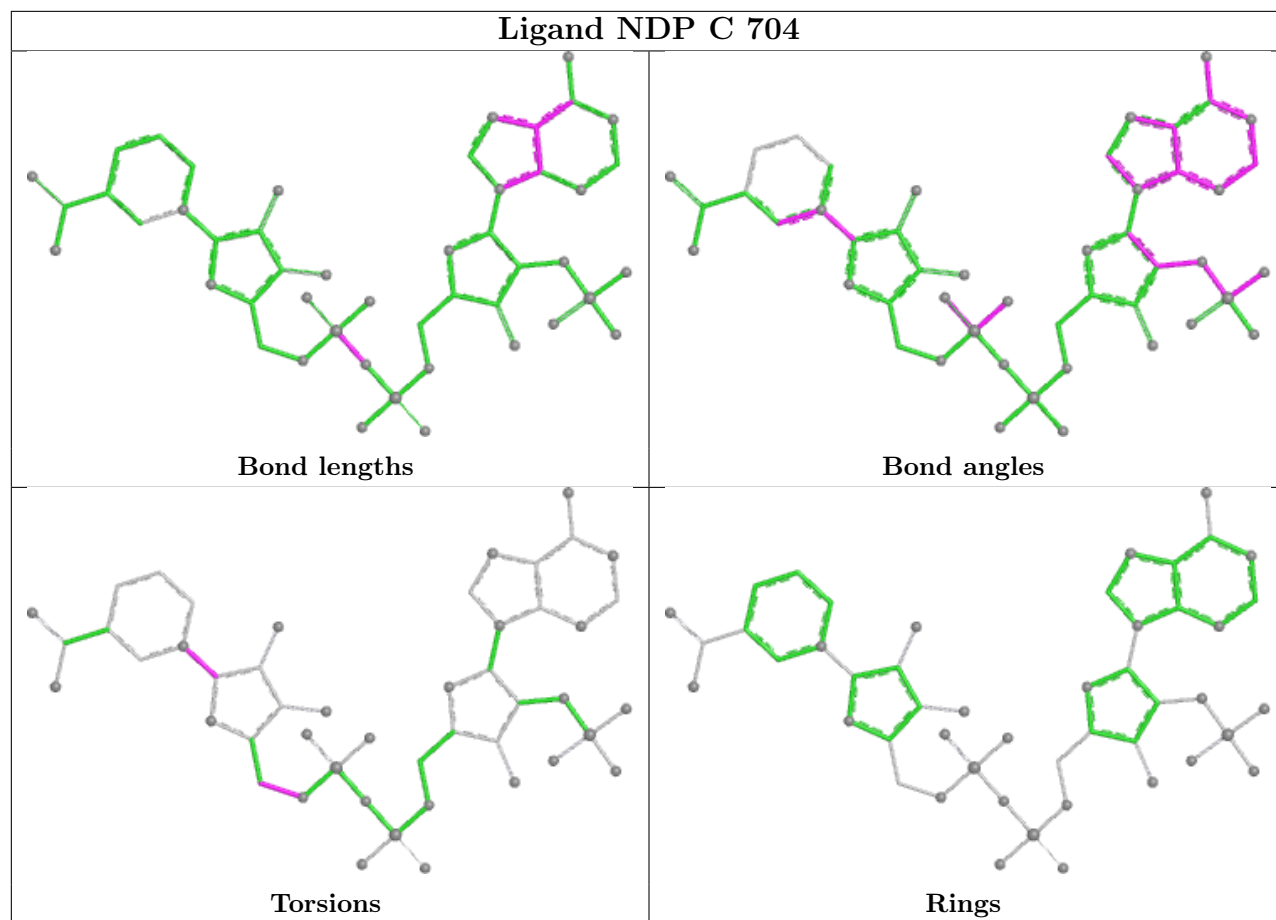
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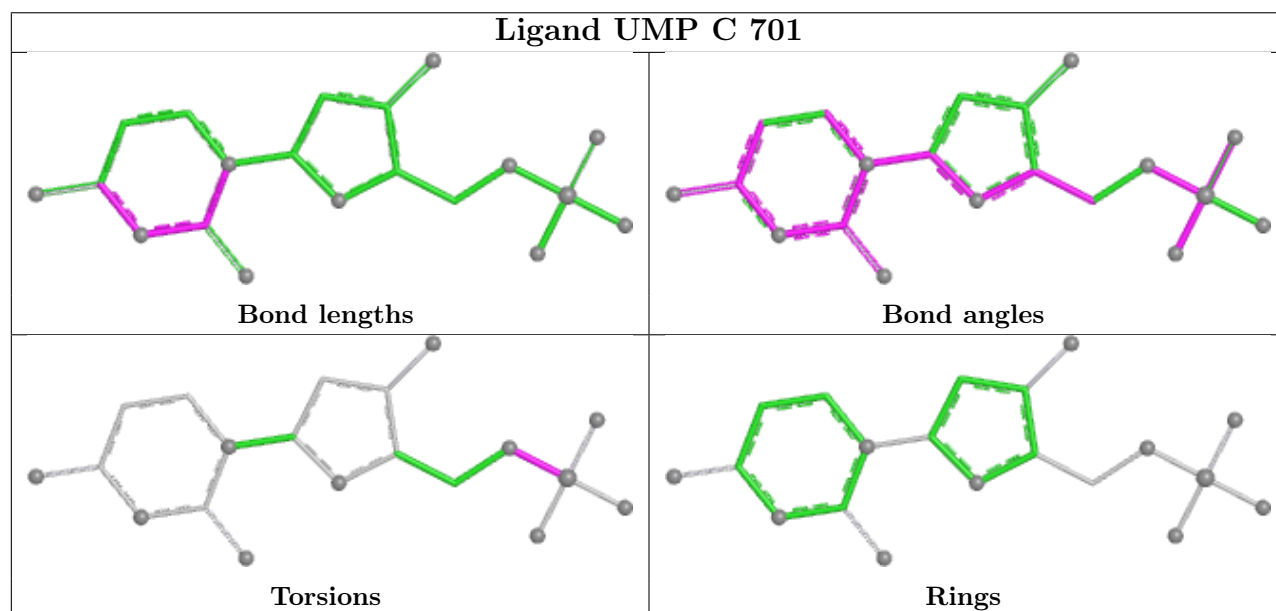
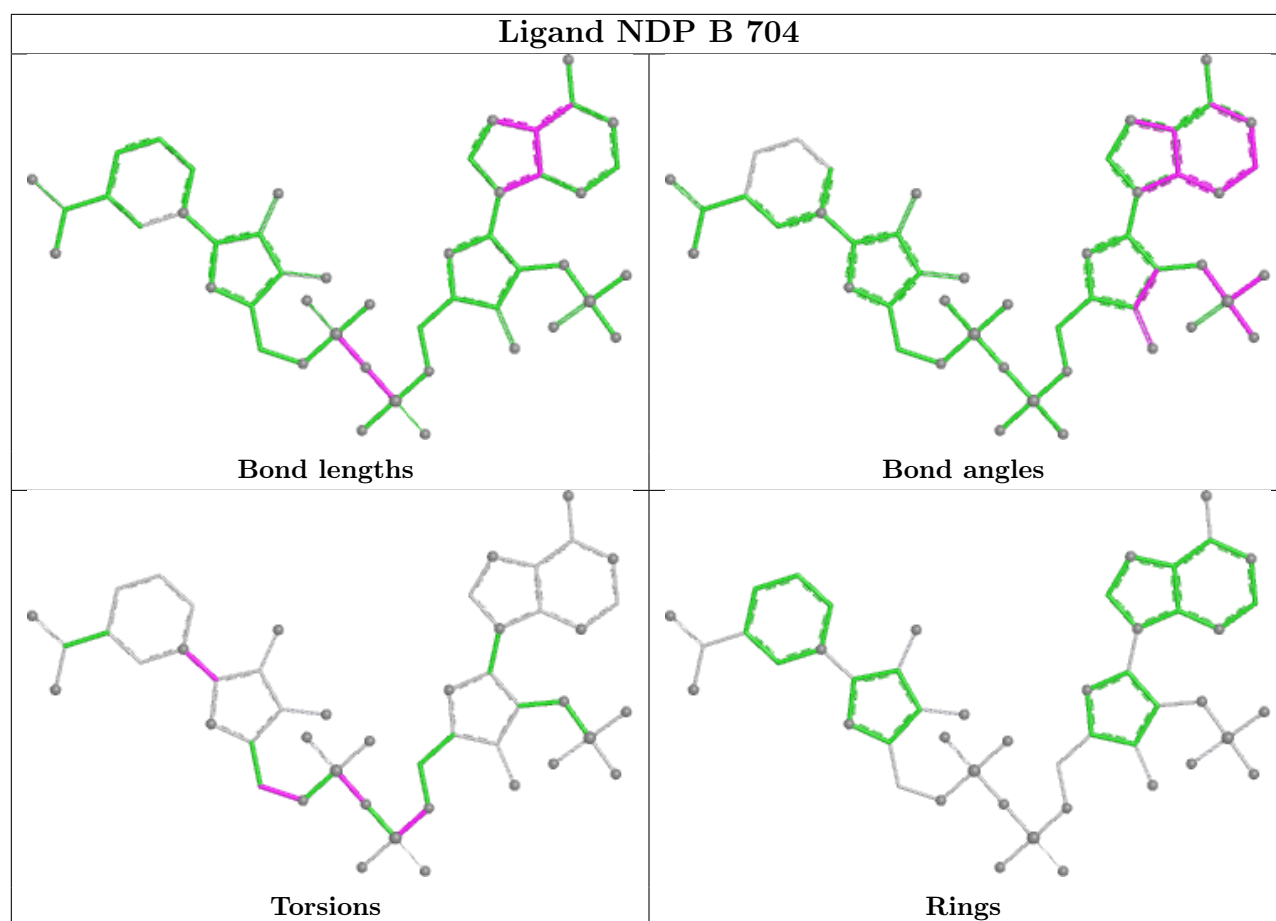
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	704	NDP	3	0
5	F	704	NDP	5	0

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.

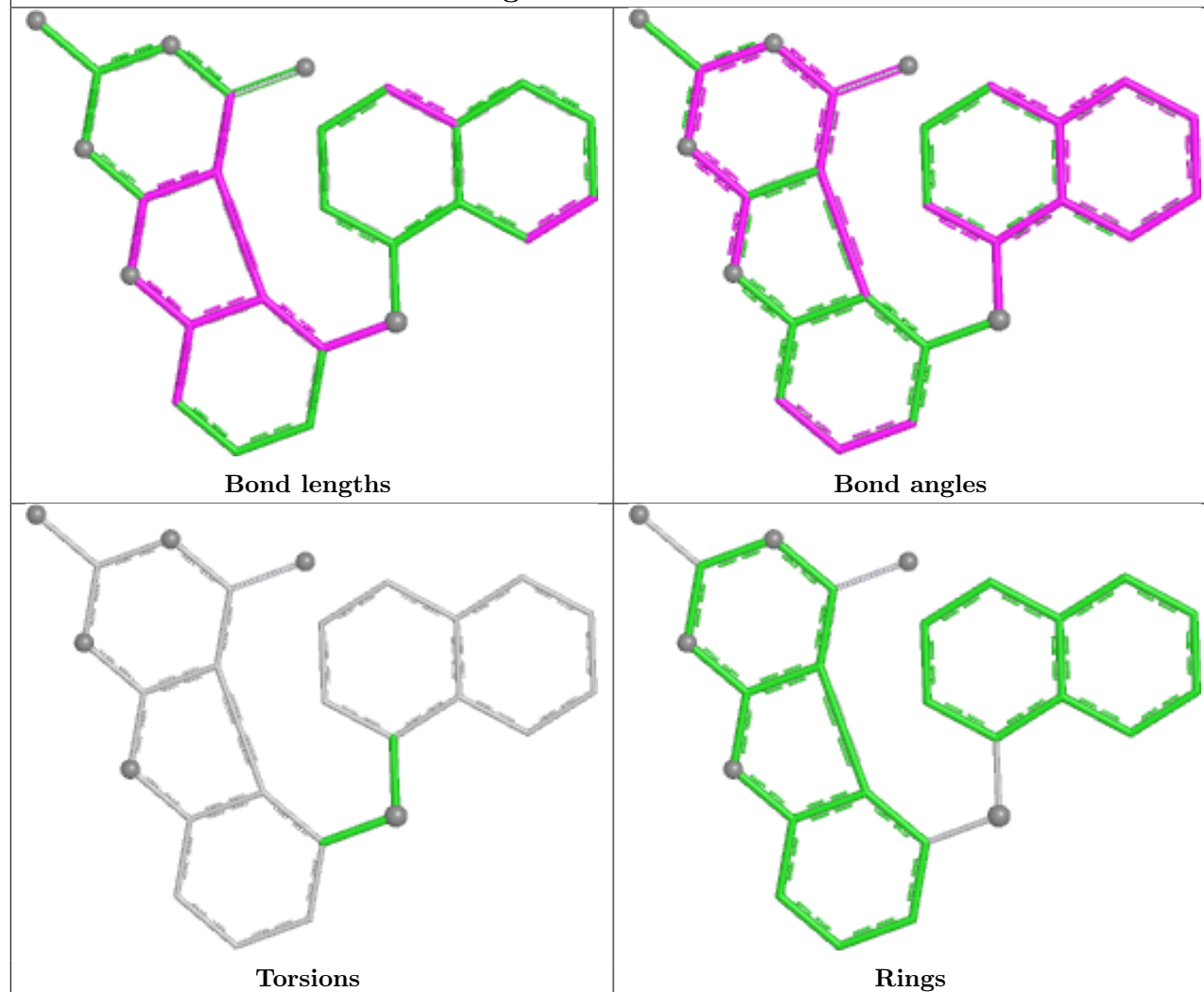




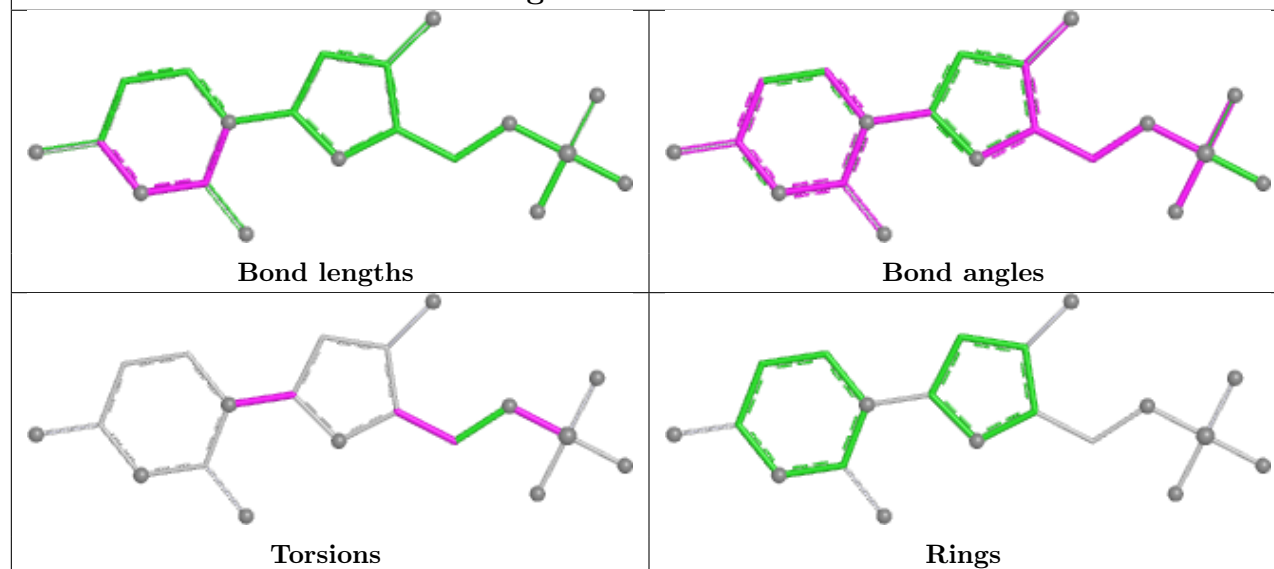


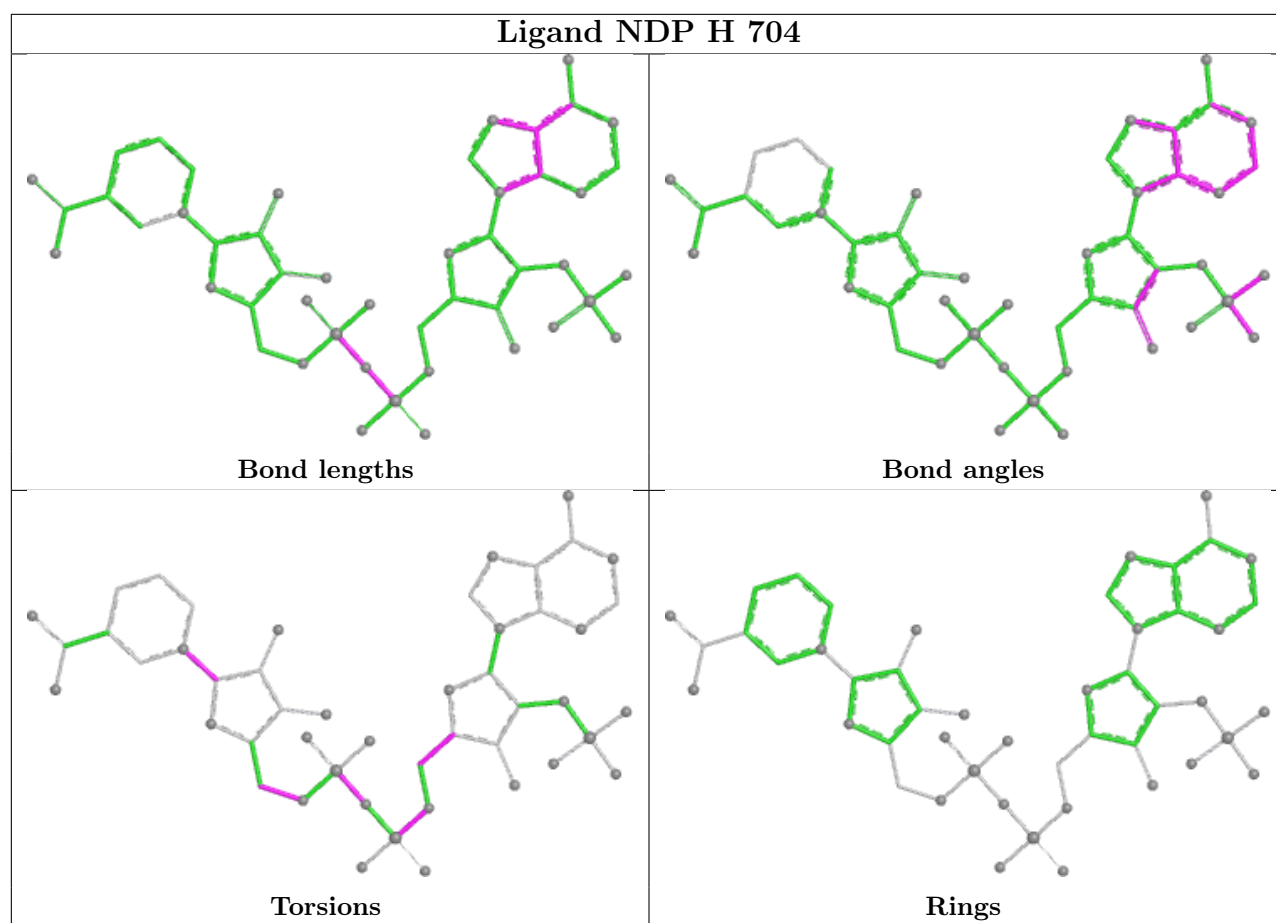


Ligand 1UG A 702

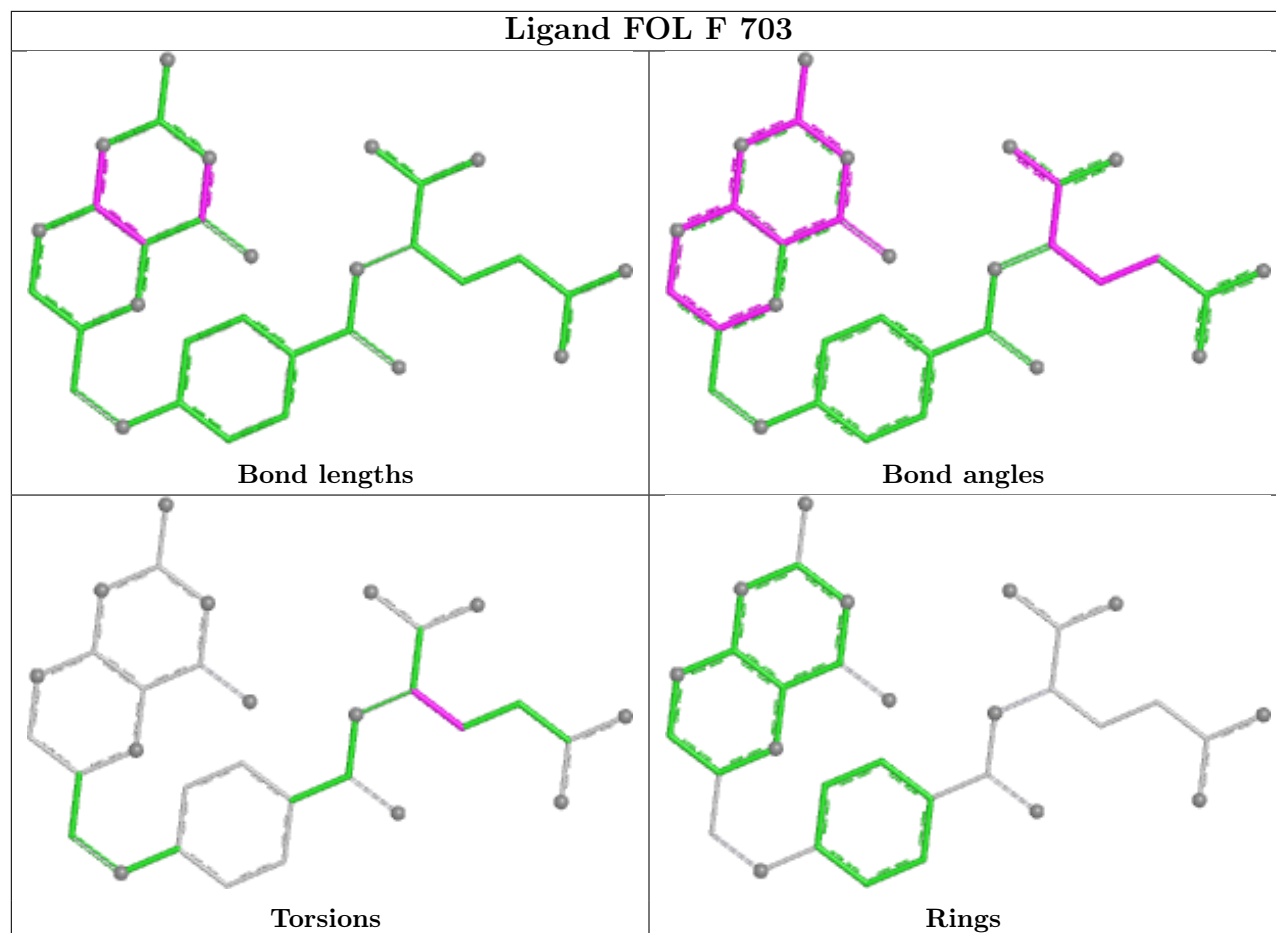


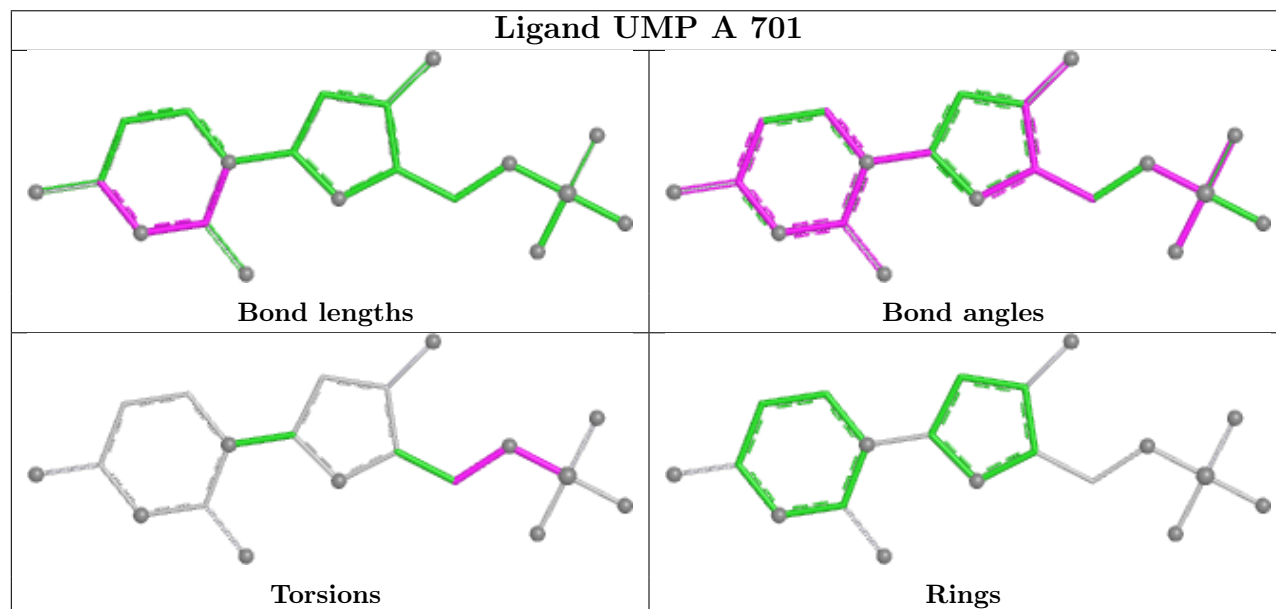
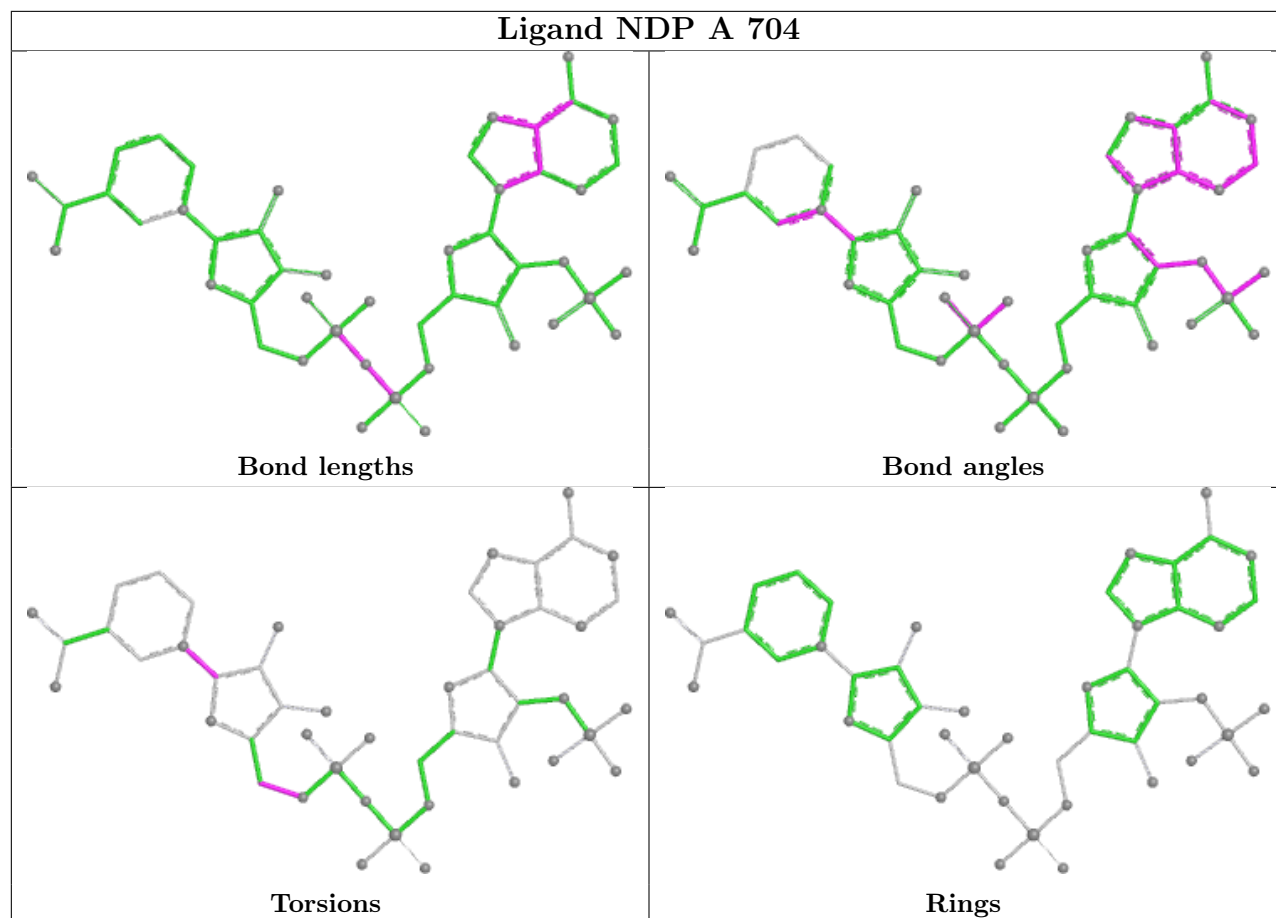
Ligand UMP B 701

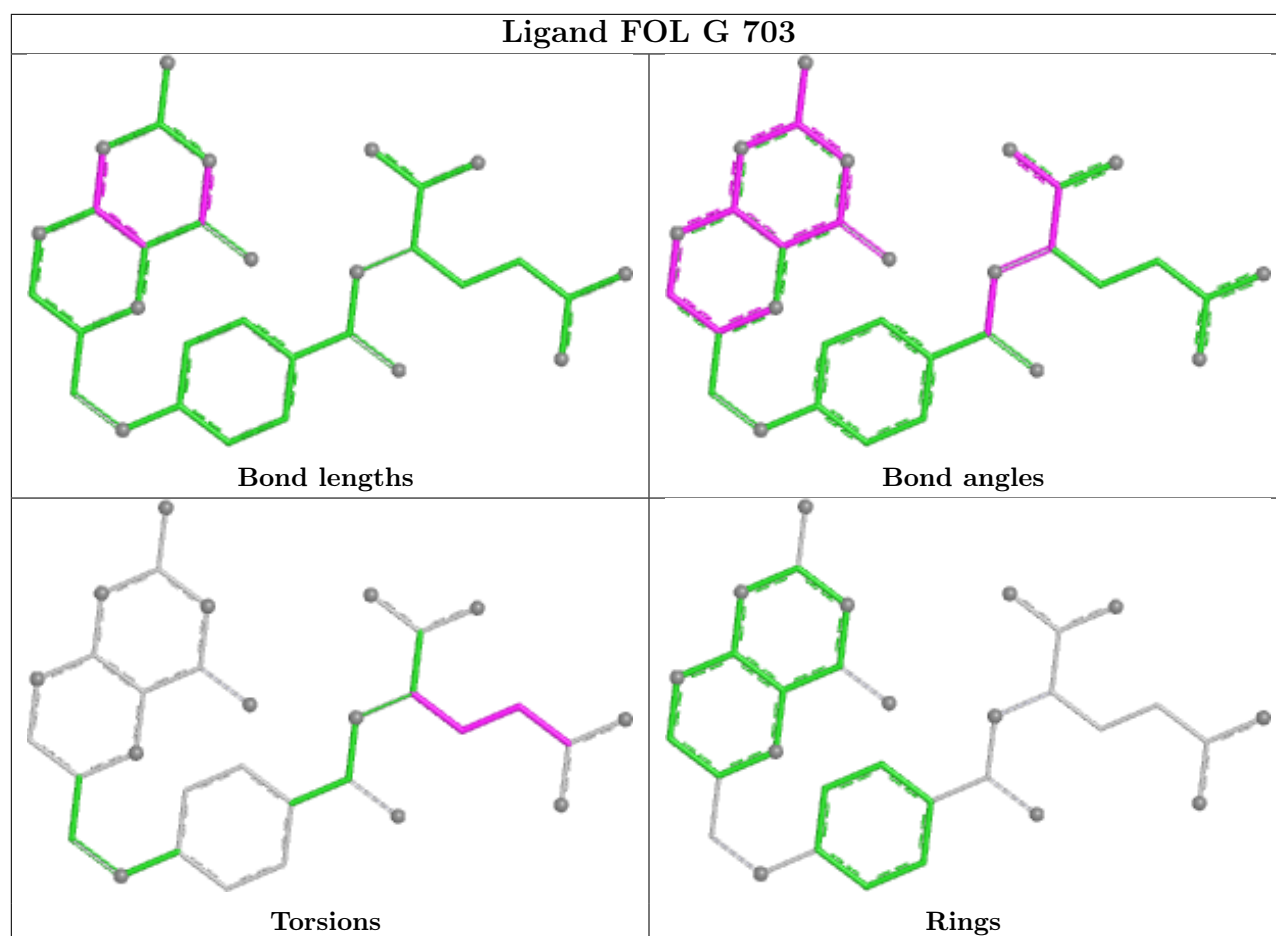


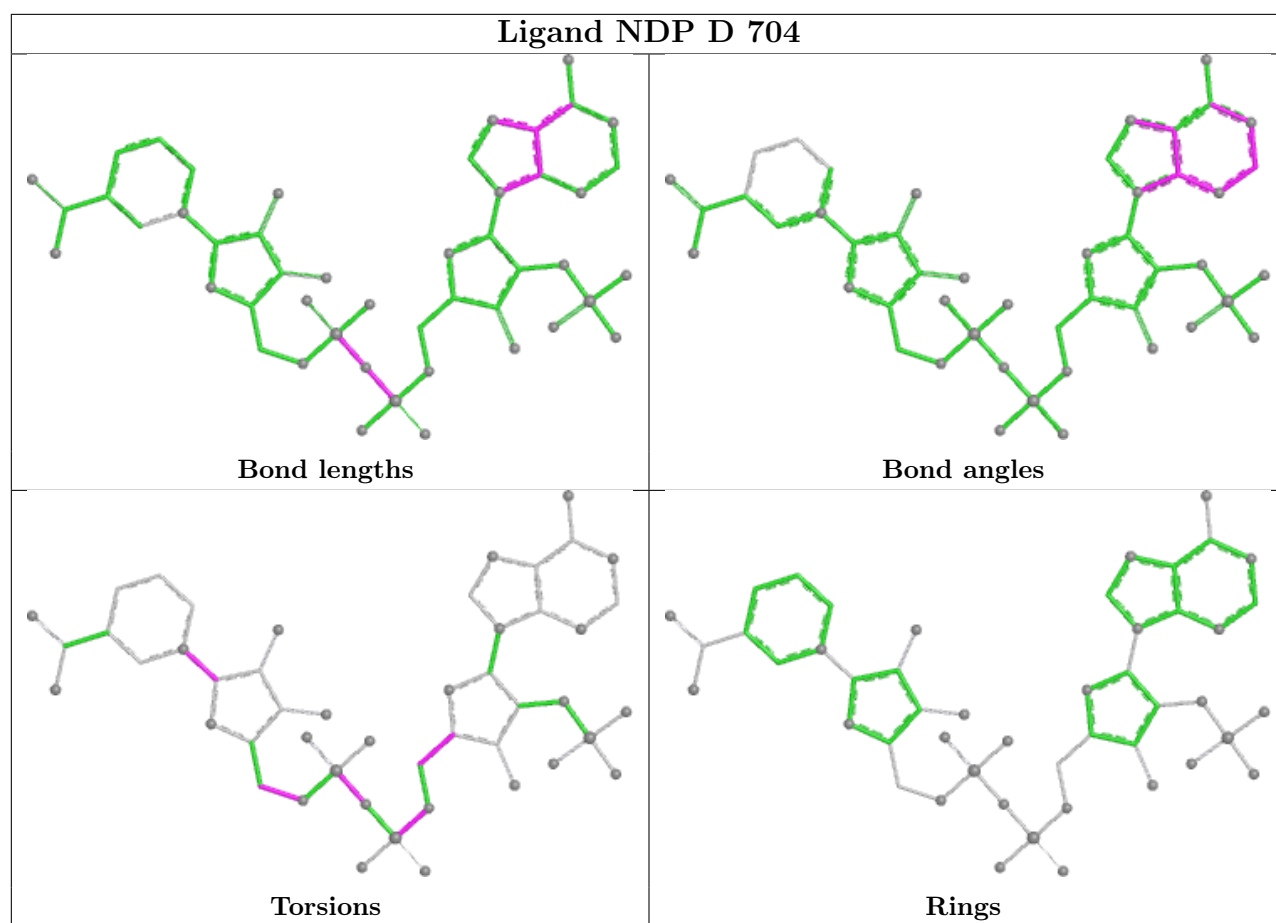


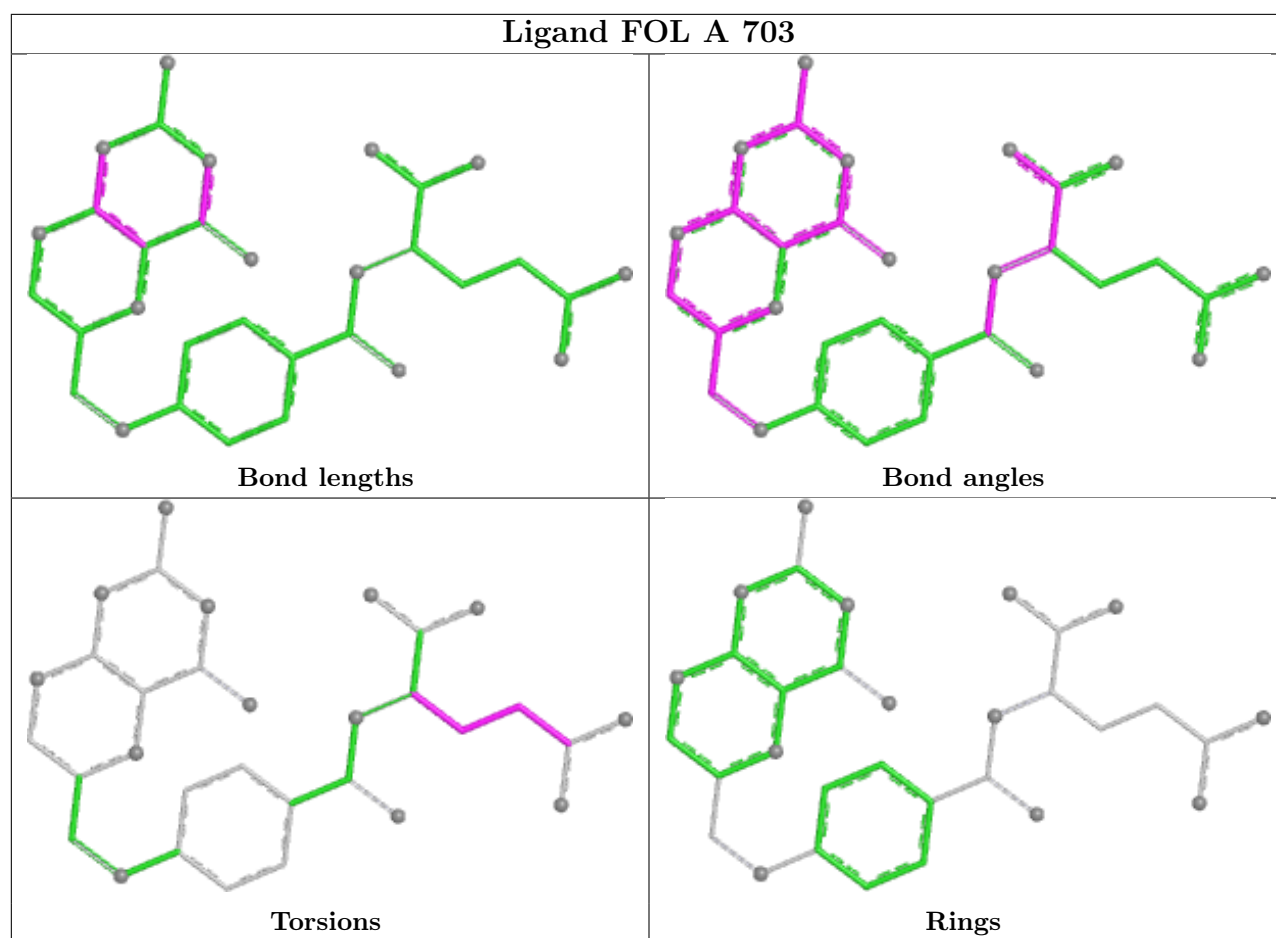
Ligand FOL F 703

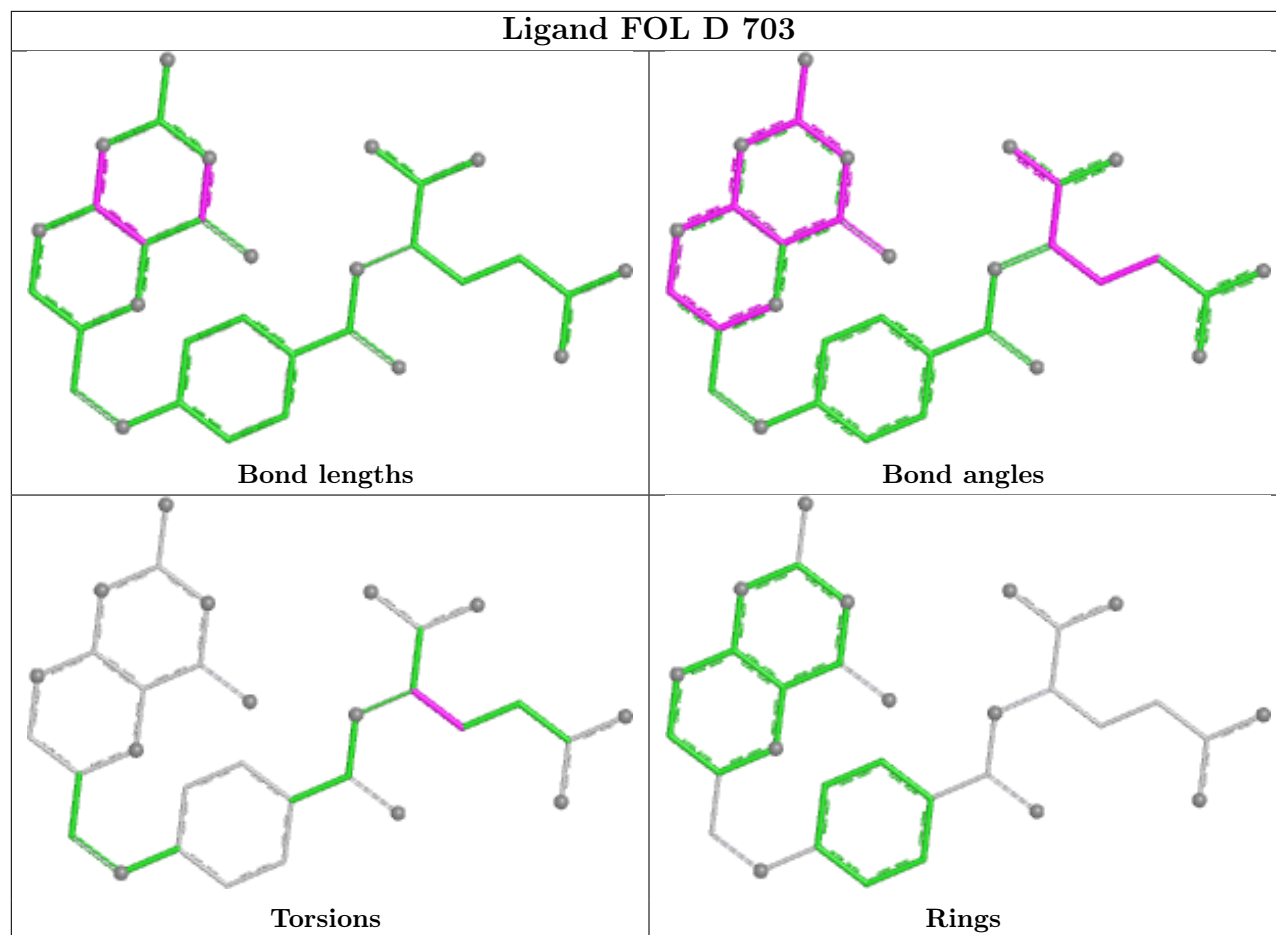




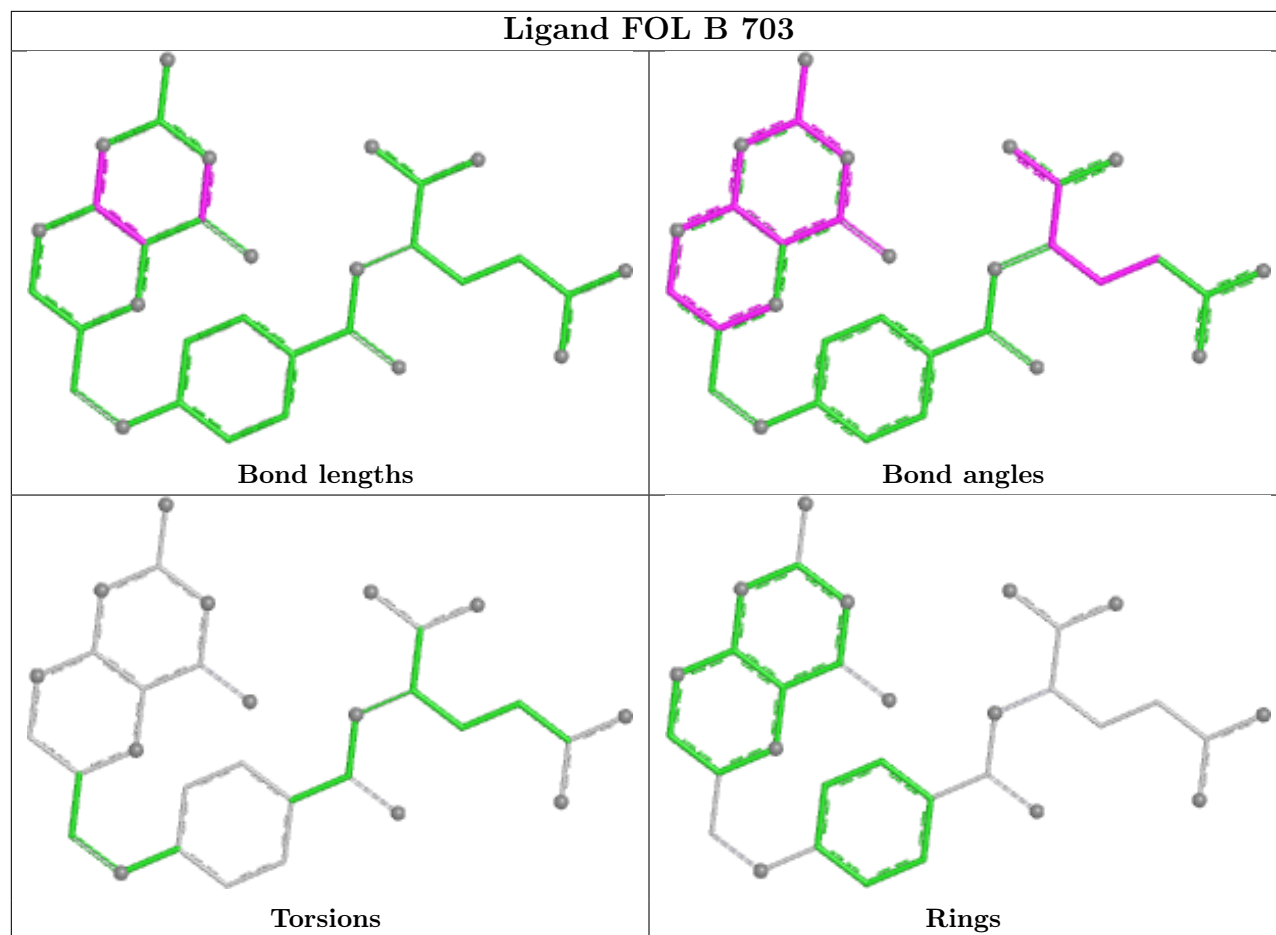




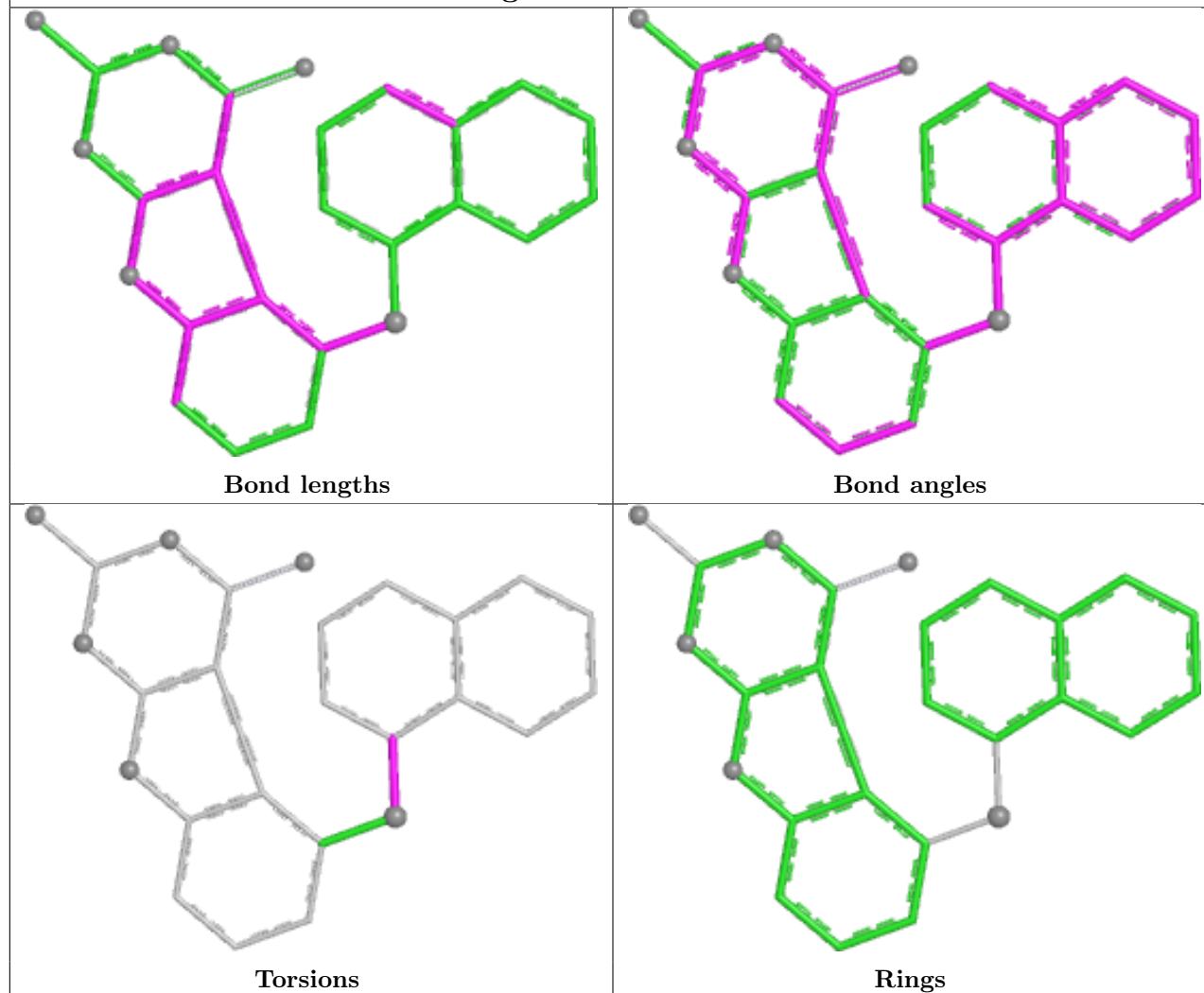




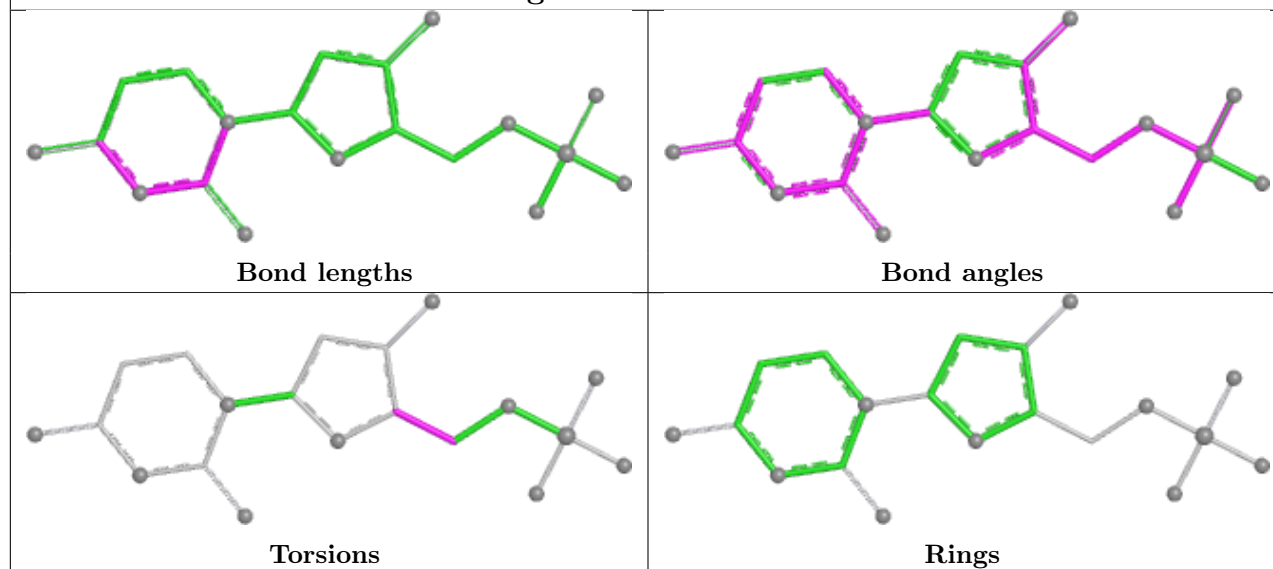
Ligand FOL B 703



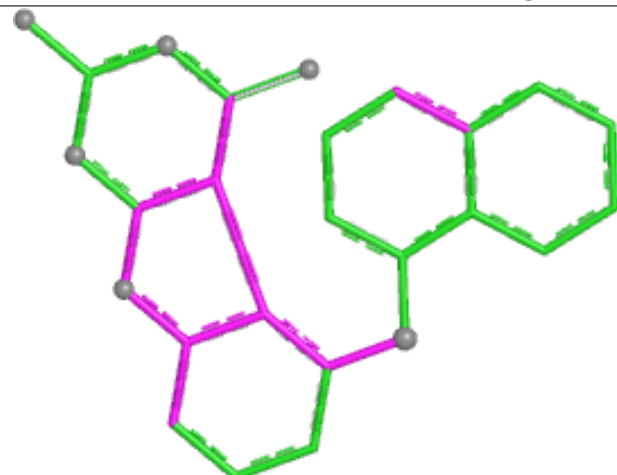
Ligand 1UG H 702



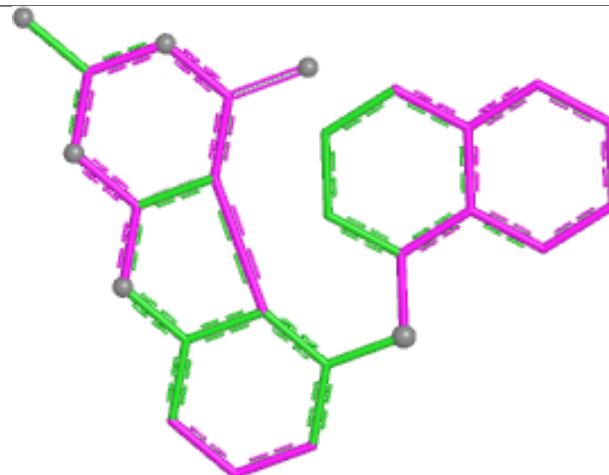
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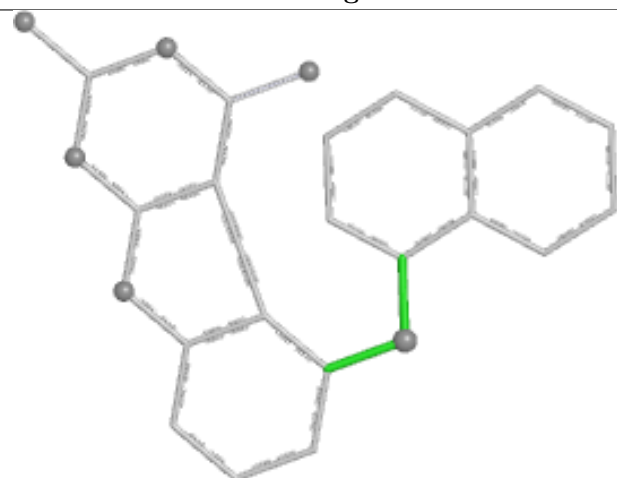
Ligand 1UG E 702



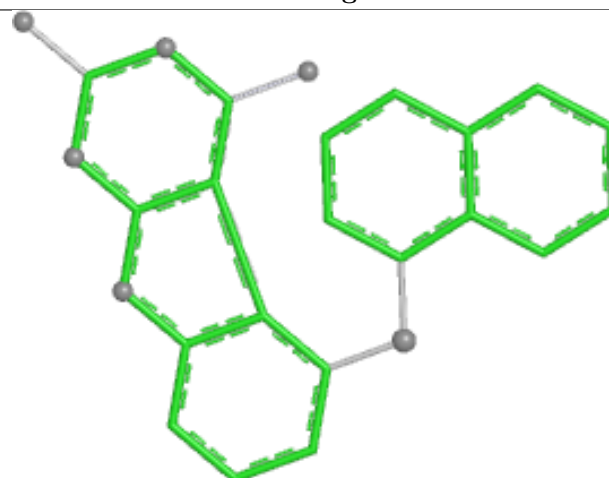
Bond lengths



Bond angles

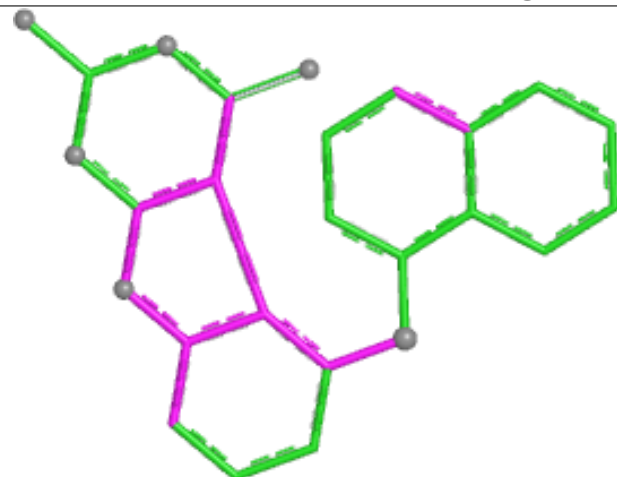


Torsions

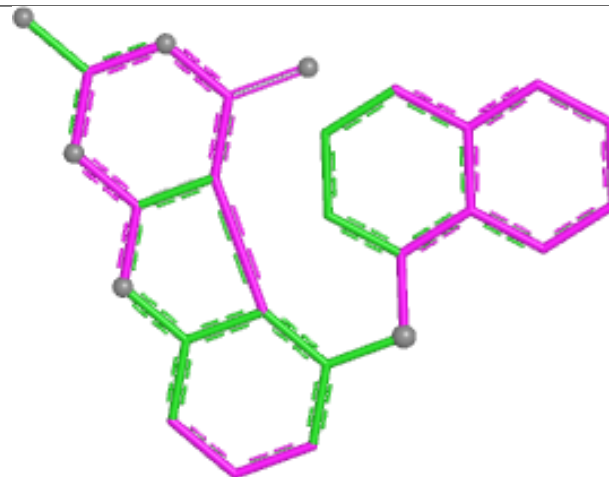


Rings

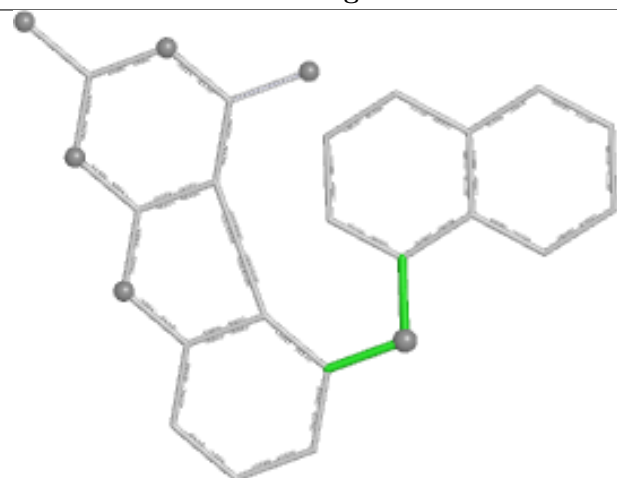
Ligand 1UG C 702



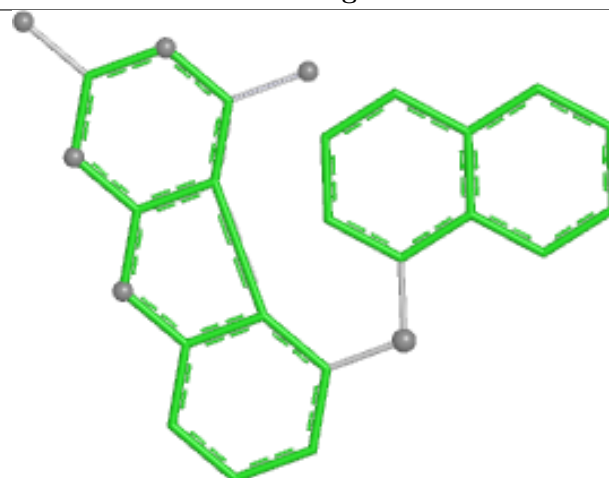
Bond lengths



Bond angles

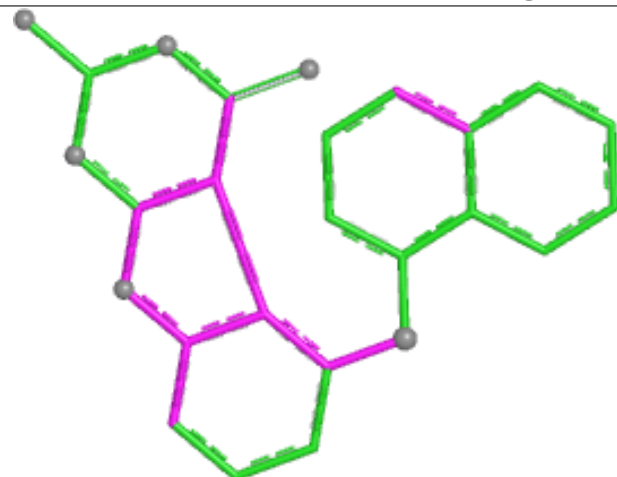


Torsions

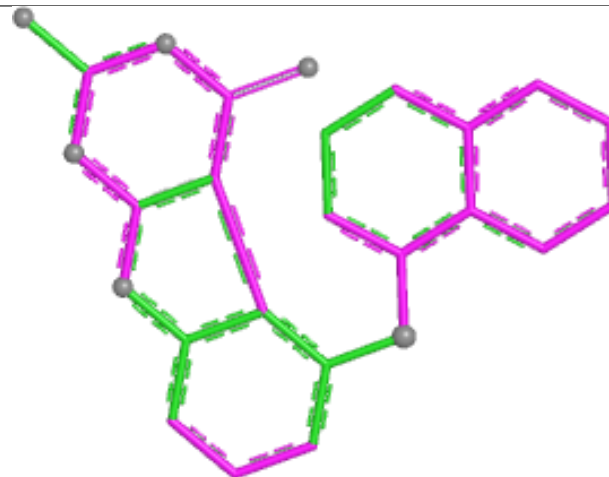


Rings

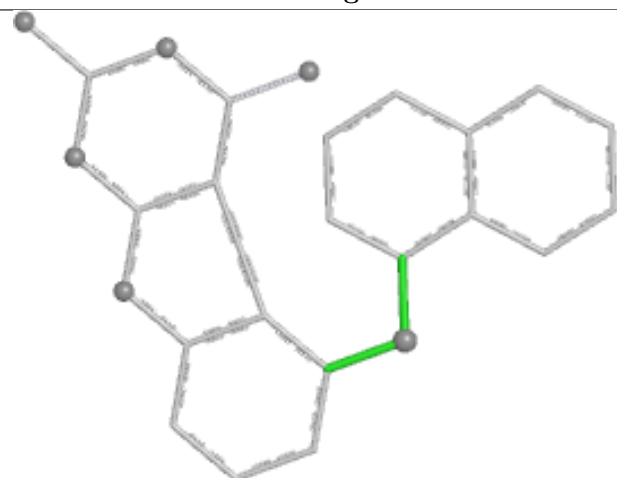
Ligand 1UG F 702



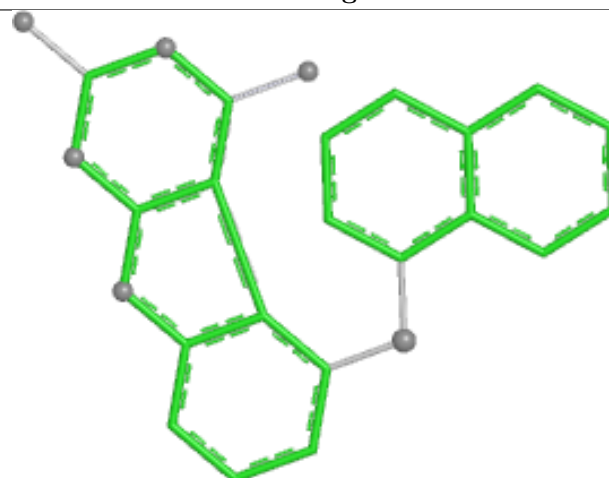
Bond lengths



Bond angles

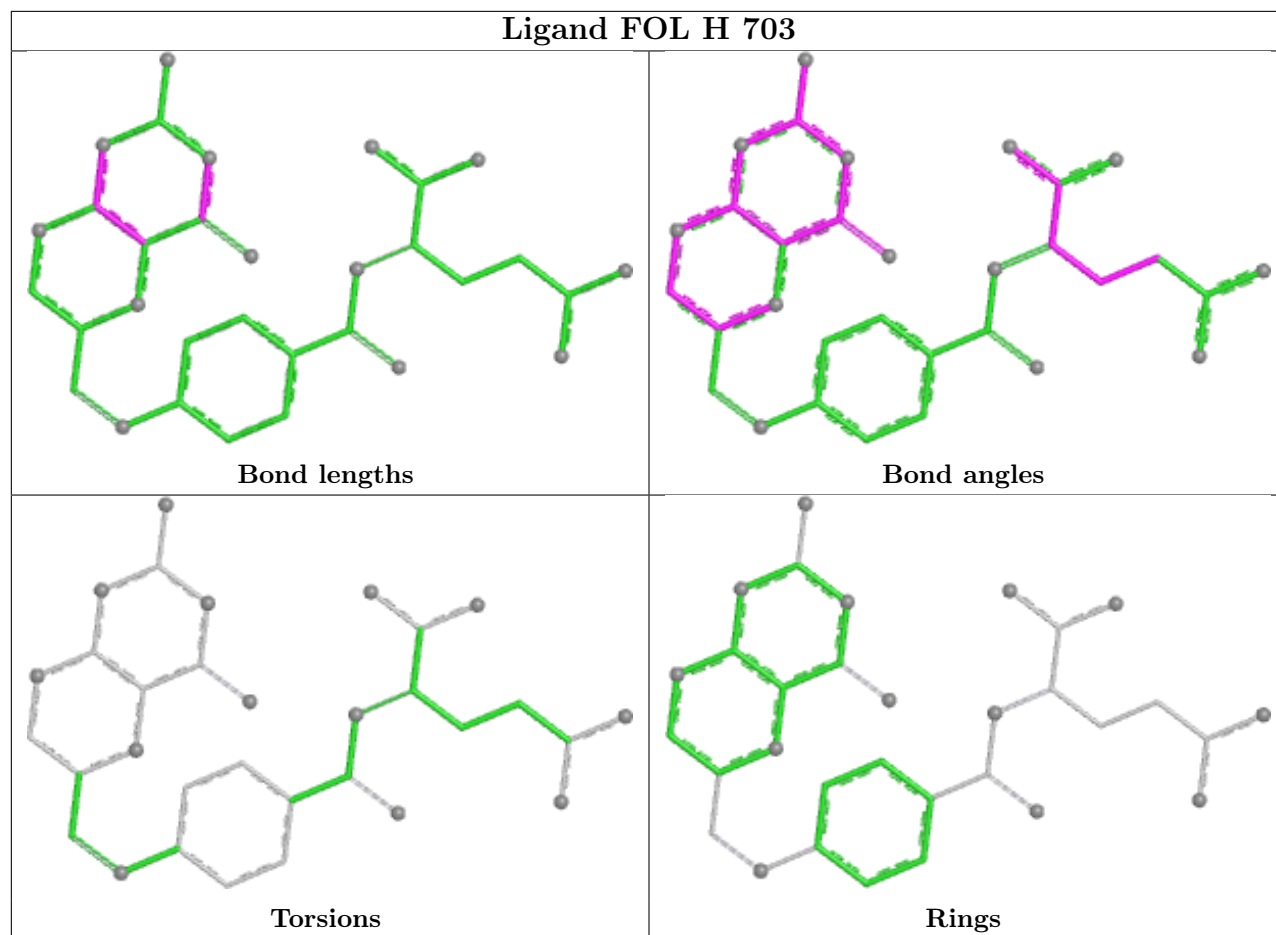


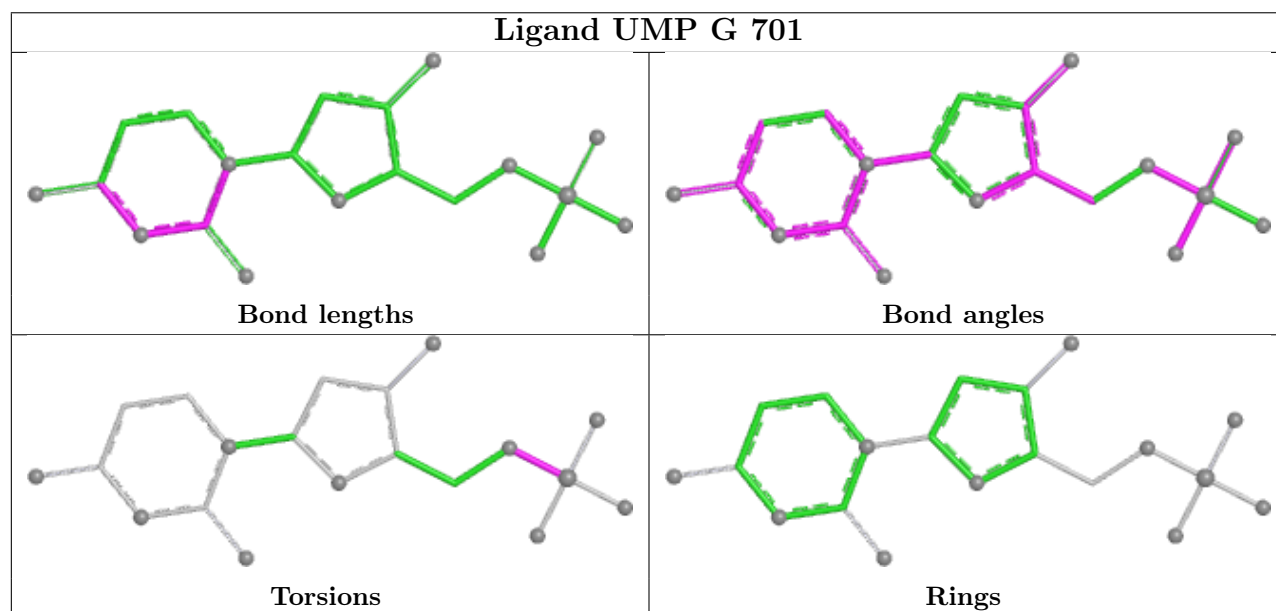
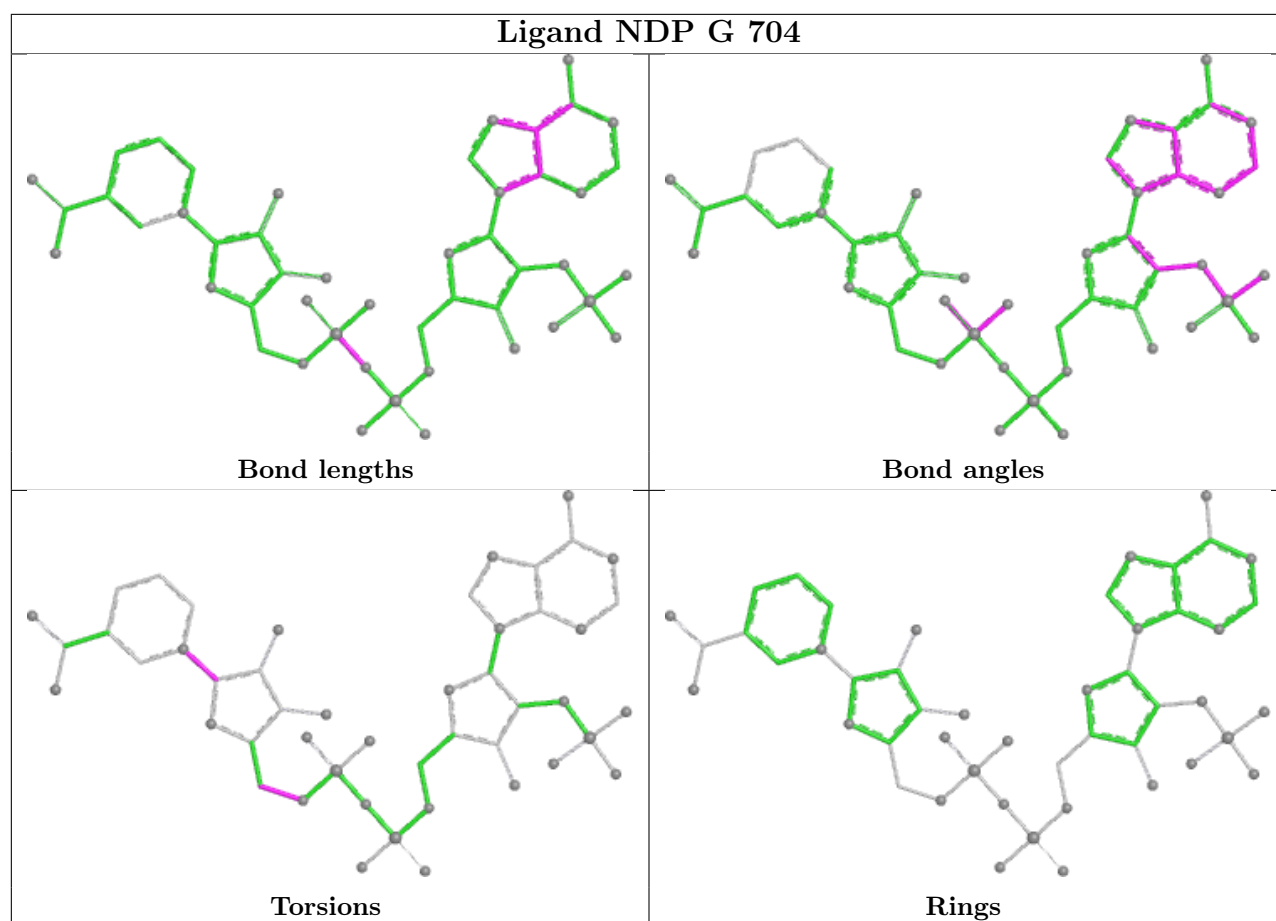
Torsions



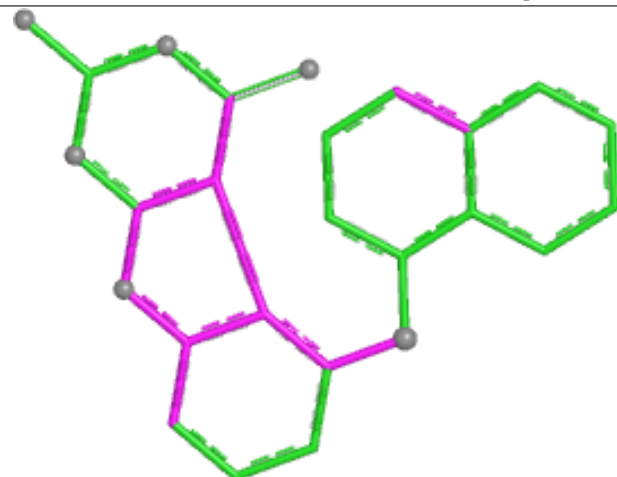
Rings

Ligand FOL H 703

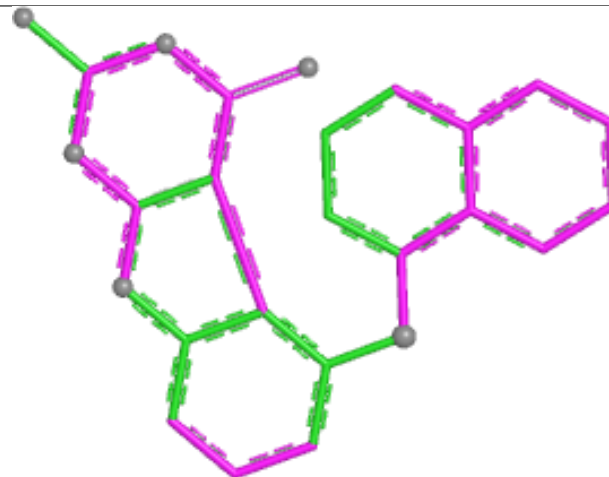




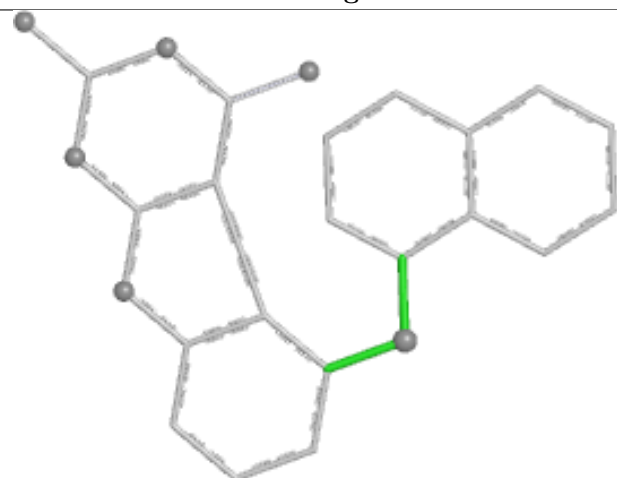
Ligand 1UG G 702



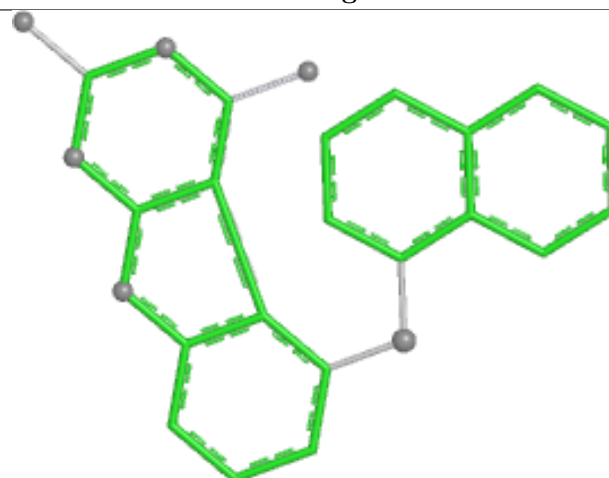
Bond lengths



Bond angles

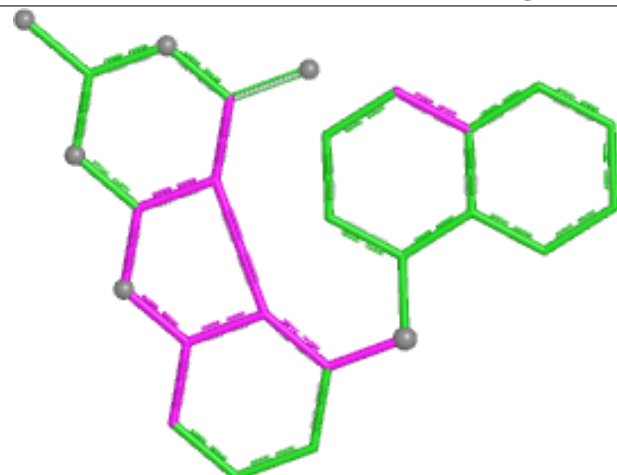


Torsions

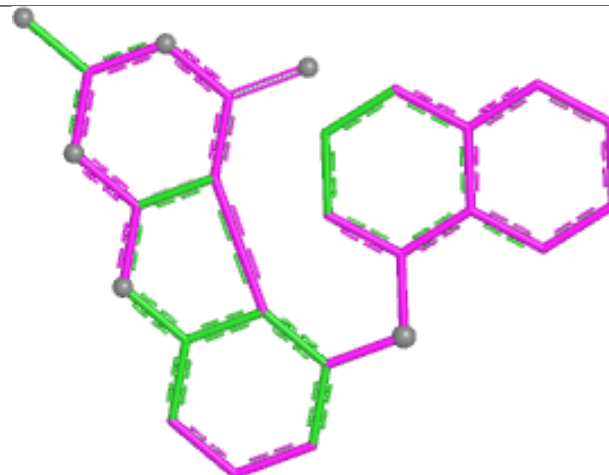


Rings

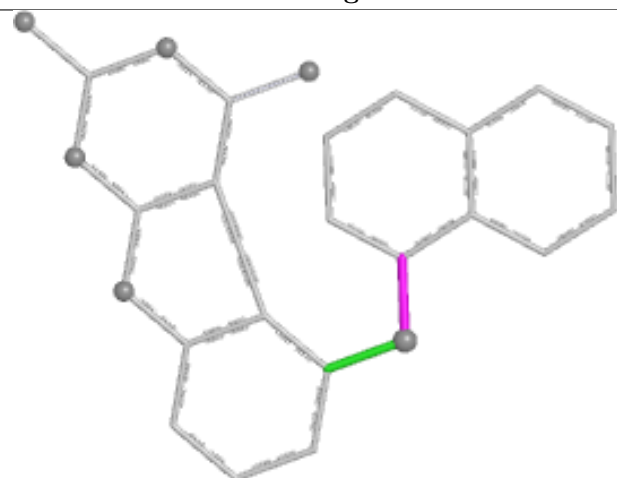
Ligand 1UG B 702



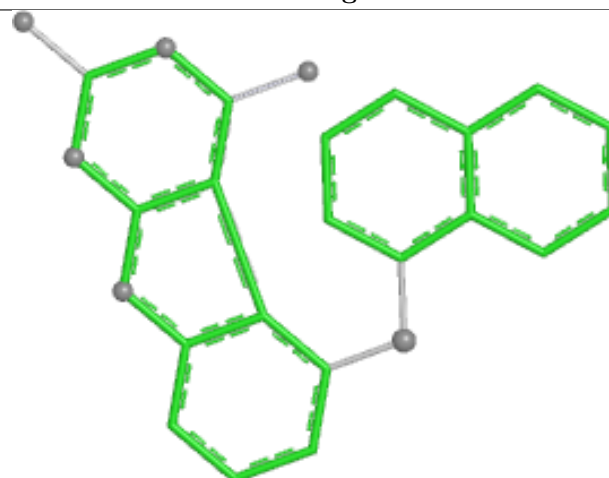
Bond lengths



Bond angles

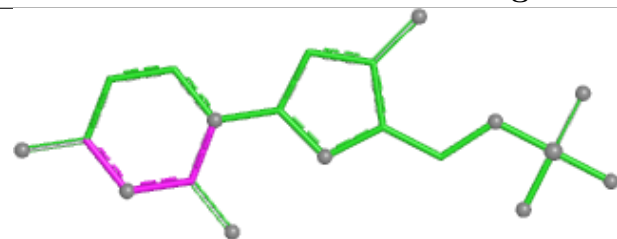


Torsions

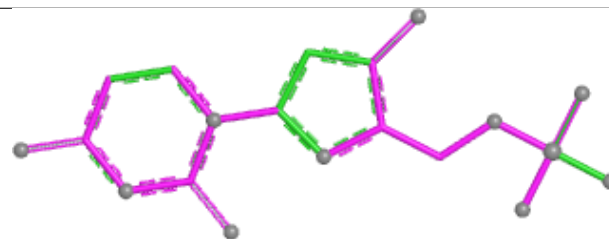


Rings

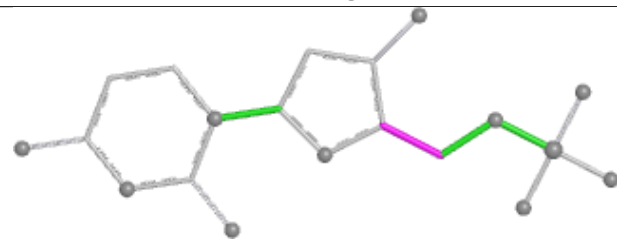
Ligand UMP H 701



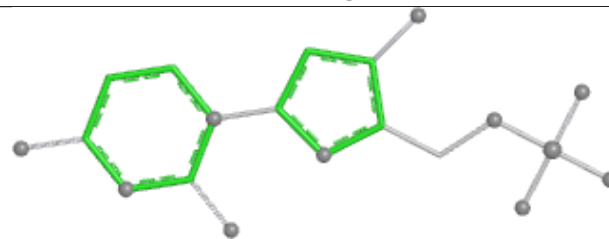
Bond lengths



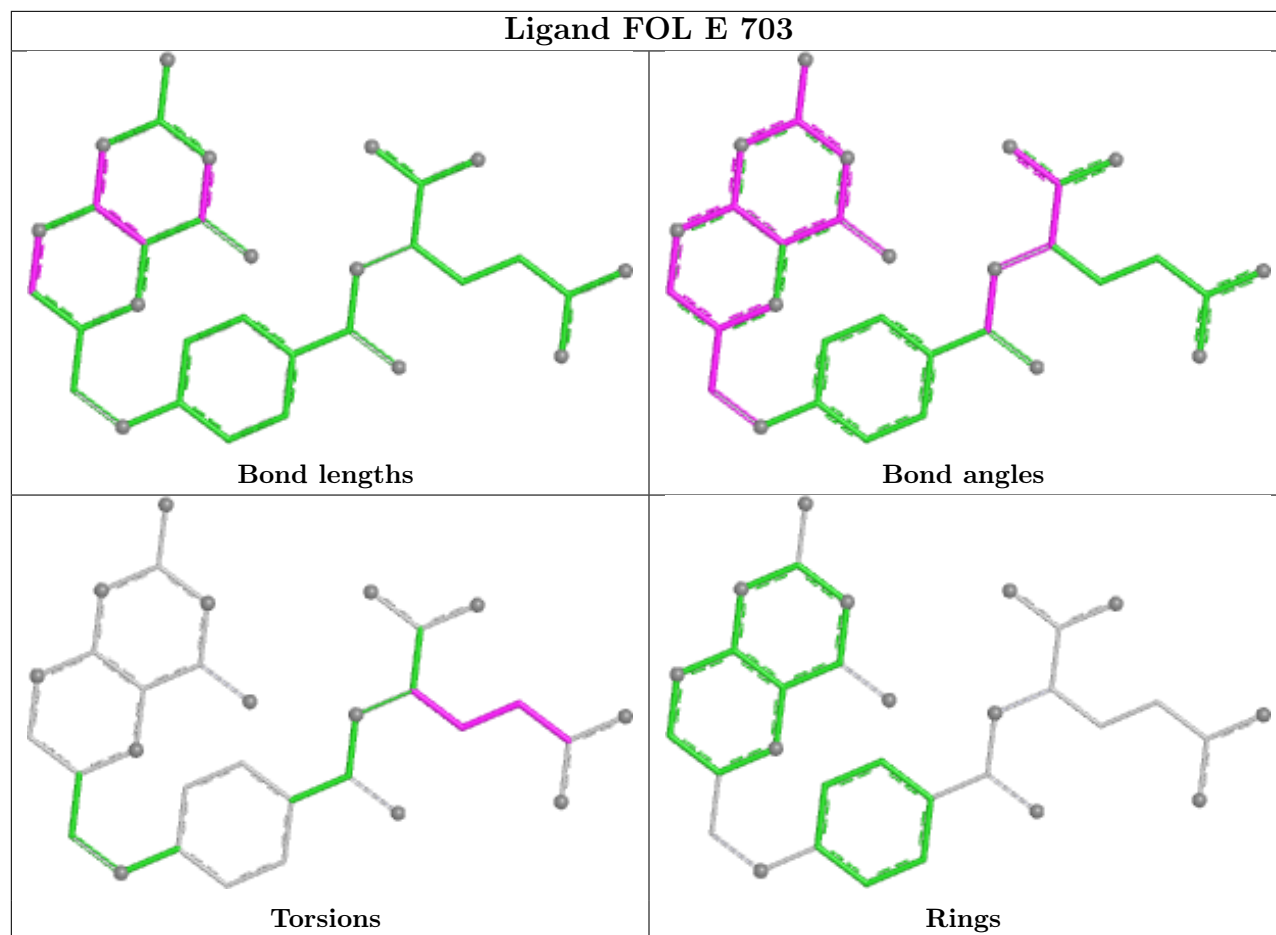
Bond angles

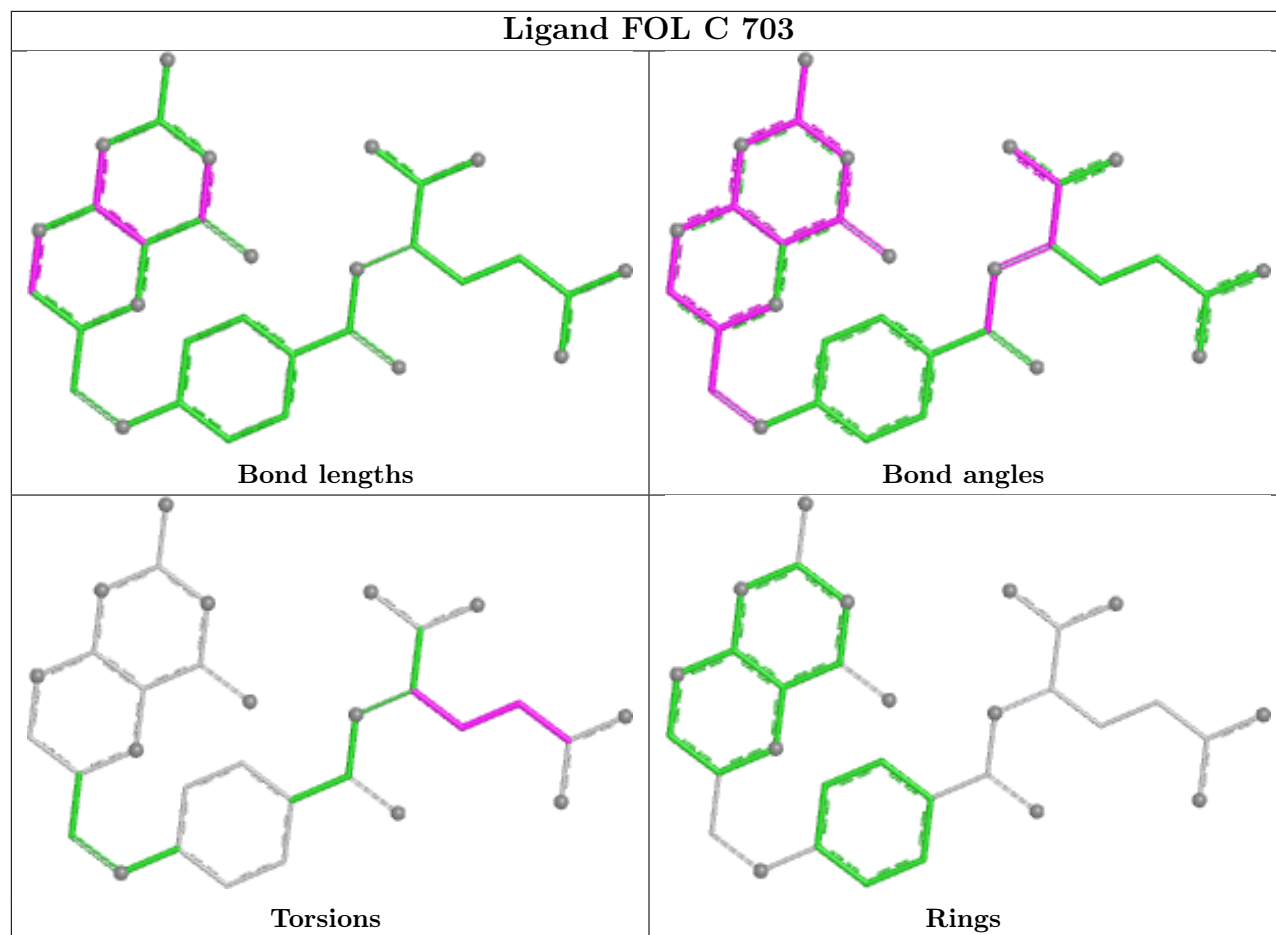


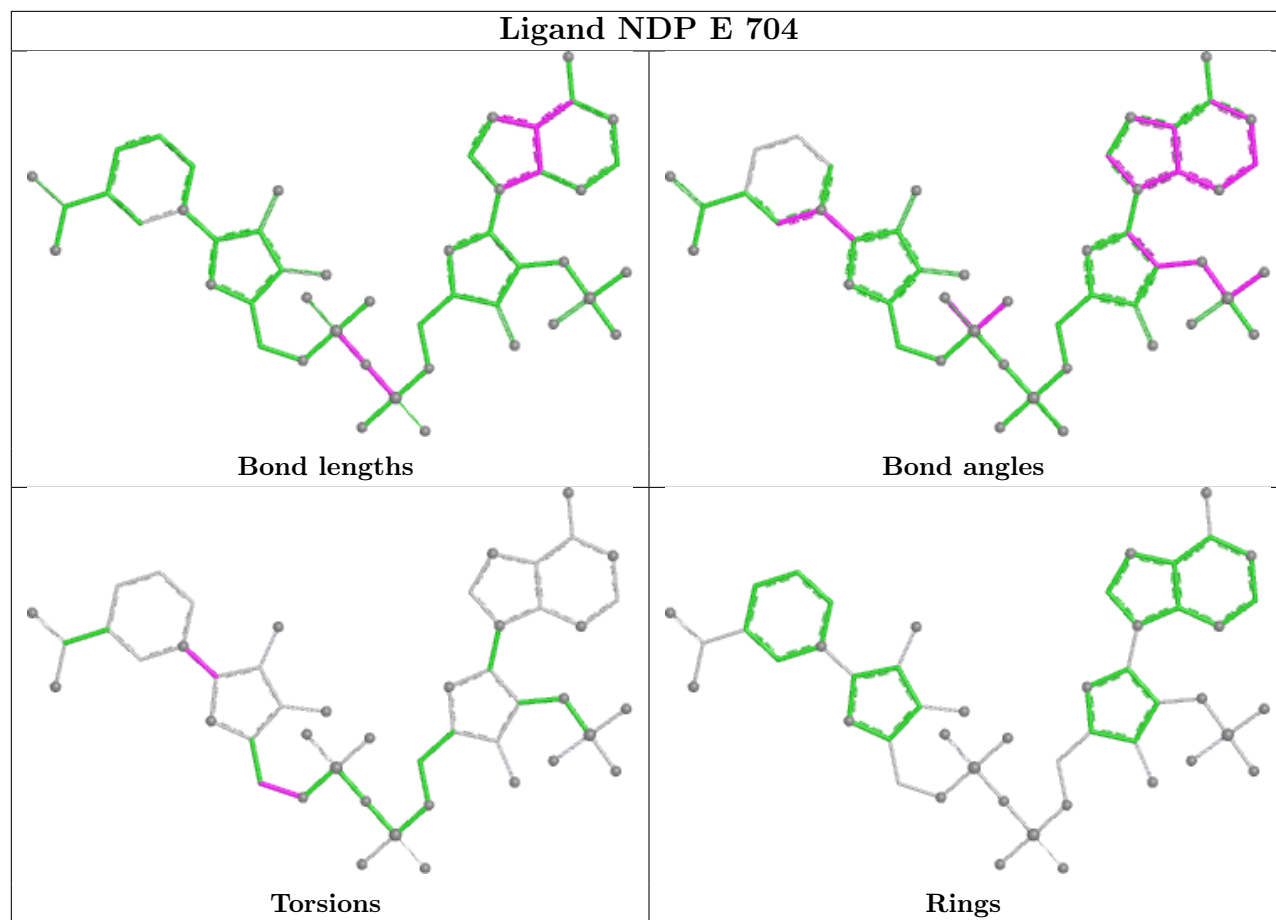
Torsions

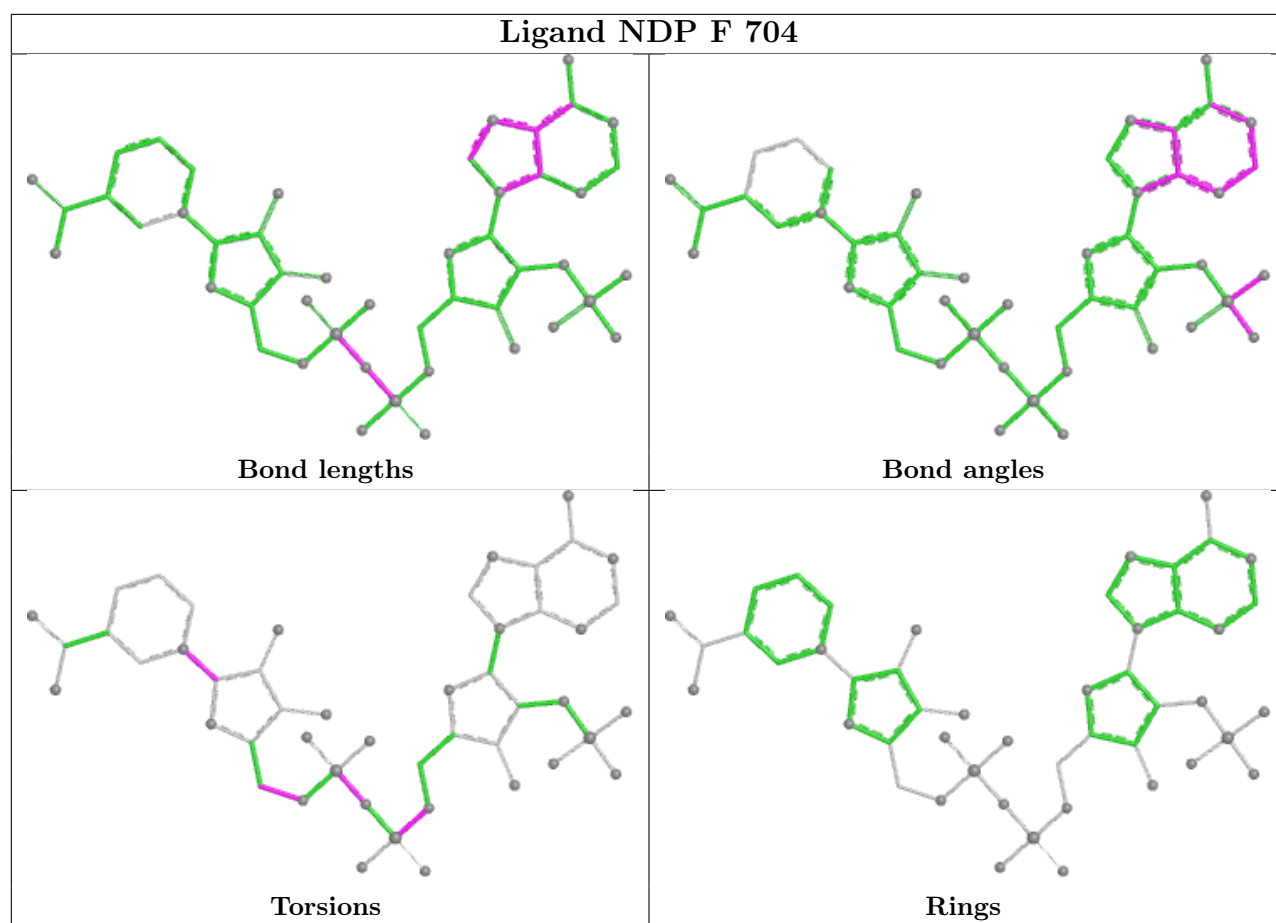


Rings









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	510/566 (90%)	-1.63	0 100 100	13, 30, 69, 99	2 (0%)
1	B	491/566 (86%)	-1.64	0 100 100	14, 32, 77, 93	1 (0%)
1	C	510/566 (90%)	-1.64	0 100 100	11, 31, 70, 100	2 (0%)
1	D	491/566 (86%)	-1.62	0 100 100	13, 32, 77, 96	1 (0%)
1	E	510/566 (90%)	-1.63	0 100 100	12, 30, 68, 98	2 (0%)
1	F	491/566 (86%)	-1.61	0 100 100	13, 32, 76, 98	1 (0%)
1	G	510/566 (90%)	-1.65	0 100 100	14, 30, 71, 104	2 (0%)
1	H	491/566 (86%)	-1.62	0 100 100	14, 33, 76, 96	1 (0%)
All	All	4004/4528 (88%)	-1.63	0 100 100	11, 31, 74, 104	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](#)

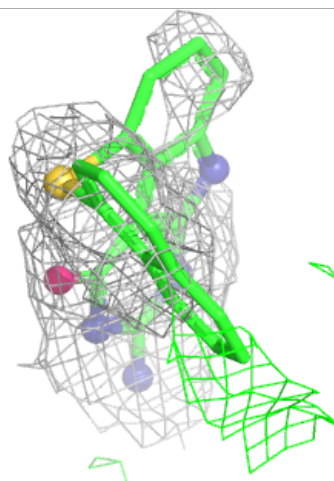
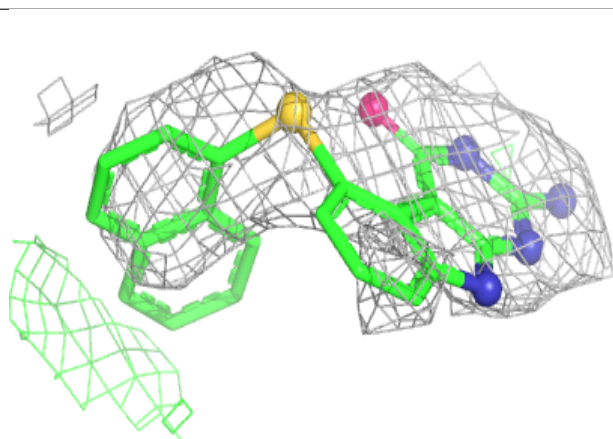
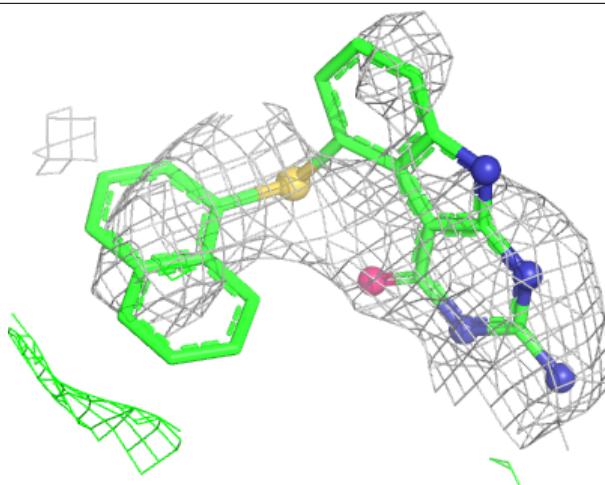
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1UG	G	702	26/26	0.98	0.07	69,105,114,116	0
2	UMP	D	701	20/20	0.99	0.03	25,46,67,73	0
2	UMP	F	701	20/20	0.99	0.03	26,43,68,70	0
2	UMP	G	701	20/20	0.99	0.03	35,56,72,72	0
2	UMP	H	701	20/20	0.99	0.03	24,46,68,70	0
3	1UG	A	702	26/26	0.99	0.06	72,99,113,115	0
3	1UG	B	702	26/26	0.99	0.05	64,89,110,111	0
3	1UG	C	702	26/26	0.99	0.07	96,114,132,133	0
3	1UG	D	702	26/26	0.99	0.05	66,83,105,106	0
3	1UG	E	702	26/26	0.99	0.05	75,101,115,117	0
3	1UG	F	702	26/26	0.99	0.05	71,86,107,110	0
2	UMP	B	701	20/20	0.99	0.03	26,47,70,71	0
3	1UG	H	702	26/26	0.99	0.05	65,82,104,105	0
4	FOL	A	703	32/32	0.99	0.04	24,45,67,89	0
4	FOL	B	703	32/32	0.99	0.04	33,60,87,93	0
4	FOL	C	703	32/32	0.99	0.03	26,48,68,95	0
4	FOL	D	703	32/32	0.99	0.04	34,59,86,91	0
4	FOL	E	703	32/32	0.99	0.03	24,45,71,90	0
4	FOL	F	703	32/32	0.99	0.04	36,63,87,91	0
4	FOL	G	703	32/32	0.99	0.04	26,41,68,86	0
4	FOL	H	703	32/32	0.99	0.04	33,60,88,93	0
5	NDP	B	704	48/48	0.99	0.03	35,69,105,110	0
5	NDP	D	704	48/48	0.99	0.03	34,65,100,106	0
5	NDP	F	704	48/48	0.99	0.03	30,65,105,108	0
5	NDP	H	704	48/48	0.99	0.03	35,63,99,108	0
2	UMP	A	701	20/20	1.00	0.03	30,57,70,70	0
5	NDP	C	704	48/48	1.00	0.02	21,32,43,51	0
2	UMP	E	701	20/20	1.00	0.03	34,57,75,78	0
5	NDP	E	704	48/48	1.00	0.03	20,33,42,48	0
2	UMP	C	701	20/20	1.00	0.03	32,62,81,82	0
5	NDP	G	704	48/48	1.00	0.03	21,32,44,56	0
5	NDP	A	704	48/48	1.00	0.03	21,34,40,56	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.

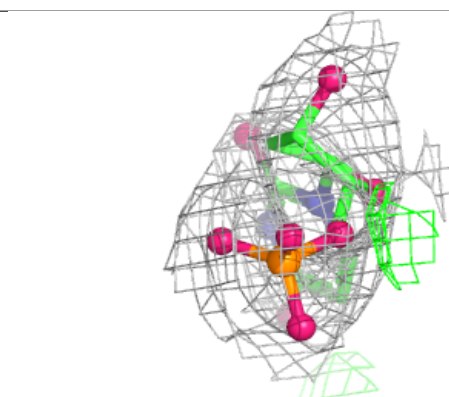
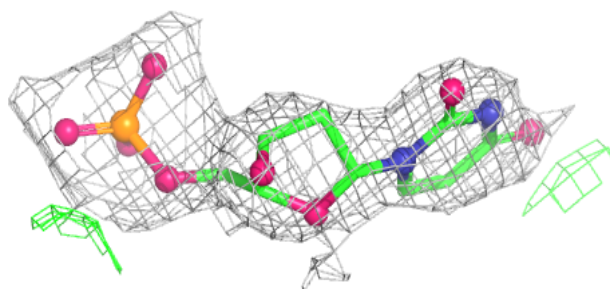
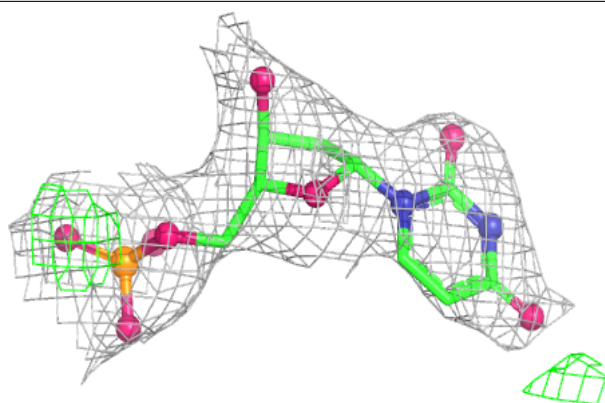
Electron density around 1UG G 702:

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

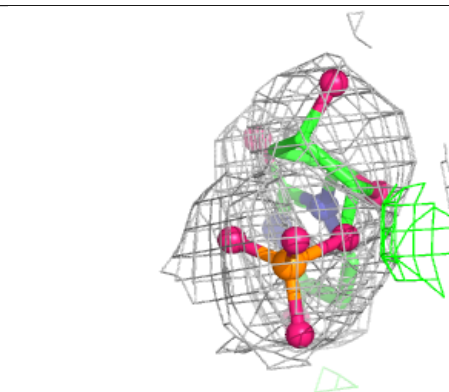
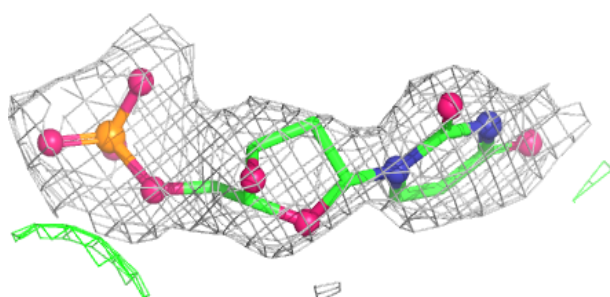
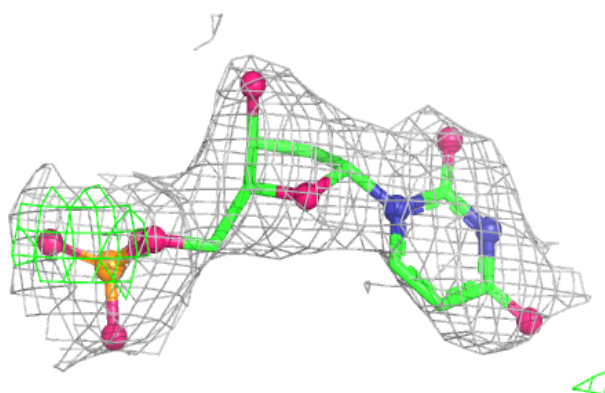


Electron density around UMP D 701:

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

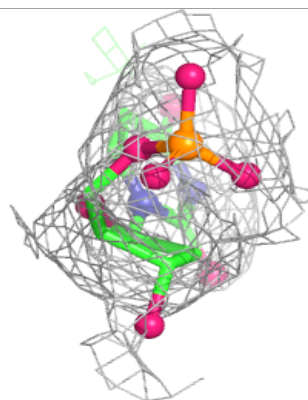
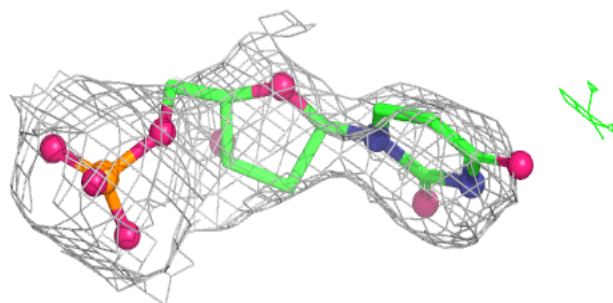
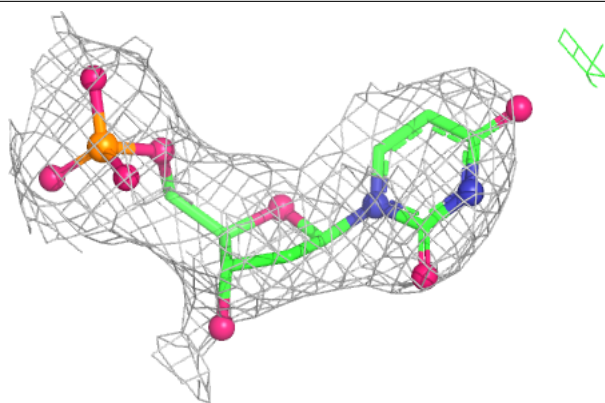
**Electron density around UMP F 701:**

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

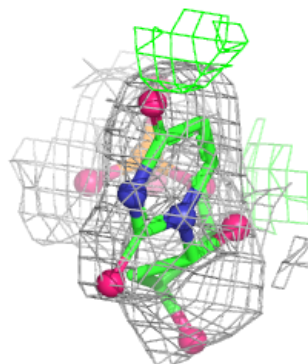
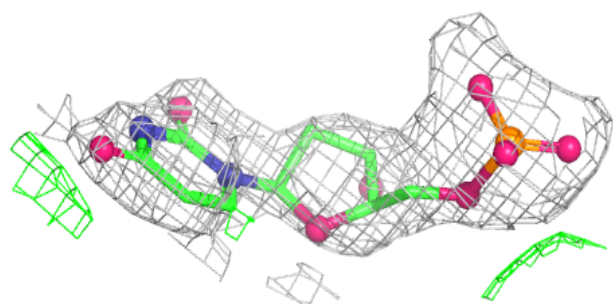
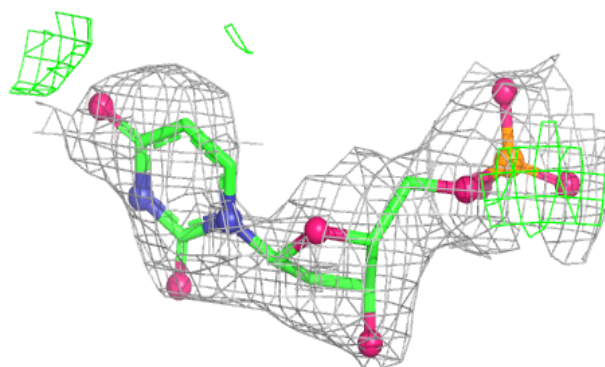


Electron density around UMP G 701:

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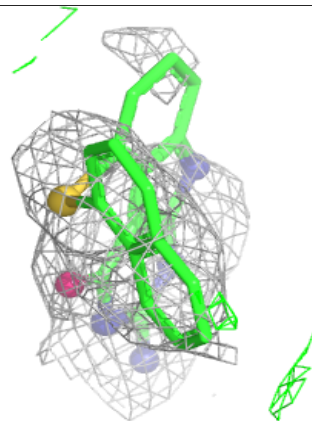
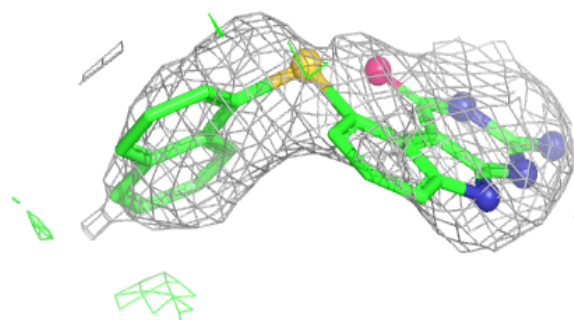
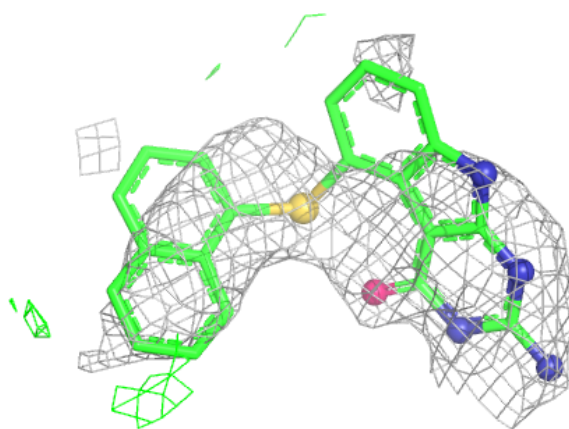
**Electron density around UMP H 701:**

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and green (positive)



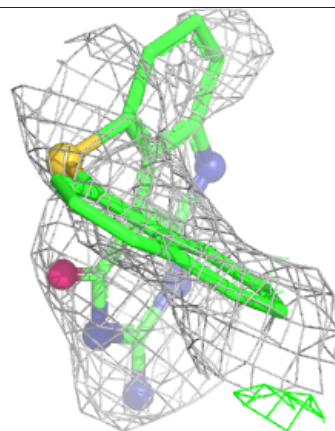
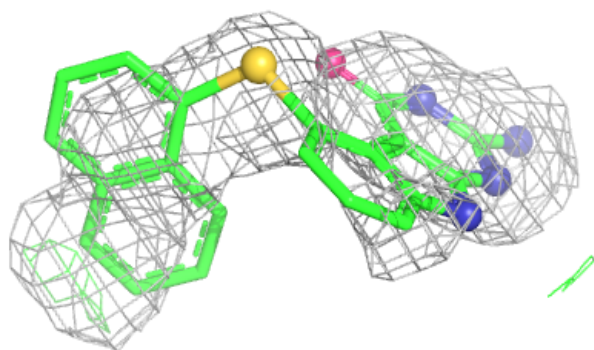
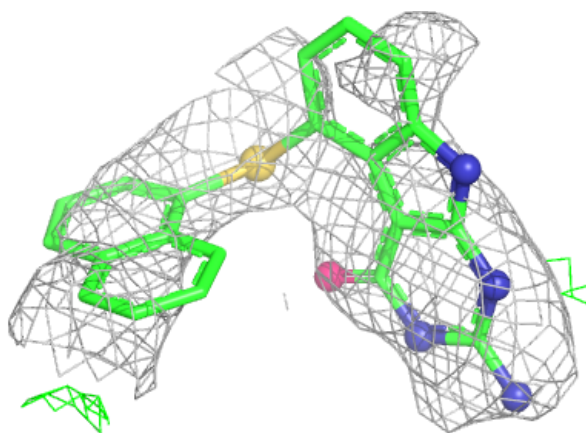
Electron density around 1UG A 702:

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



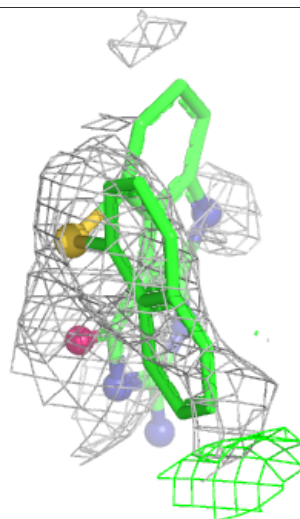
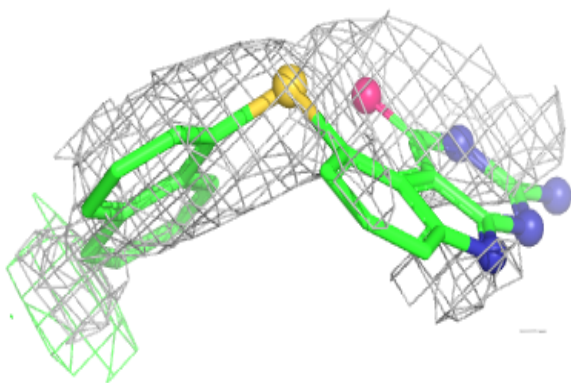
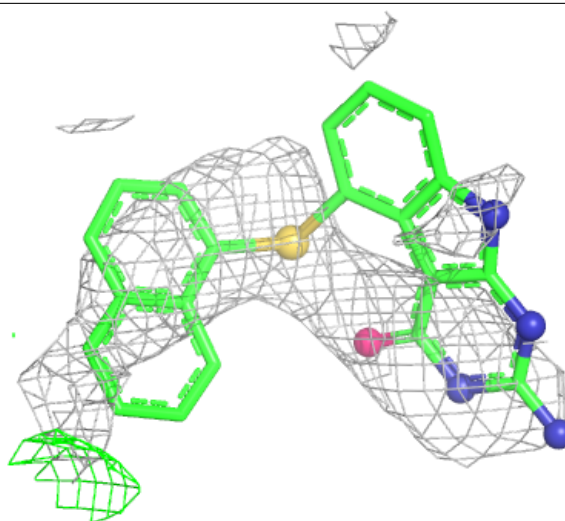
Electron density around 1UG B 702:

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and green (positive)



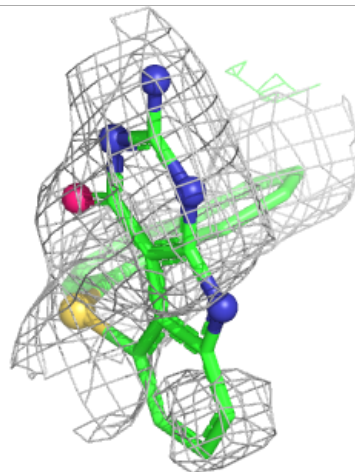
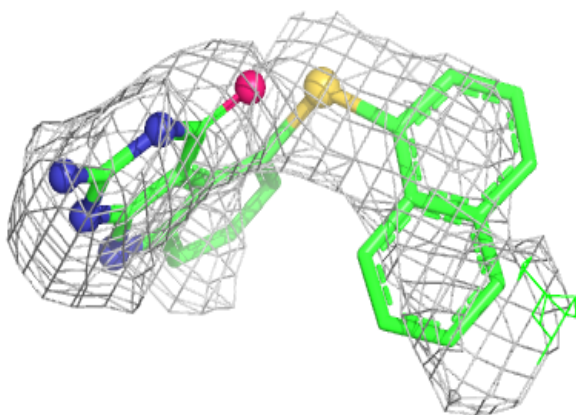
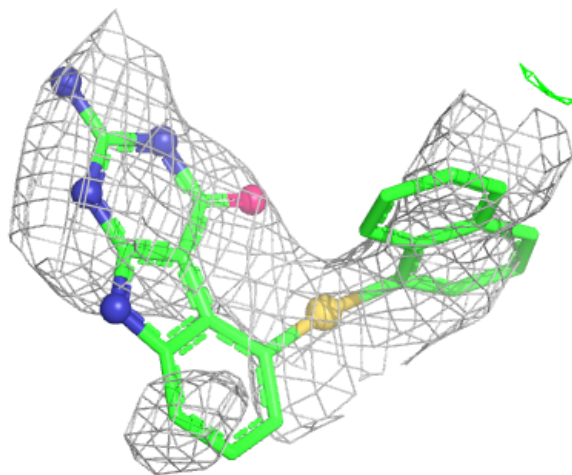
Electron density around 1UG C 702:

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and green (positive)



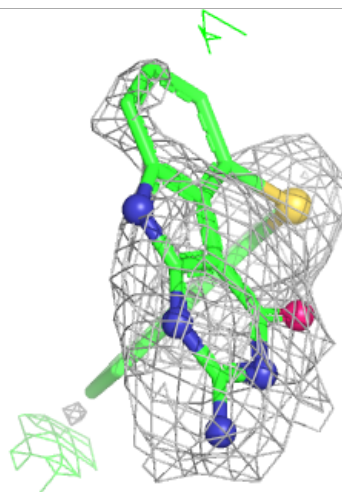
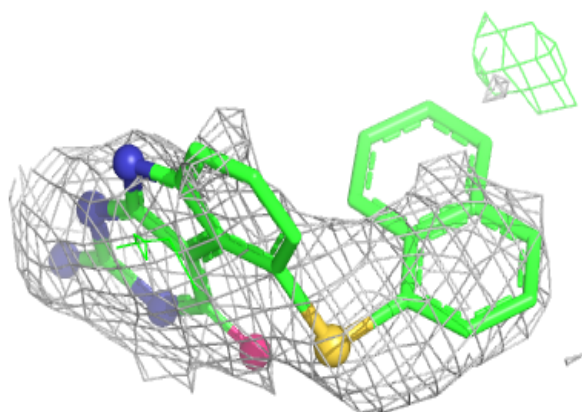
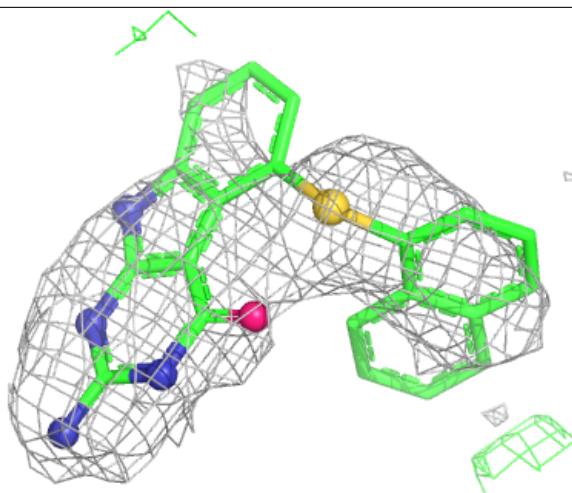
Electron density around 1UG D 702:

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



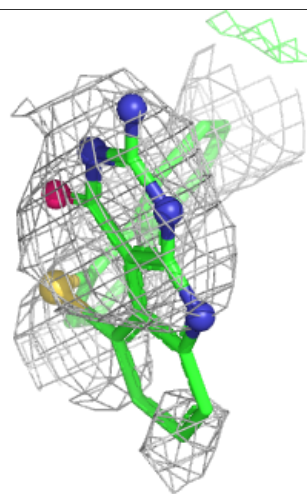
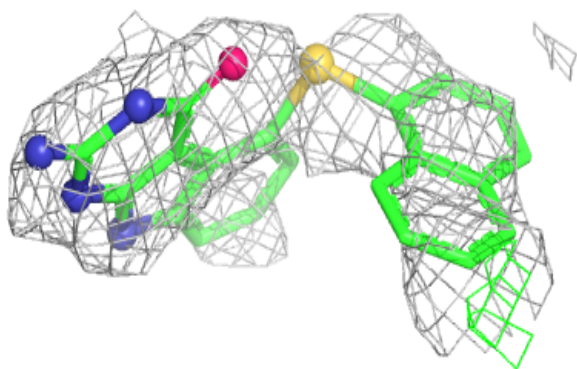
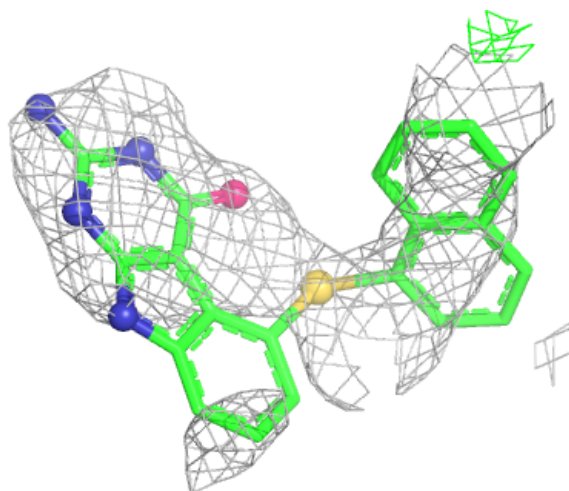
Electron density around 1UG E 702:

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and green (positive)



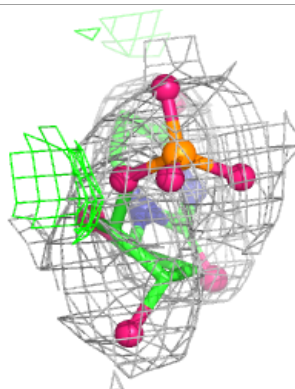
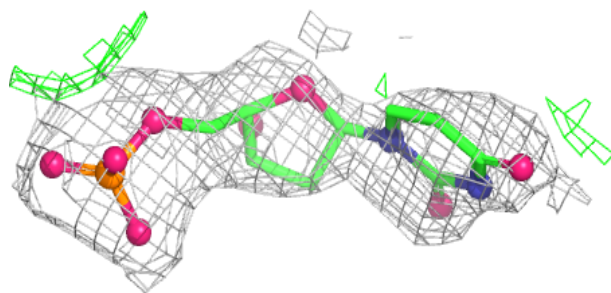
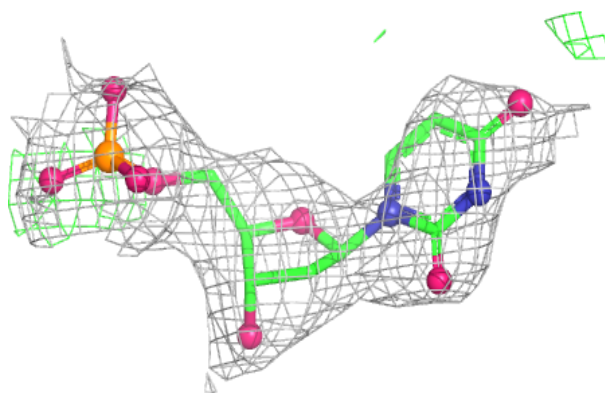
Electron density around 1UG F 702:

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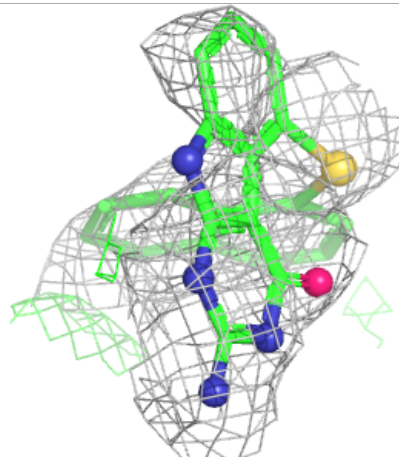
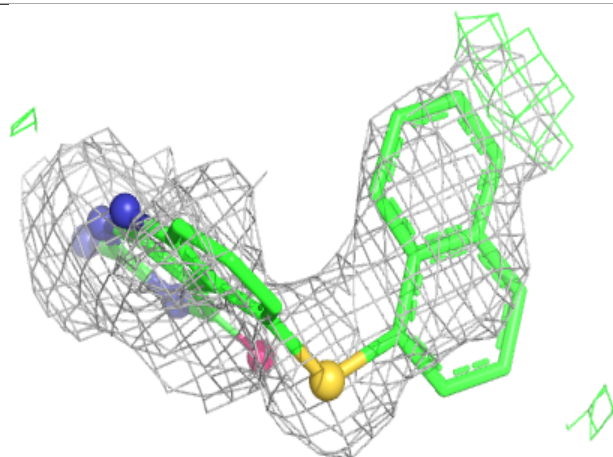
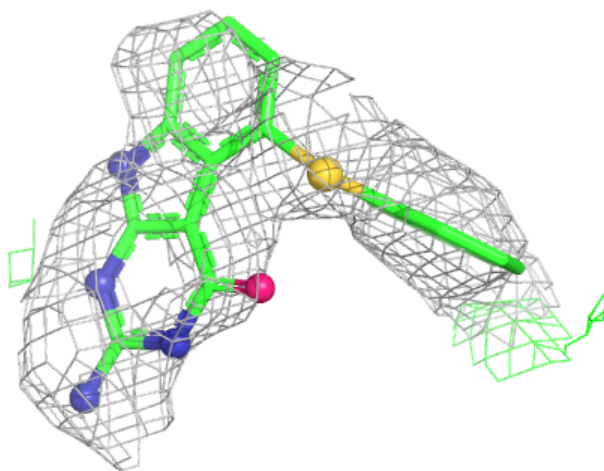
Electron density around UMP B 701:

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and green (positive)



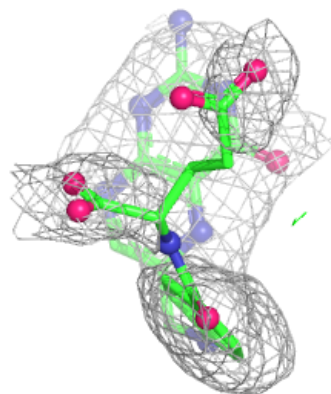
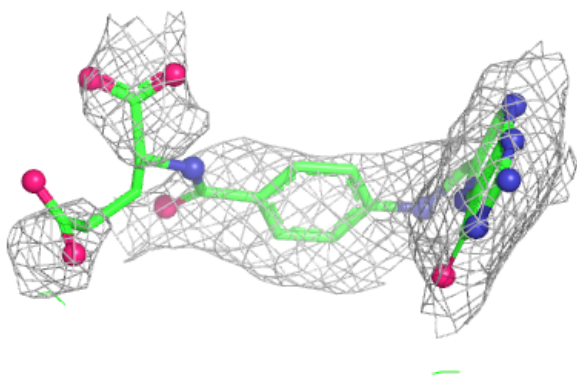
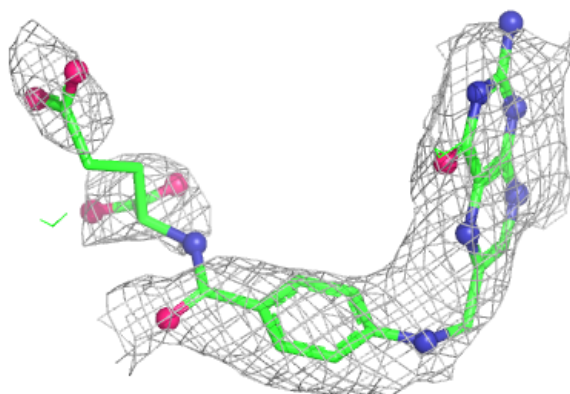
Electron density around 1UG H 702:

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and green (positive)

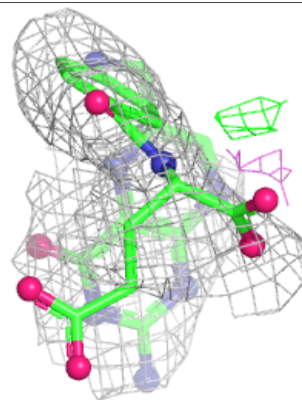
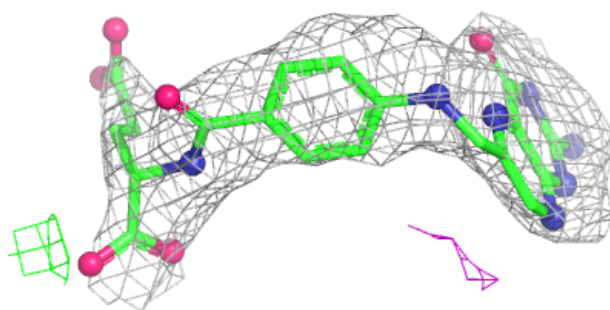
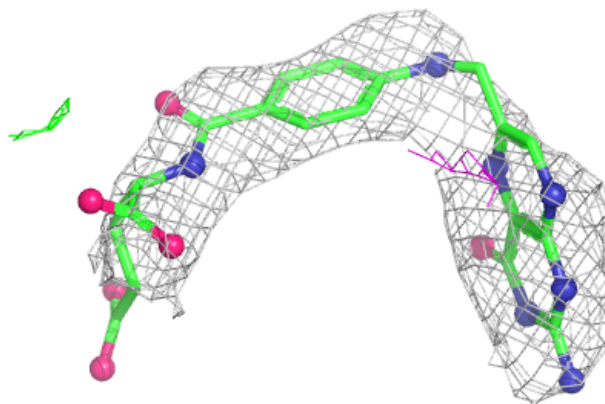


Electron density around FOL A 703:

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and green (positive)

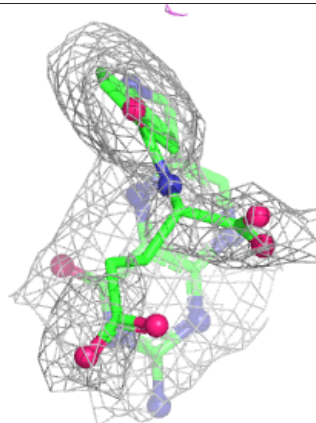
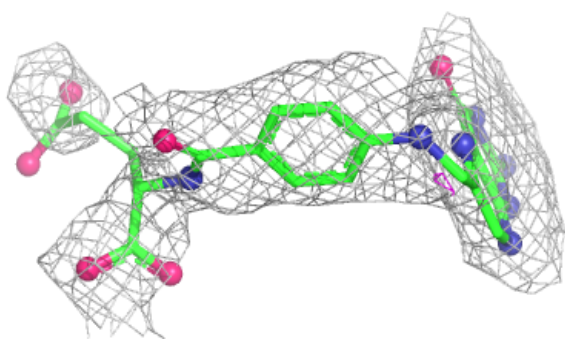
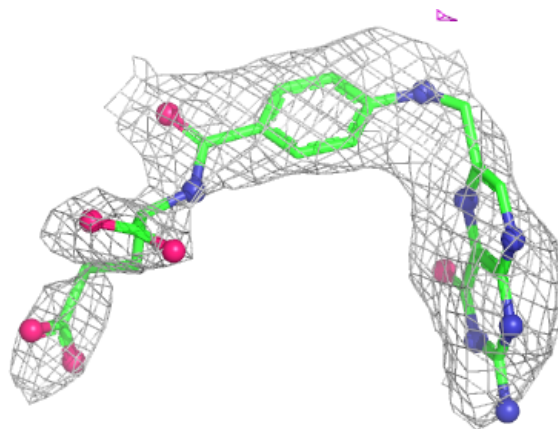
**Electron density around FOL B 703:**

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and green (positive)



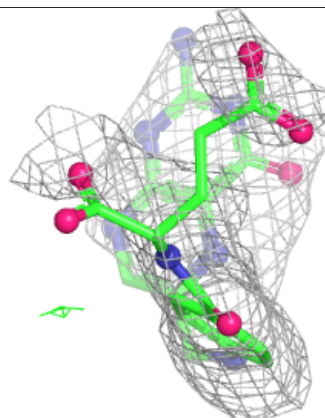
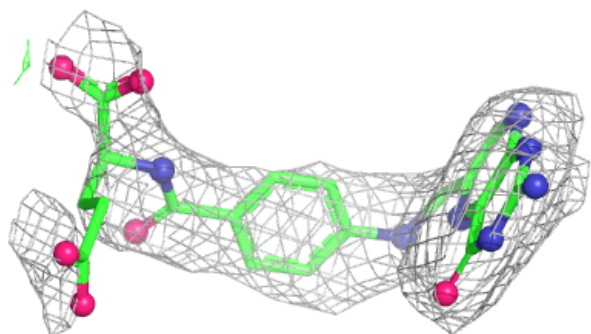
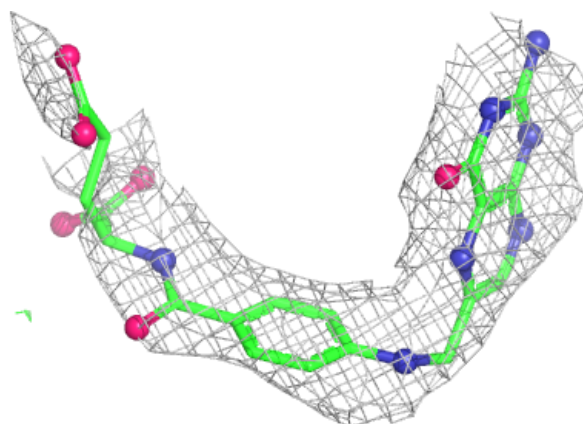
Electron density around FOL C 703:

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

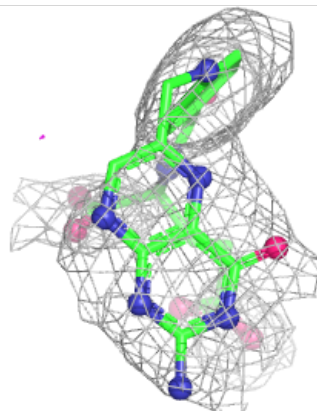
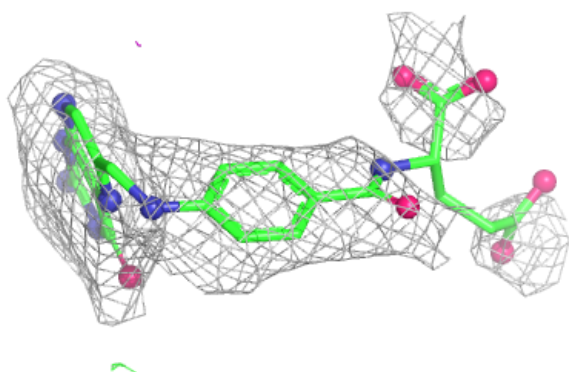
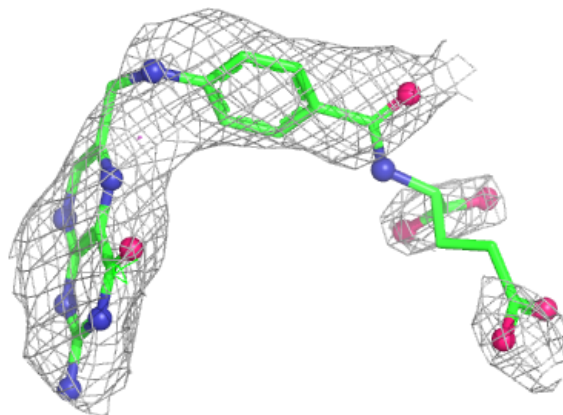


Electron density around FOL D 703:

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

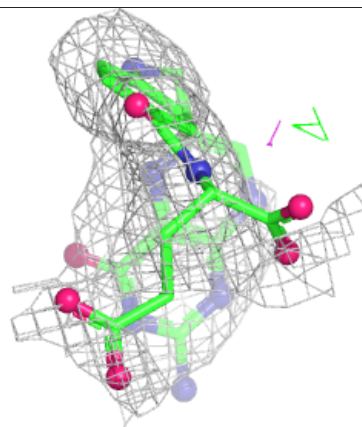
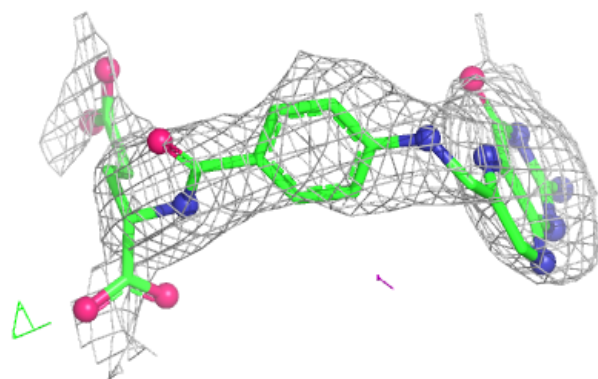
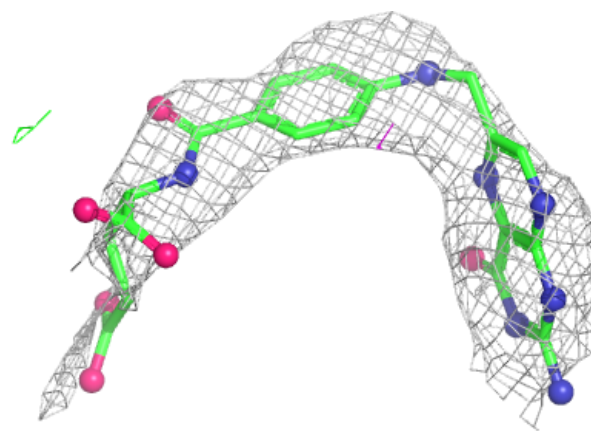
**Electron density around FOL E 703:**

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

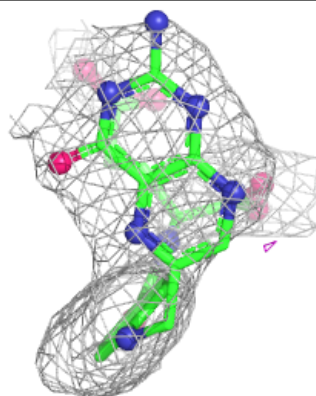
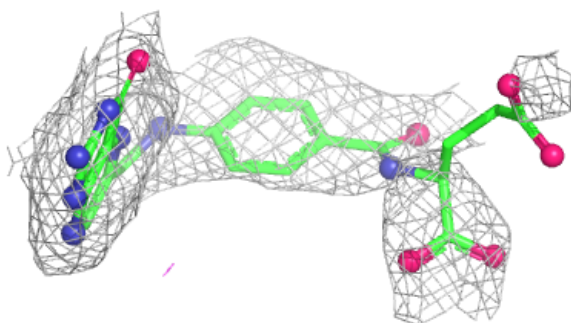
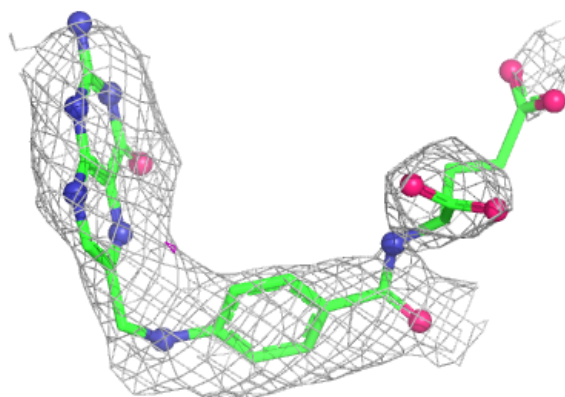


Electron density around FOL F 703:

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

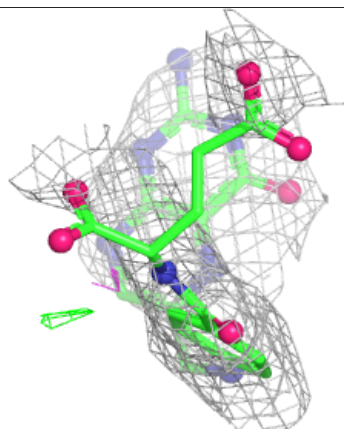
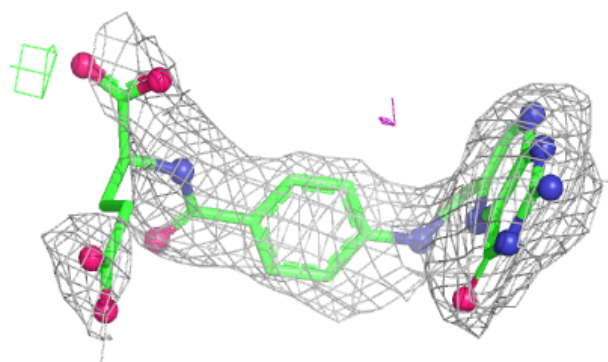
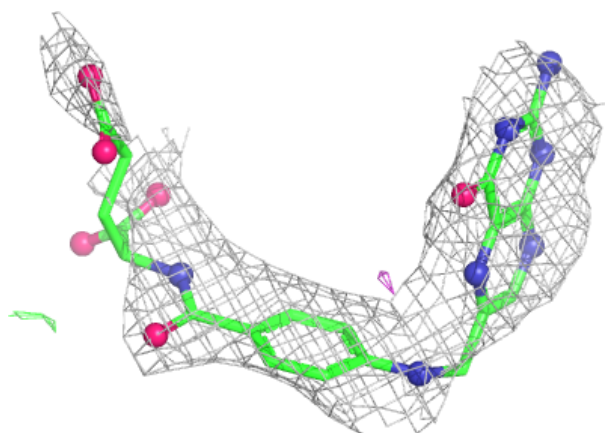
**Electron density around FOL G 703:**

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

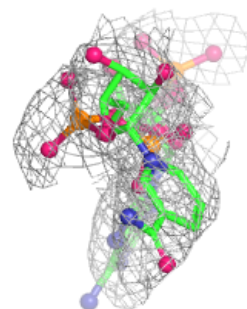
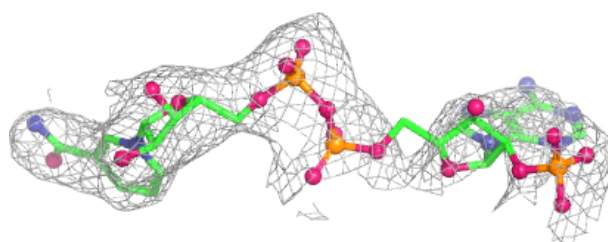
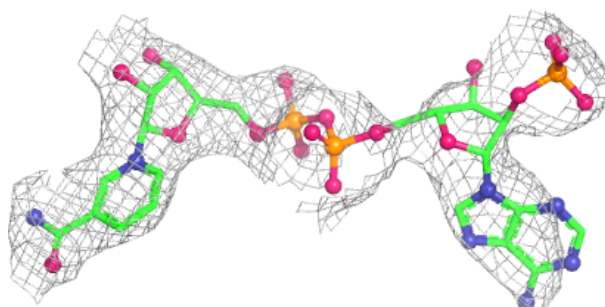


Electron density around FOL H 703:

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

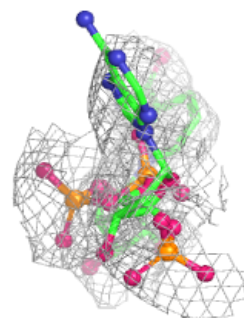
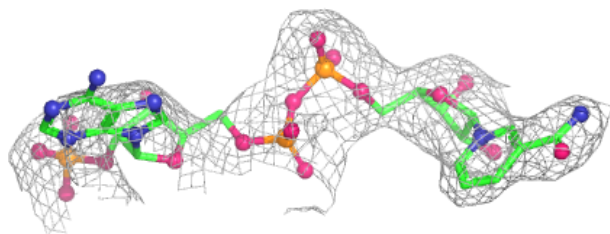
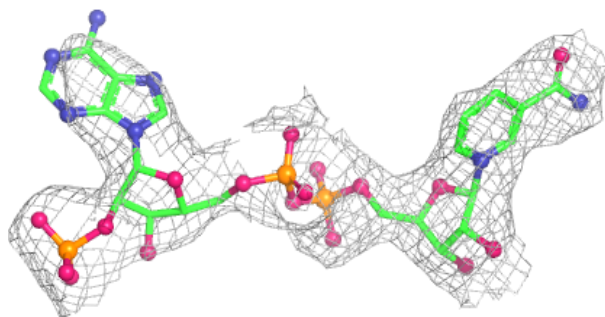
**Electron density around NDP B 704:**

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

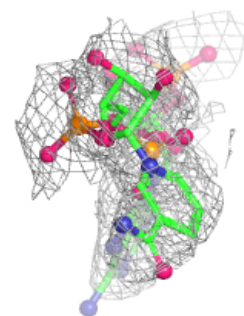
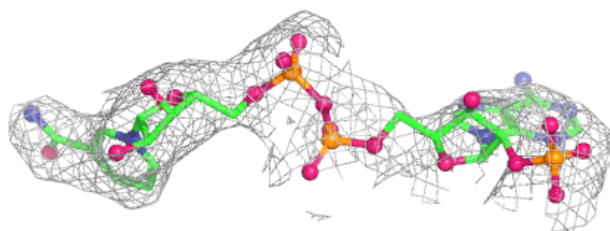
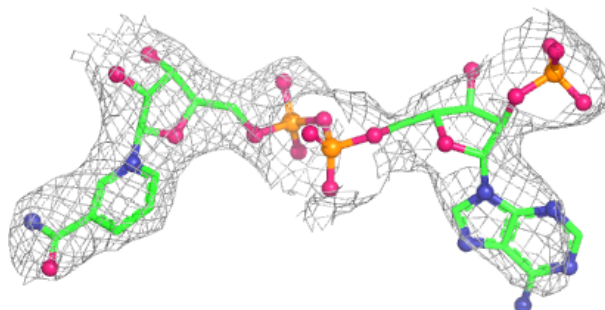


Electron density around NDP D 704:

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

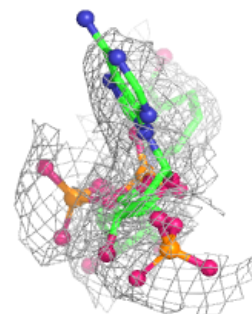
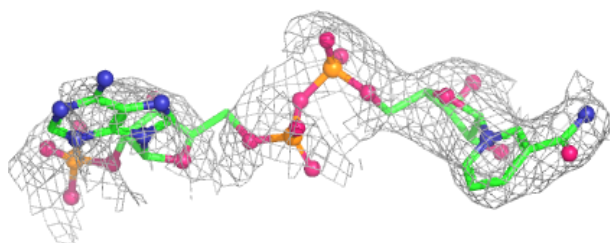
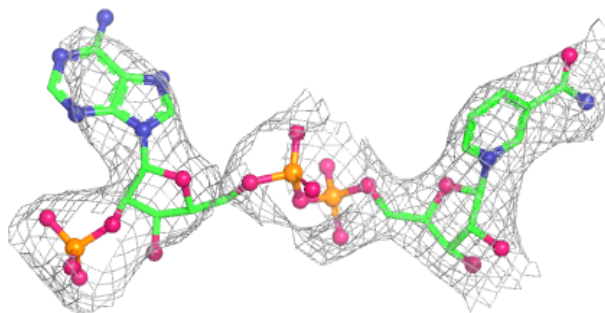
**Electron density around NDP F 704:**

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

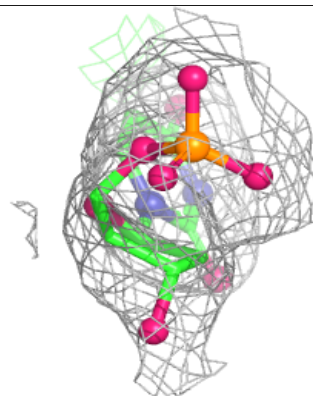
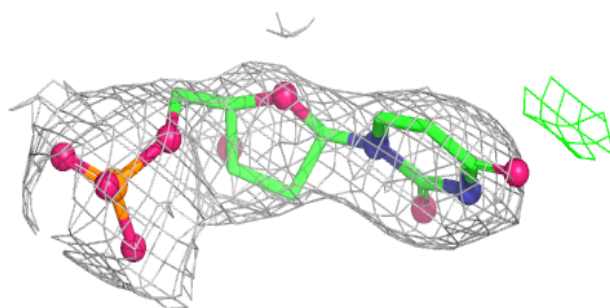
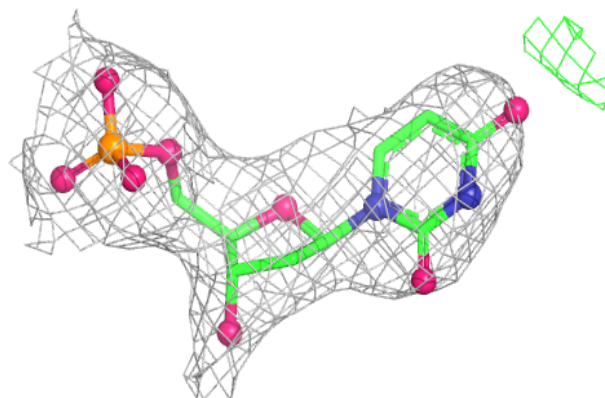


Electron density around NDP H 704:

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

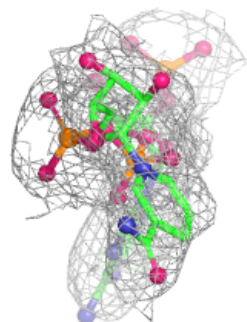
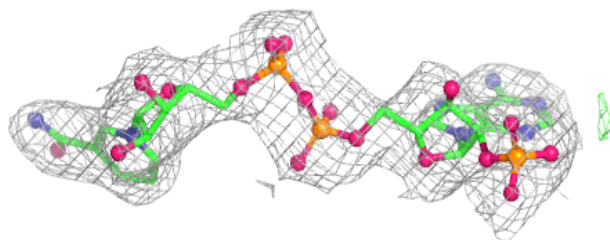
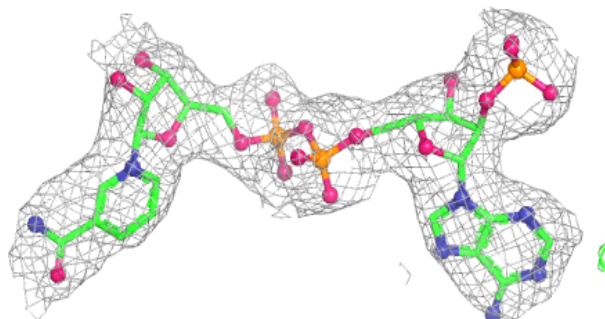
**Electron density around UMP A 701:**

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

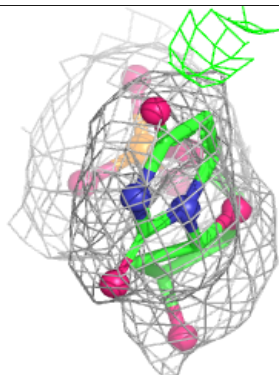
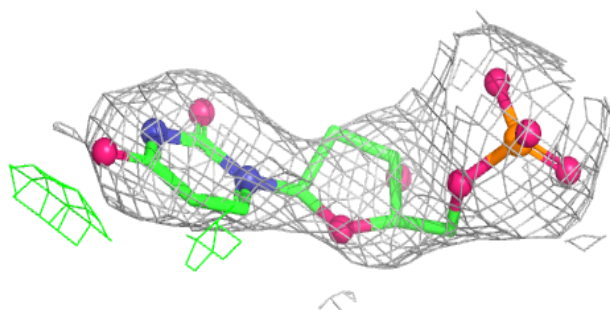
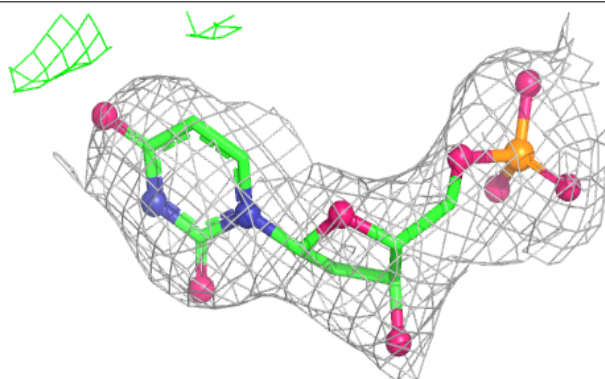


Electron density around NDP C 704:

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

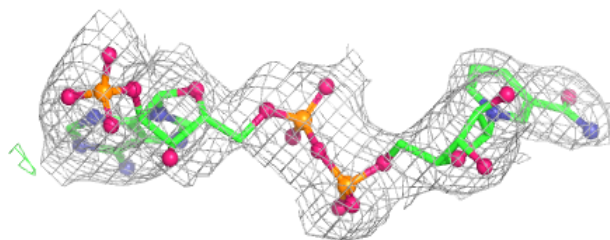
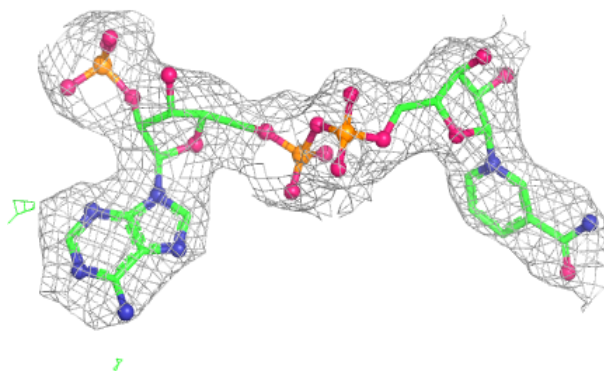
**Electron density around UMP E 701:**

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

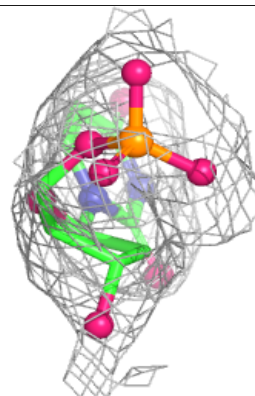
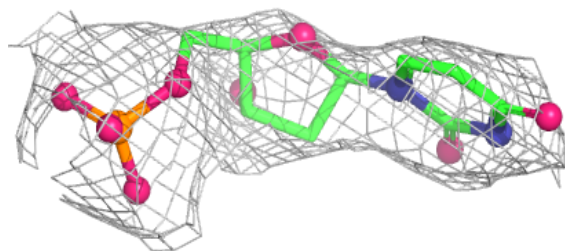
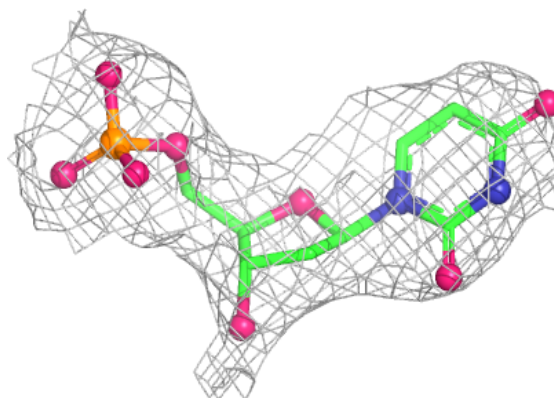


Electron density around NDP E 704:

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

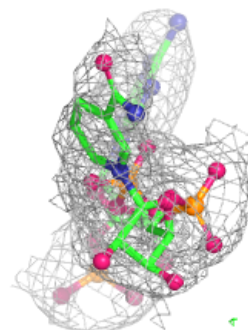
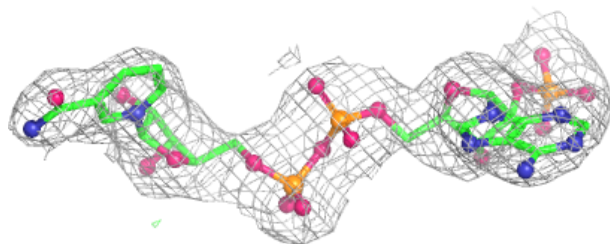
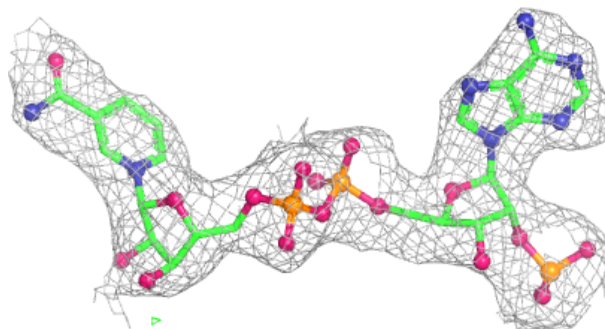
**Electron density around UMP C 701:**

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

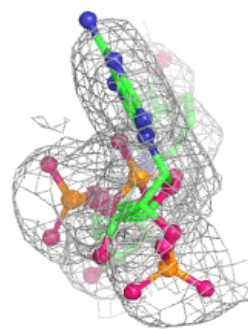
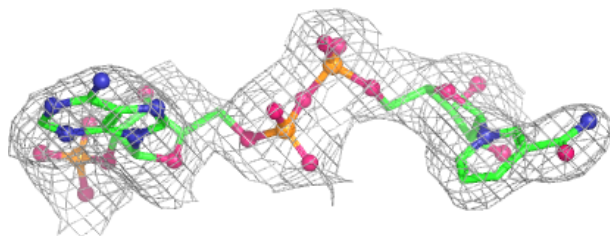
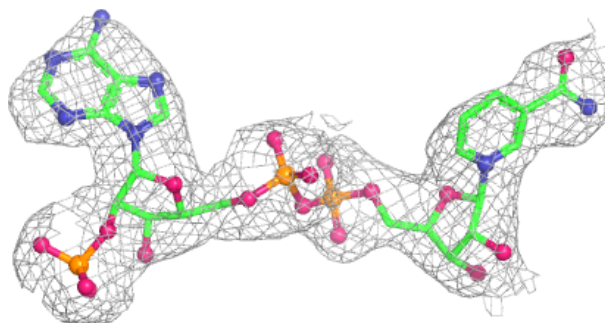


Electron density around NDP G 704:

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

**Electron density around NDP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.