



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 04:25 pm BST

PDB ID : 4KYA
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.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

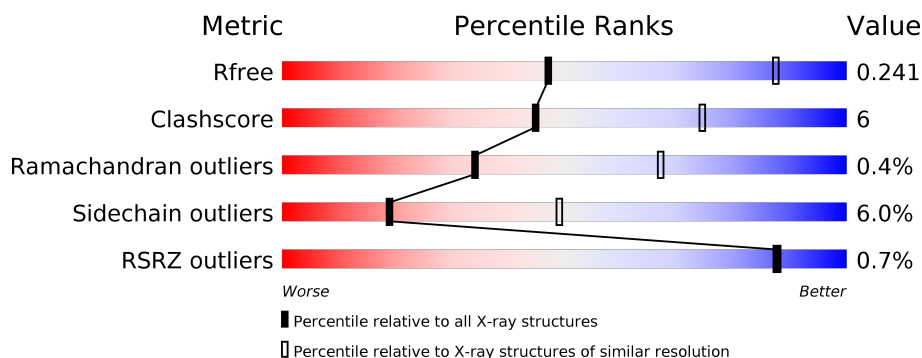
1 Overall quality at a glance

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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 on 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 74%, yellow 15%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 74% 15% 10% </div> </div>
1	B	566	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 72%, yellow 14%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 14% 13% </div> </div>
1	C	566	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 73%, yellow 17%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 73% 17% 10% </div> </div>
1	D	566	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 69%, yellow 16%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 69% 16% 13% </div> </div>
1	E	566	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 73%, yellow 16%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 73% 16% 10% </div> </div>
1	F	566	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 69%, yellow 16%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 69% 16% 13% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	566	 % 73% 16% 10%
1	H	566	 69% 16% 13%

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
3	1UG	C	702	-	-	-	X

2 Entry composition

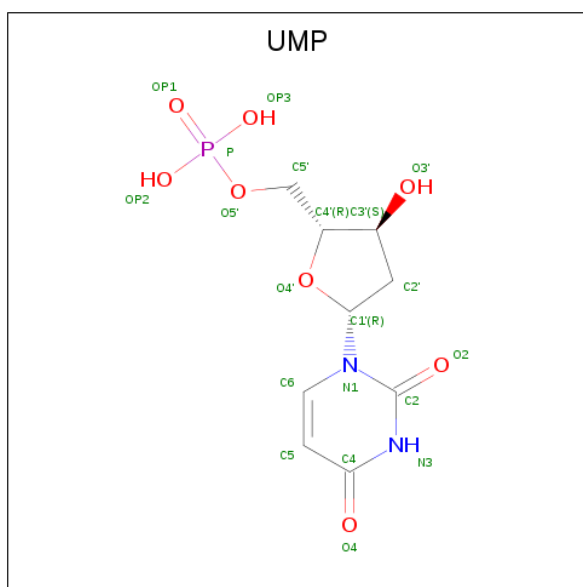
There are 5 unique types of molecules in this entry. The entry contains 33184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

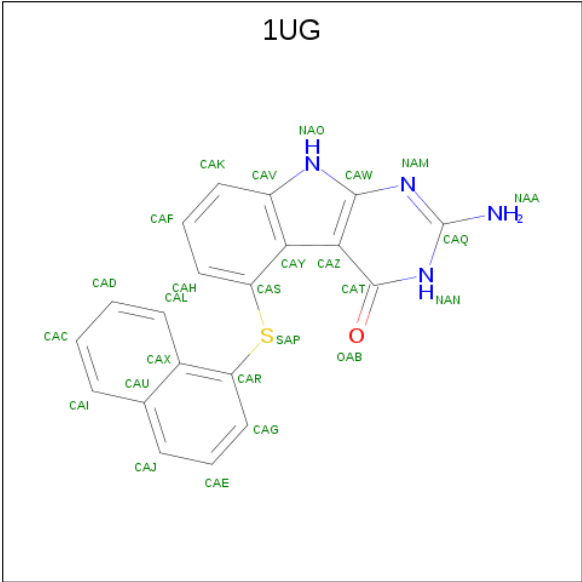
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	B	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	C	510	Total	C	N	O	S	0	2	0
			4096	2618	718	735	25			
1	D	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	E	510	Total	C	N	O	S	0	2	0
			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 (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



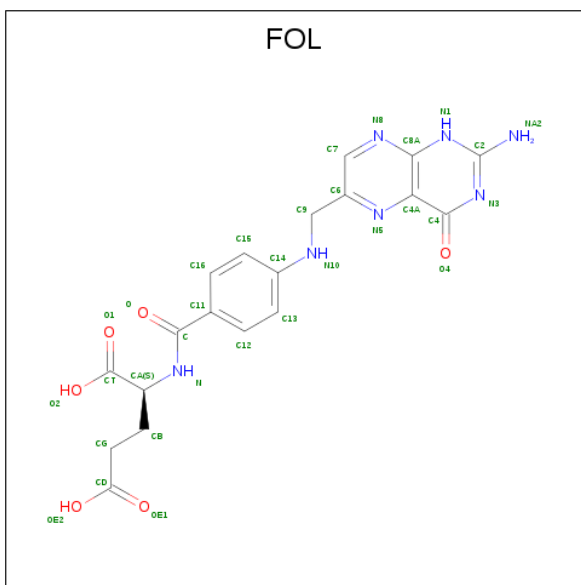
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	G	1	Total	C	N	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 (three-letter code: 1UG) (formula: C₂₀H₁₄N₄OS).



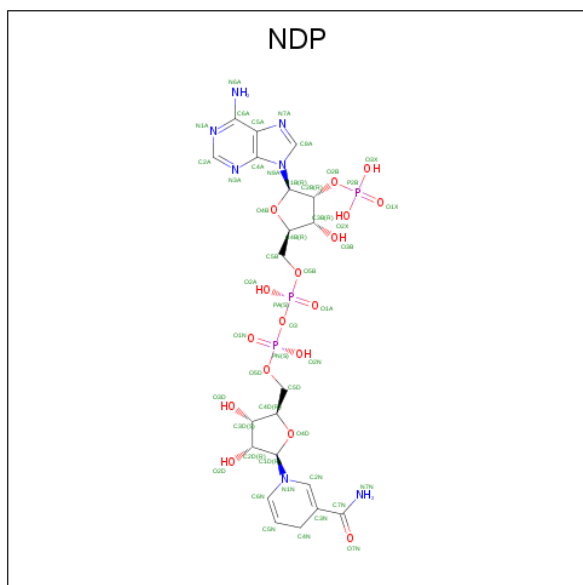
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	B	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	C	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	D	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	E	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	F	1	Total	C	N	O	S	0	0
			26	20	4	1	1		
3	G	1	Total	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 (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).

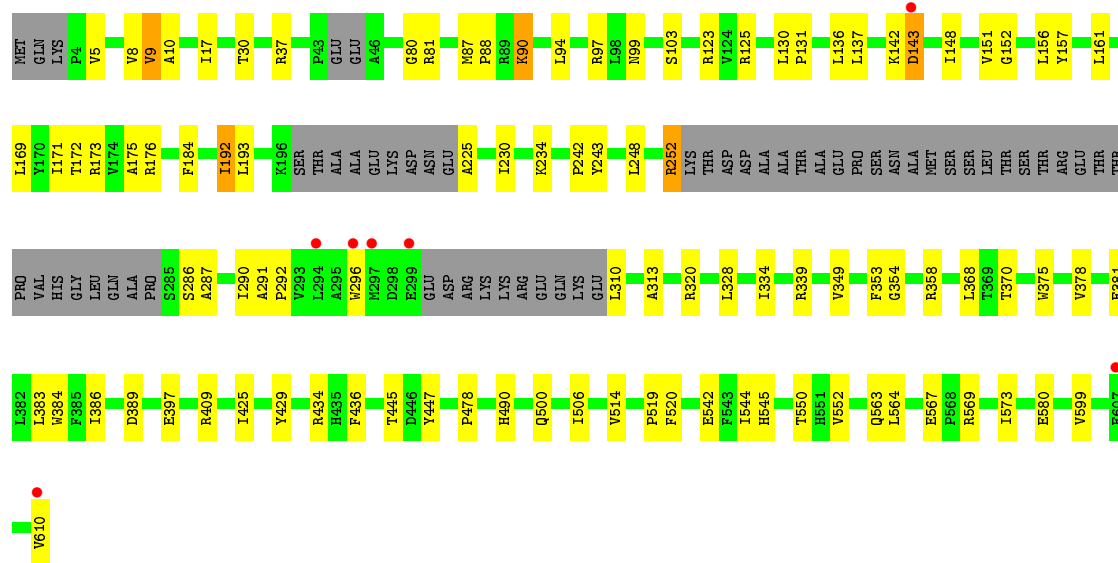


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 32	C 19	N 7	O 6	0	0
4	B	1	Total 32	C 19	N 7	O 6	0	0
4	C	1	Total 32	C 19	N 7	O 6	0	0
4	D	1	Total 32	C 19	N 7	O 6	0	0
4	E	1	Total 32	C 19	N 7	O 6	0	0
4	F	1	Total 32	C 19	N 7	O 6	0	0
4	G	1	Total 32	C 19	N 7	O 6	0	0
4	H	1	Total 32	C 19	N 7	O 6	0	0

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

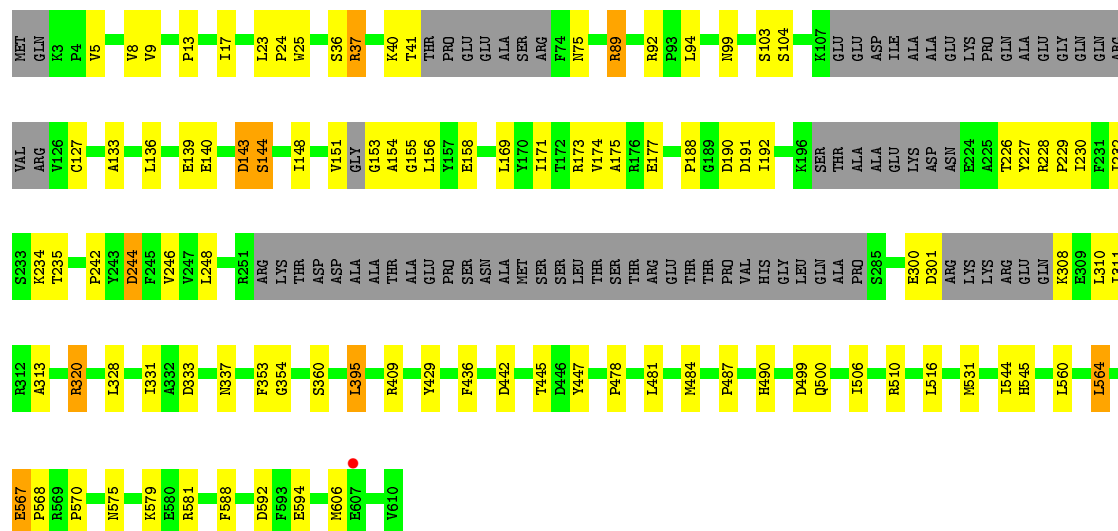


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	G	1	Total 48	C 21	N 7	O 17	P 3	0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



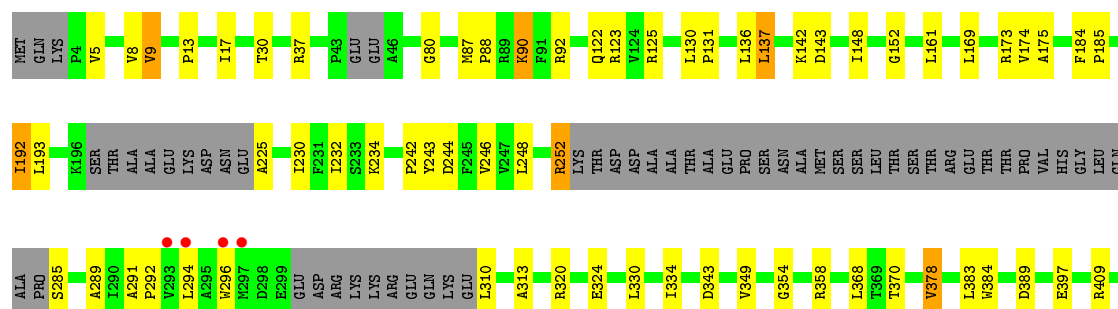
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

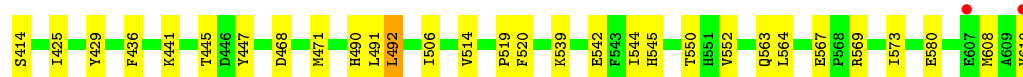
Chain D: 69% 16% 13%



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

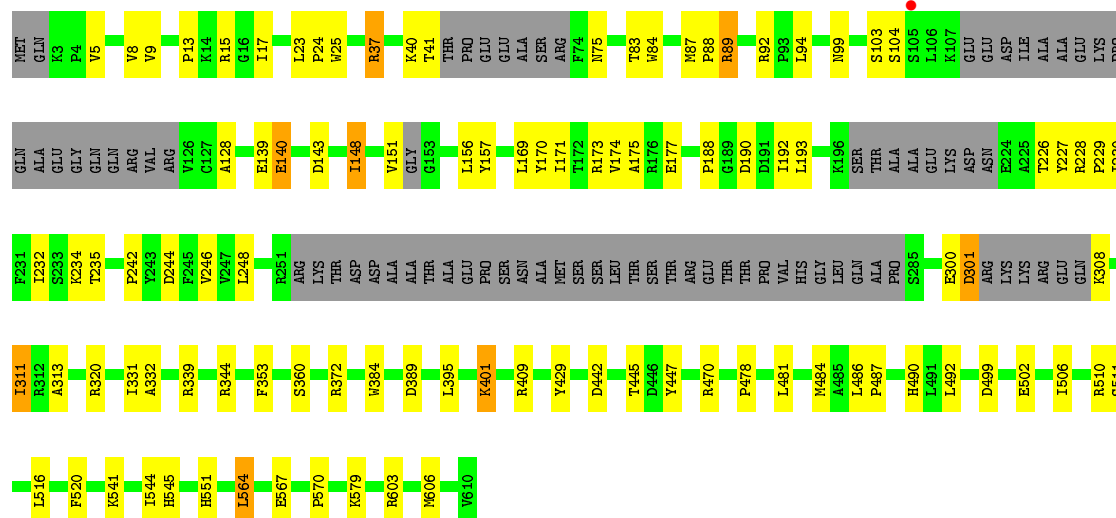
Chain E: 73% 16% 10%





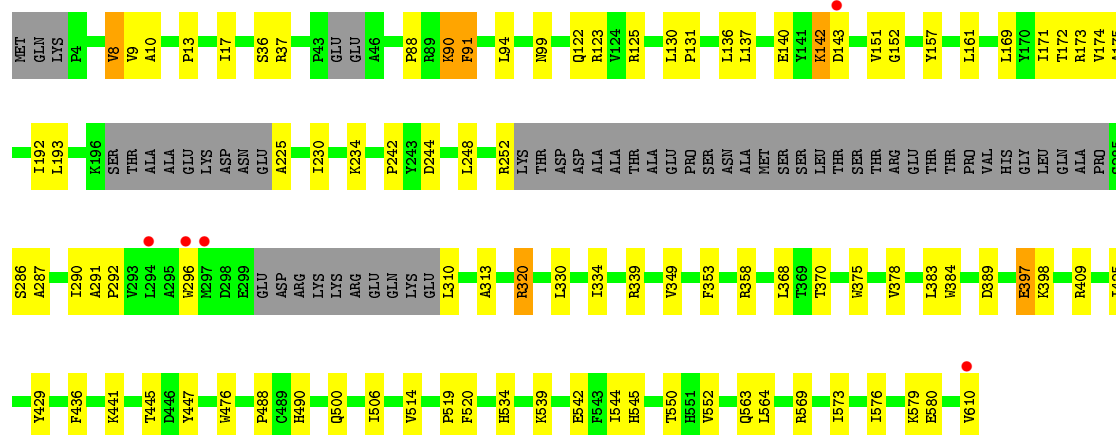
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

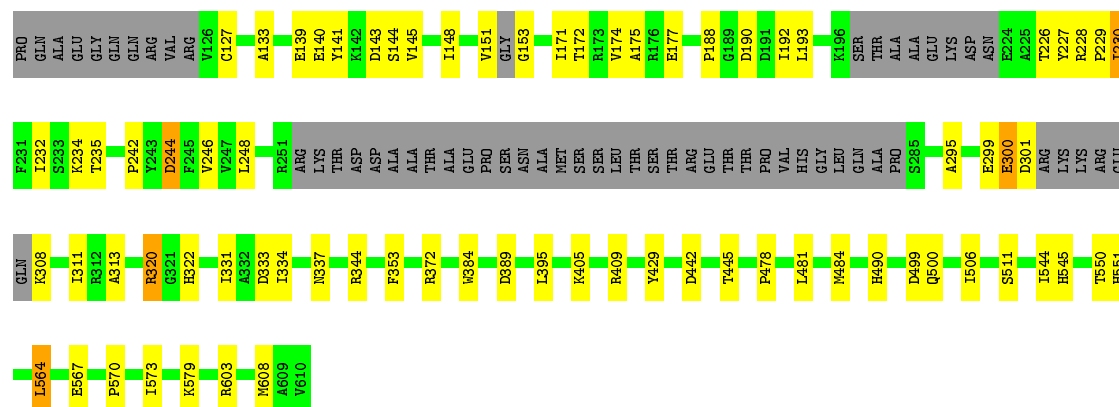
Chain F: 69% 16% 13%



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain G: 73% 16% 10%





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 48.36 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.66-3.26) 98.5 (48.36-3.26)	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 0.183 , 0.241	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)	0.30 , -5.3	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	0.91	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, NDP, UMP, 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	0.24	0/4196	0.42	0/5683
1	B	0.24	0/4043	0.43	0/5473
1	C	0.24	0/4196	0.42	0/5683
1	D	0.23	0/4043	0.43	0/5473
1	E	0.24	0/4196	0.42	0/5683
1	F	0.24	0/4043	0.43	0/5473
1	G	0.24	0/4196	0.42	0/5683
1	H	0.24	0/4043	0.43	0/5473
All	All	0.24	0/32956	0.43	0/44624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4096	0	4058	47	0
1	B	3948	0	3910	50	0
1	C	4096	0	4058	58	0
1	D	3948	0	3910	59	0
1	E	4096	0	4058	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3948	0	3910	57	0
1	G	4096	0	4058	56	0
1	H	3948	0	3910	49	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	3	0
3	C	26	0	14	4	0
3	D	26	0	14	1	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	1	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	3	0
All	All	33184	0	32416	425	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 6.

The worst 5 of 425 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:E:313:ALA:O	1:E:320:ARG:NH2	2.14	0.79
1:A:313:ALA:O	1:A:320:ARG:NH2	2.16	0.77
1:F:244:ASP:HB2	1:F:570:PRO:HG3	1.66	0.76
1:G:313:ALA:O	1:G:320:ARG:NH2	2.17	0.76
1:B:313:ALA:O	1:B:320:ARG:NH1	2.19	0.74

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%)	47	77
1	B	478/566 (84%)	447 (94%)	29 (6%)	2 (0%)	34	67
1	C	502/566 (89%)	485 (97%)	15 (3%)	2 (0%)	34	67
1	D	478/566 (84%)	448 (94%)	27 (6%)	3 (1%)	25	59
1	E	502/566 (89%)	486 (97%)	15 (3%)	1 (0%)	47	77
1	F	478/566 (84%)	448 (94%)	28 (6%)	2 (0%)	34	67
1	G	502/566 (89%)	485 (97%)	15 (3%)	2 (0%)	34	67
1	H	478/566 (84%)	449 (94%)	25 (5%)	4 (1%)	19	52
All	All	3920/4528 (87%)	3730 (95%)	173 (4%)	17 (0%)	34	67

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	429	TYR
1	H	429	TYR
1	E	429	TYR
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%)	417 (94%)	27 (6%)	18	49
1	B	431/491 (88%)	409 (95%)	22 (5%)	24	54
1	C	444/491 (90%)	420 (95%)	24 (5%)	22	53
1	D	431/491 (88%)	406 (94%)	25 (6%)	20	50
1	E	444/491 (90%)	412 (93%)	32 (7%)	14	41
1	F	431/491 (88%)	404 (94%)	27 (6%)	18	47
1	G	444/491 (90%)	418 (94%)	26 (6%)	19	50
1	H	431/491 (88%)	403 (94%)	28 (6%)	17	46
All	All	3500/3928 (89%)	3289 (94%)	211 (6%)	19	49

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	564	LEU
1	E	378	VAL
1	H	228	ARG
1	E	5	VAL
1	E	143	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	563	GLN
1	E	99	ASN
1	G	563	GLN
1	D	99	ASN
1	E	117	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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	1UG	G	702	-	28,30,30	1.76	6 (21%)	31,44,44	2.59	14 (45%)
4	FOL	A	703	-	28,34,34	1.53	4 (14%)	36,47,47	2.48	12 (33%)
4	FOL	F	703	-	28,34,34	1.47	4 (14%)	36,47,47	2.33	12 (33%)
3	1UG	H	702	-	28,30,30	1.74	6 (21%)	31,44,44	2.74	15 (48%)
5	NDP	H	704	-	45,52,52	1.04	2 (4%)	53,80,80	1.20	4 (7%)
5	NDP	G	704	-	45,52,52	1.04	2 (4%)	53,80,80	1.25	4 (7%)
2	UMP	E	701	-	18,21,21	1.14	1 (5%)	21,31,31	1.47	4 (19%)
5	NDP	F	704	-	45,52,52	1.04	2 (4%)	53,80,80	1.20	3 (5%)
4	FOL	B	703	-	28,34,34	1.48	4 (14%)	36,47,47	2.33	12 (33%)
3	1UG	D	702	-	28,30,30	1.74	7 (25%)	31,44,44	2.74	15 (48%)
5	NDP	E	704	-	45,52,52	1.05	2 (4%)	53,80,80	1.25	5 (9%)
2	UMP	C	701	-	18,21,21	1.13	1 (5%)	21,31,31	1.49	4 (19%)
2	UMP	F	701	-	18,21,21	1.16	1 (5%)	21,31,31	1.40	5 (23%)
5	NDP	D	704	-	45,52,52	1.04	2 (4%)	53,80,80	1.19	2 (3%)
5	NDP	C	704	-	45,52,52	1.03	2 (4%)	53,80,80	1.26	7 (13%)
4	FOL	H	703	-	28,34,34	1.48	4 (14%)	36,47,47	2.34	12 (33%)
2	UMP	H	701	-	18,21,21	1.15	1 (5%)	21,31,31	1.41	5 (23%)
3	1UG	E	702	-	28,30,30	1.75	7 (25%)	31,44,44	2.57	12 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FOL	C	703	-	28,34,34	1.52	4 (14%)	36,47,47	2.47	12 (33%)
3	1UG	B	702	-	28,30,30	1.74	7 (25%)	31,44,44	2.70	15 (48%)
3	1UG	C	702	-	28,30,30	1.77	6 (21%)	31,44,44	2.59	13 (41%)
5	NDP	B	704	-	45,52,52	1.04	2 (4%)	53,80,80	1.21	4 (7%)
4	FOL	D	703	-	28,34,34	1.48	4 (14%)	36,47,47	2.31	12 (33%)
2	UMP	B	701	-	18,21,21	1.15	1 (5%)	21,31,31	1.41	5 (23%)
2	UMP	A	701	-	18,21,21	1.14	1 (5%)	21,31,31	1.48	4 (19%)
3	1UG	A	702	-	28,30,30	1.79	7 (25%)	31,44,44	2.73	14 (45%)
4	FOL	G	703	-	28,34,34	1.51	4 (14%)	36,47,47	2.44	11 (30%)
2	UMP	D	701	-	18,21,21	1.15	1 (5%)	21,31,31	1.42	4 (19%)
5	NDP	A	704	-	45,52,52	1.03	2 (4%)	53,80,80	1.25	6 (11%)
4	FOL	E	703	-	28,34,34	1.52	4 (14%)	36,47,47	2.45	12 (33%)
2	UMP	G	701	-	18,21,21	1.15	1 (5%)	21,31,31	1.47	4 (19%)
3	1UG	F	702	-	28,30,30	1.74	6 (21%)	31,44,44	2.63	14 (45%)

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	1UG	G	702	-	-	0/4/4/4	0/5/5/5
4	FOL	A	703	-	-	3/16/22/22	0/3/3/3
4	FOL	F	703	-	-	2/16/22/22	0/3/3/3
3	1UG	H	702	-	-	2/4/4/4	0/5/5/5
5	NDP	H	704	-	-	8/30/77/77	0/5/5/5
5	NDP	G	704	-	-	3/30/77/77	0/5/5/5
2	UMP	E	701	-	-	3/7/22/22	0/2/2/2
5	NDP	F	704	-	-	7/30/77/77	0/5/5/5
4	FOL	B	703	-	-	2/16/22/22	0/3/3/3
3	1UG	D	702	-	-	2/4/4/4	0/5/5/5
5	NDP	E	704	-	-	3/30/77/77	0/5/5/5
2	UMP	C	701	-	-	4/7/22/22	0/2/2/2
2	UMP	F	701	-	-	2/7/22/22	0/2/2/2
5	NDP	D	704	-	-	9/30/77/77	0/5/5/5
5	NDP	C	704	-	-	3/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FOL	H	703	-	-	2/16/22/22	0/3/3/3
2	UMP	H	701	-	-	2/7/22/22	0/2/2/2
3	1UG	E	702	-	-	0/4/4/4	0/5/5/5
4	FOL	C	703	-	-	3/16/22/22	0/3/3/3
3	1UG	B	702	-	-	2/4/4/4	0/5/5/5
3	1UG	C	702	-	-	0/4/4/4	0/5/5/5
5	NDP	B	704	-	-	7/30/77/77	0/5/5/5
4	FOL	D	703	-	-	2/16/22/22	0/3/3/3
2	UMP	B	701	-	-	3/7/22/22	0/2/2/2
2	UMP	A	701	-	-	4/7/22/22	0/2/2/2
3	1UG	A	702	-	-	2/4/4/4	0/5/5/5
4	FOL	G	703	-	-	3/16/22/22	0/3/3/3
2	UMP	D	701	-	-	3/7/22/22	0/2/2/2
5	NDP	A	704	-	-	3/30/77/77	0/5/5/5
4	FOL	E	703	-	-	3/16/22/22	0/3/3/3
2	UMP	G	701	-	-	3/7/22/22	0/2/2/2
3	1UG	F	702	-	-	1/4/4/4	0/5/5/5

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	FOL	C4A-C8A	4.41	1.49	1.40
4	E	703	FOL	C4A-C8A	4.38	1.49	1.40
3	H	702	1UG	CAT-NAN	4.37	1.40	1.33
3	B	702	1UG	CAT-NAN	4.35	1.40	1.33
4	C	703	FOL	C4A-C8A	4.35	1.49	1.40

The worst 5 of 277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	703	FOL	N8-C8A-N1	7.64	124.54	115.82
4	B	703	FOL	N8-C8A-N1	7.57	124.46	115.82
4	F	703	FOL	N8-C8A-N1	7.49	124.37	115.82
4	D	703	FOL	N8-C8A-N1	7.48	124.36	115.82
4	G	703	FOL	N8-C8A-N1	6.99	123.80	115.82

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	FOL	CT-CA-CB-CG
4	A	703	FOL	CA-CB-CG-CD
3	H	702	1UG	CAG-CAR-SAP-CAS
3	H	702	1UG	CAX-CAR-SAP-CAS
5	H	704	NDP	C5B-O5B-PA-O3

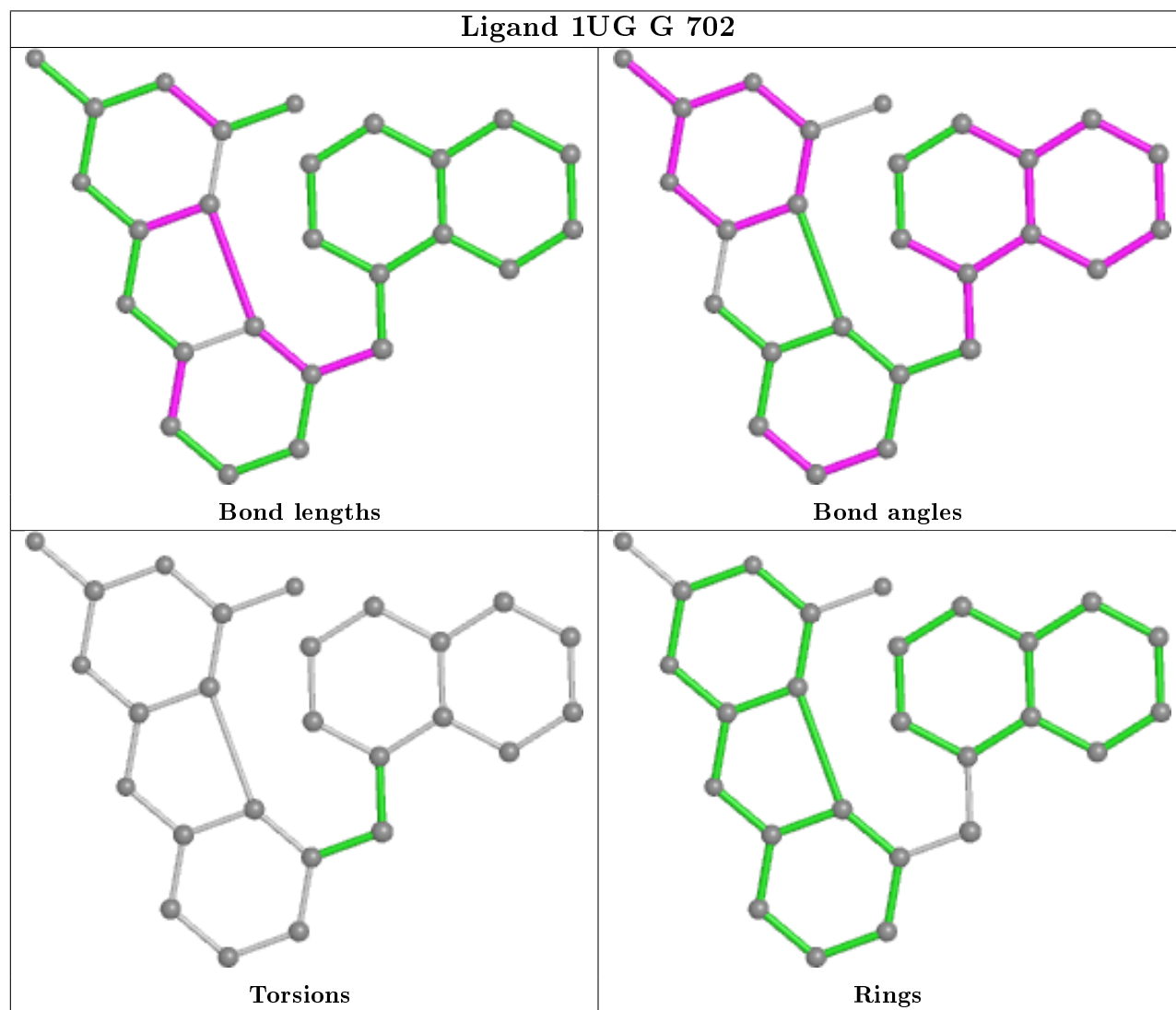
There are no ring outliers.

24 monomers are involved in 63 short contacts:

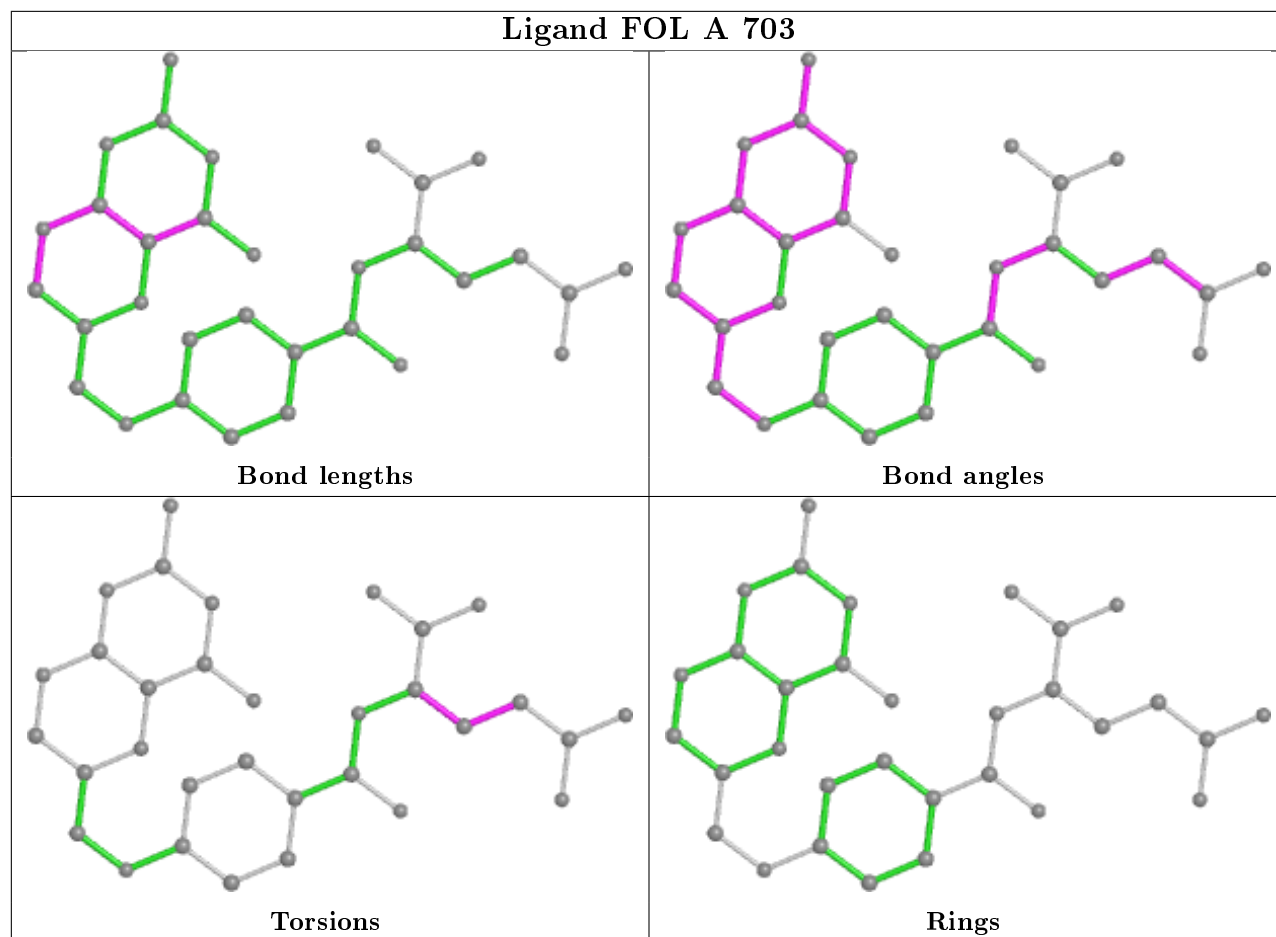
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	702	1UG	3	0
4	A	703	FOL	1	0
4	F	703	FOL	4	0
3	H	702	1UG	1	0
5	H	704	NDP	3	0
5	G	704	NDP	3	0
5	F	704	NDP	5	0
4	B	703	FOL	4	0
3	D	702	1UG	1	0
5	E	704	NDP	3	0
5	D	704	NDP	4	0
5	C	704	NDP	3	0
4	H	703	FOL	4	0
3	E	702	1UG	5	0
4	C	703	FOL	1	0
3	B	702	1UG	3	0
3	C	702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

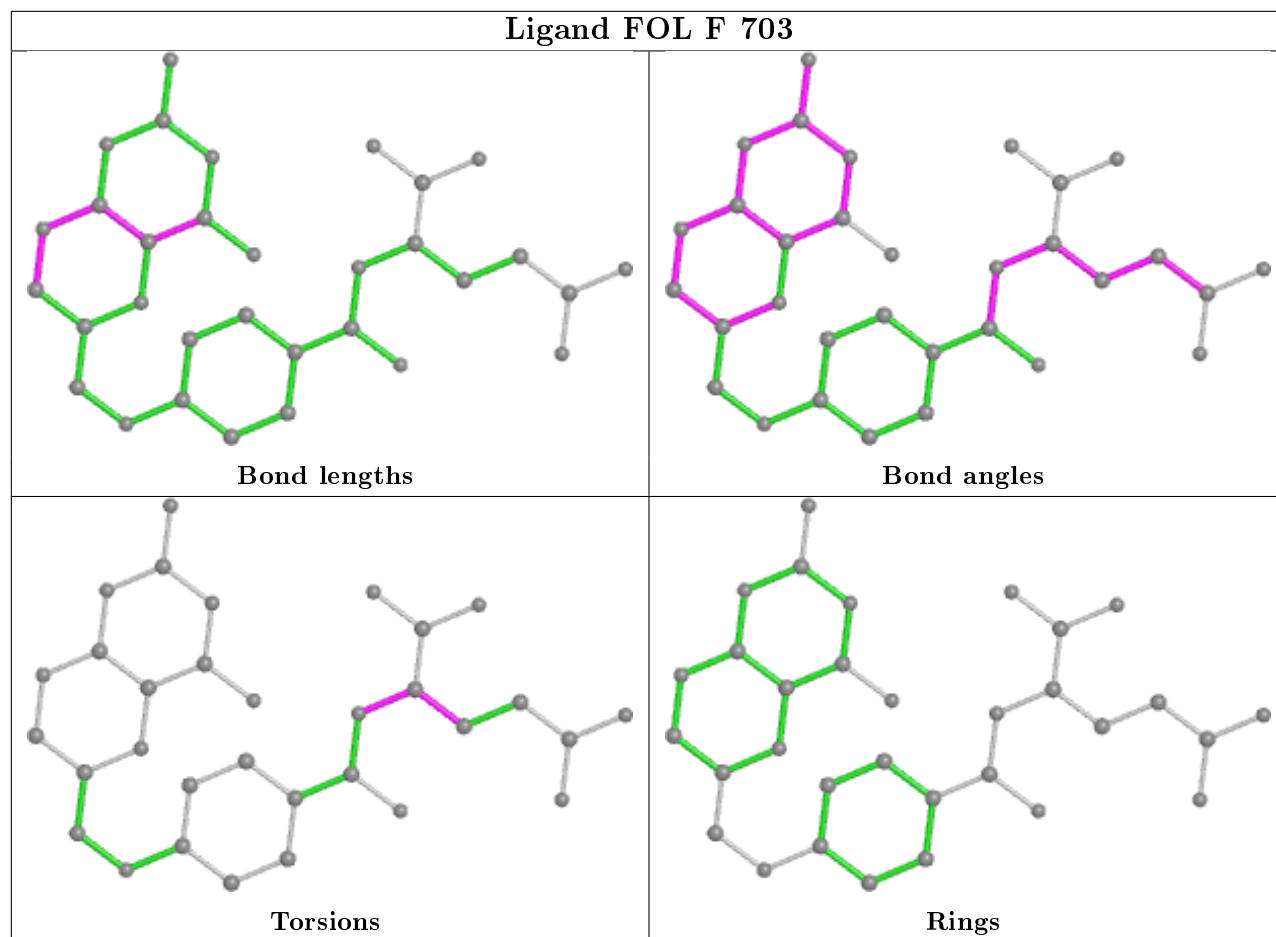
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

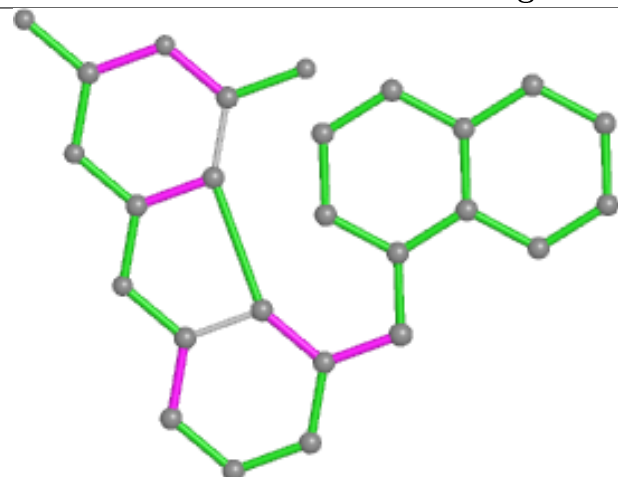


Ligand FOL A 703

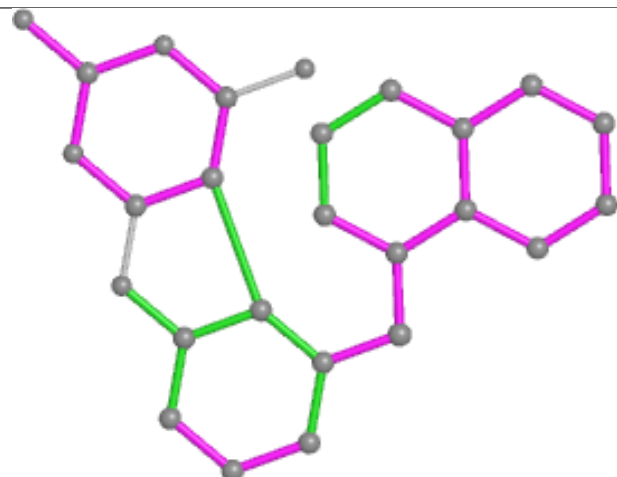




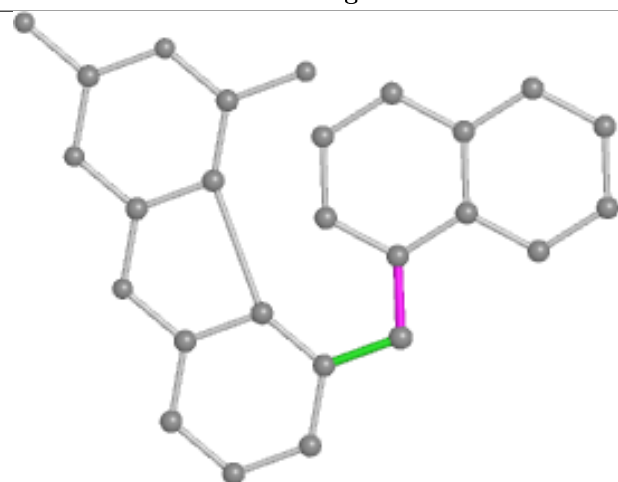
Ligand 1UG H 702



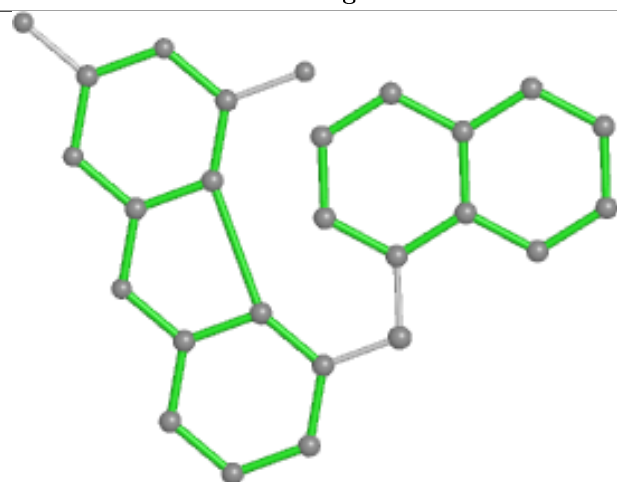
Bond lengths



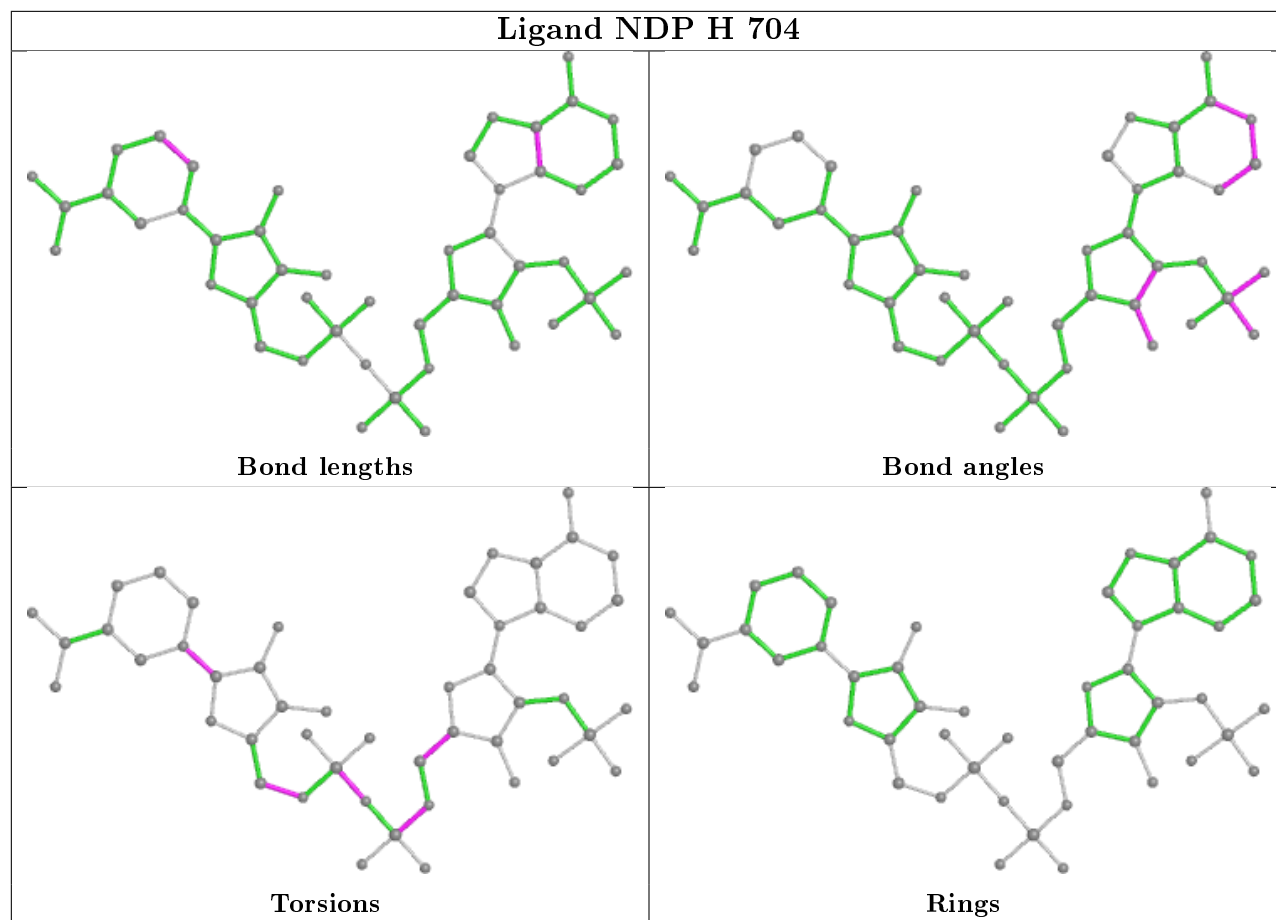
Bond angles

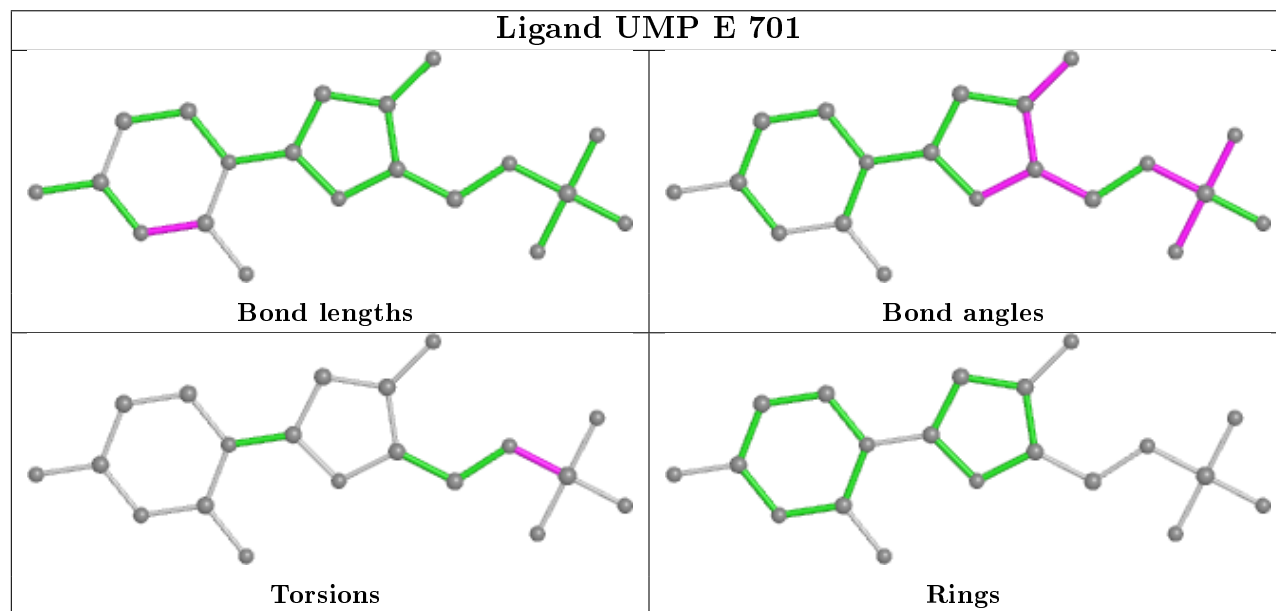
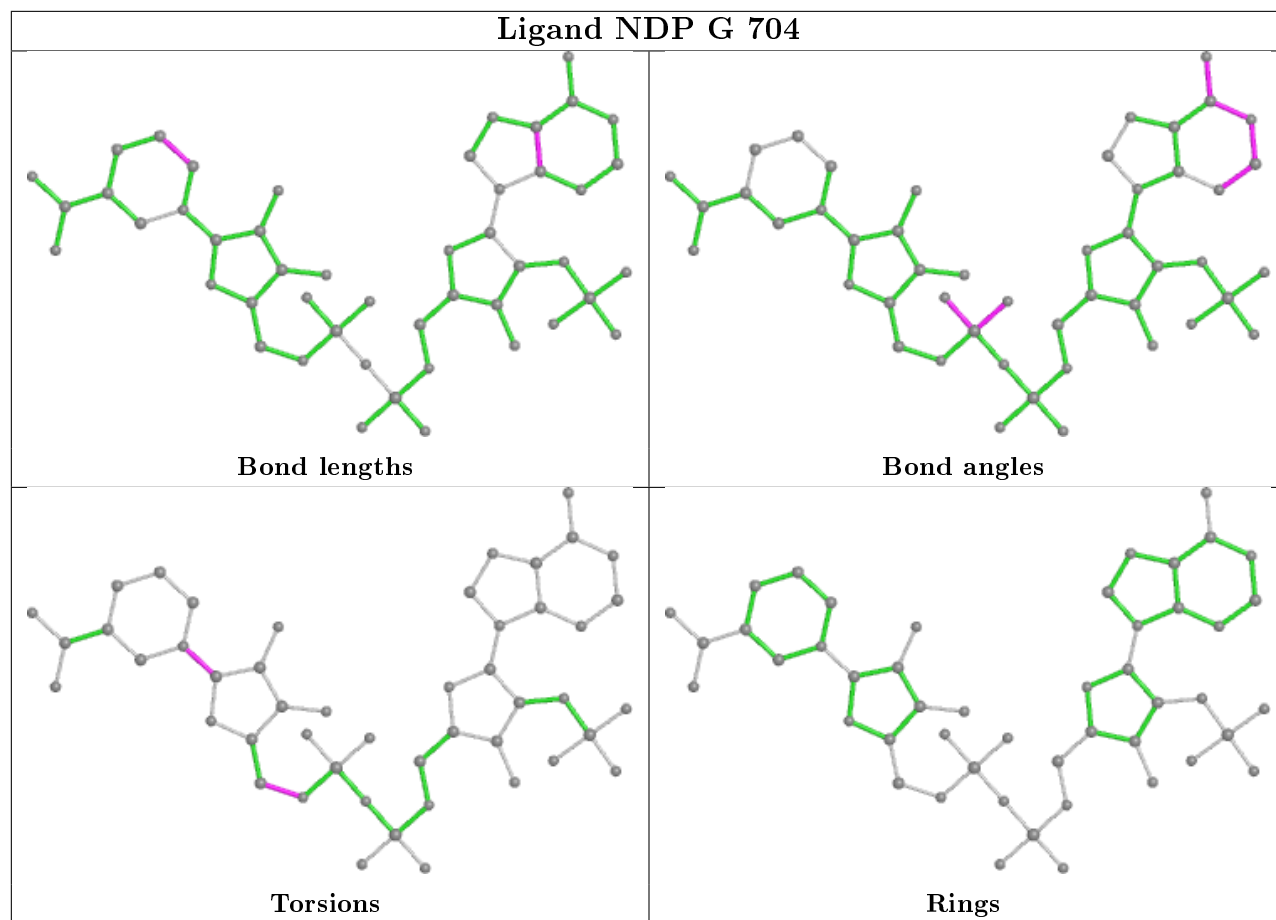


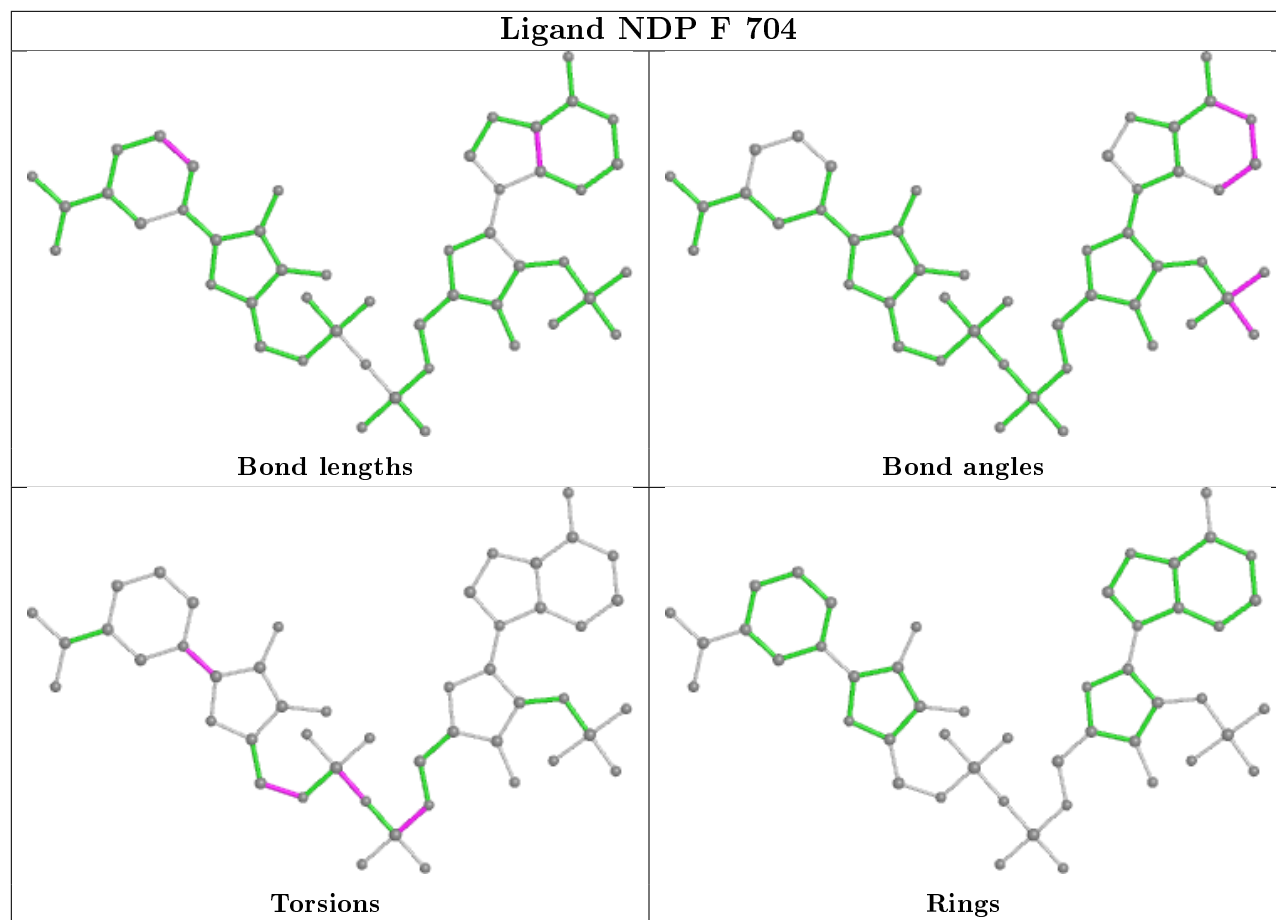
Torsions

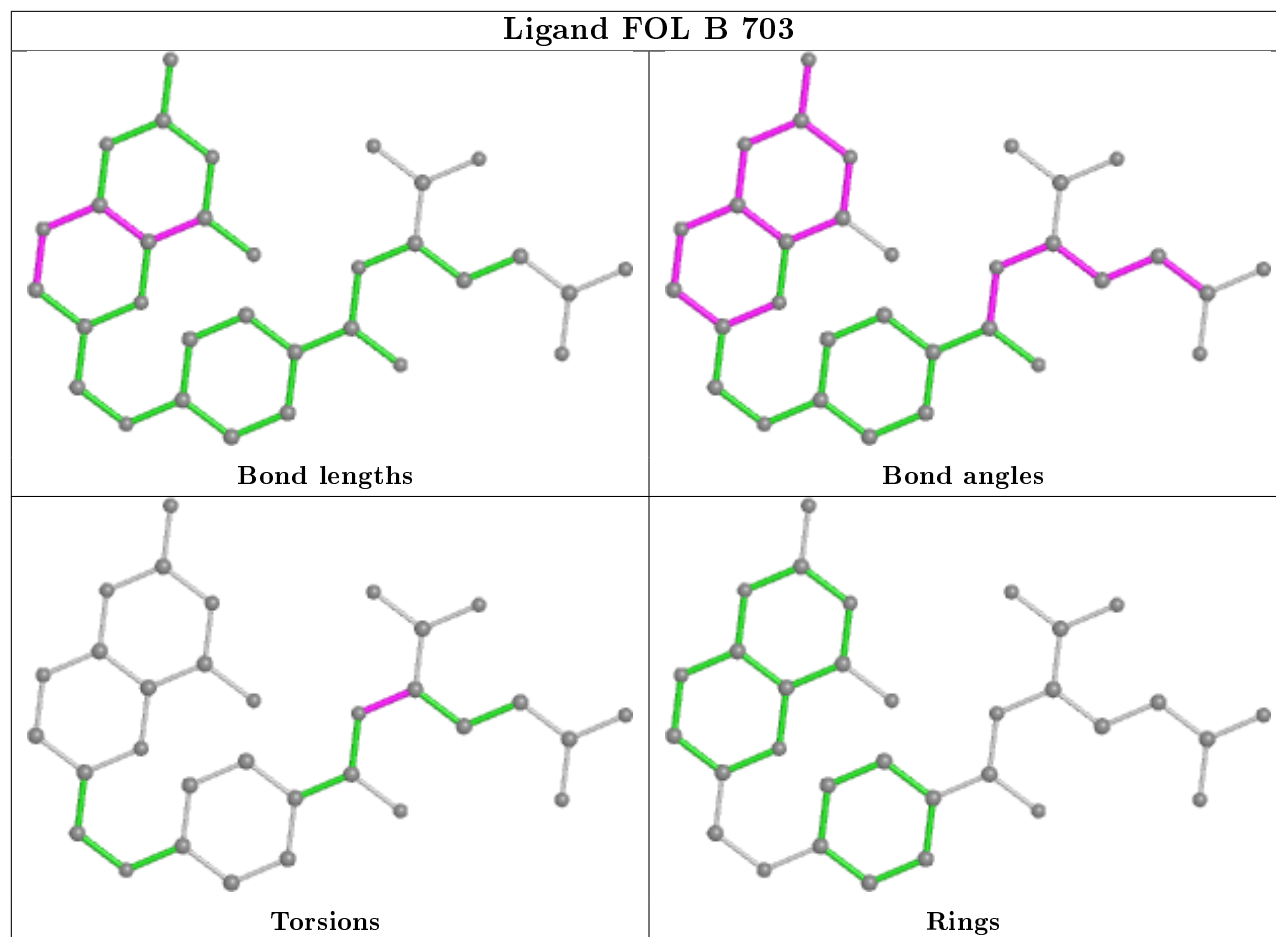


Rings

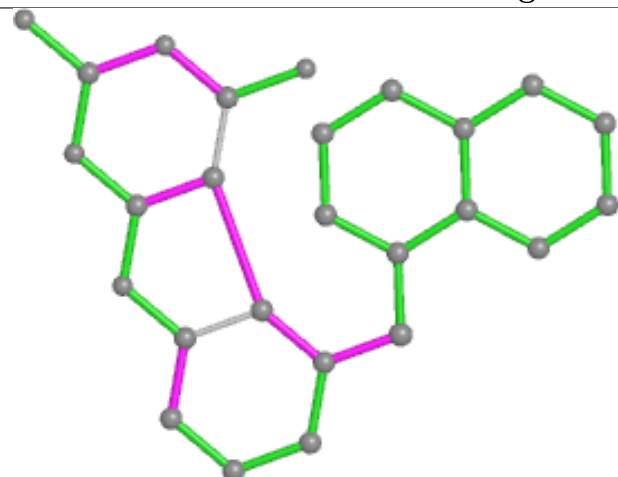




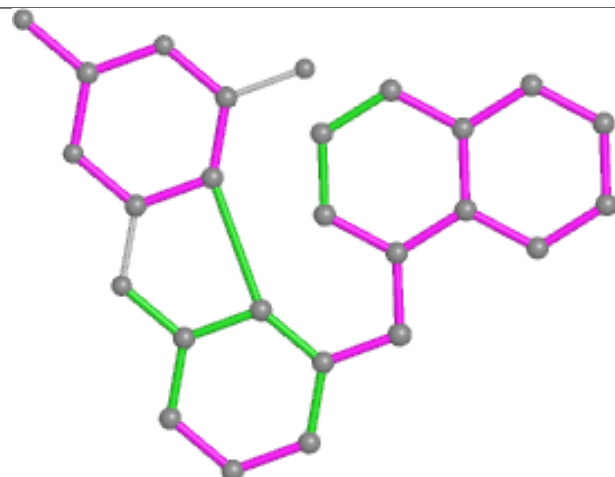




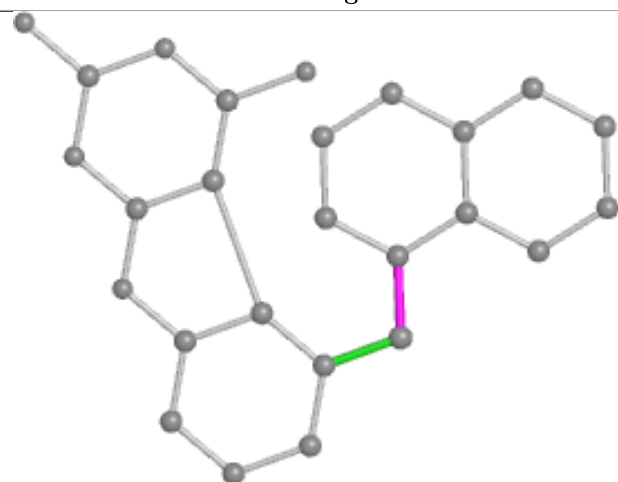
Ligand 1UG D 702



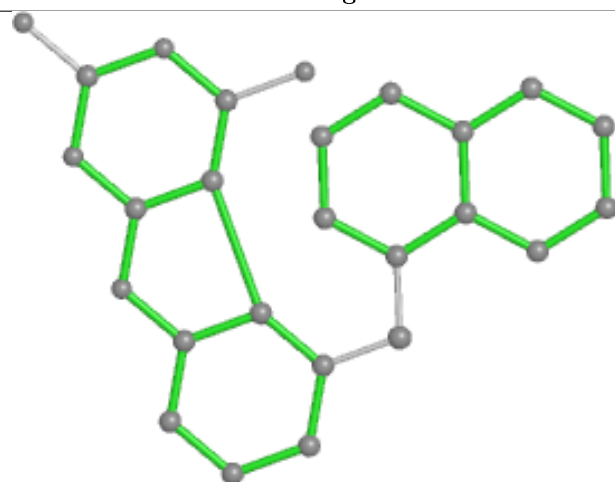
Bond lengths



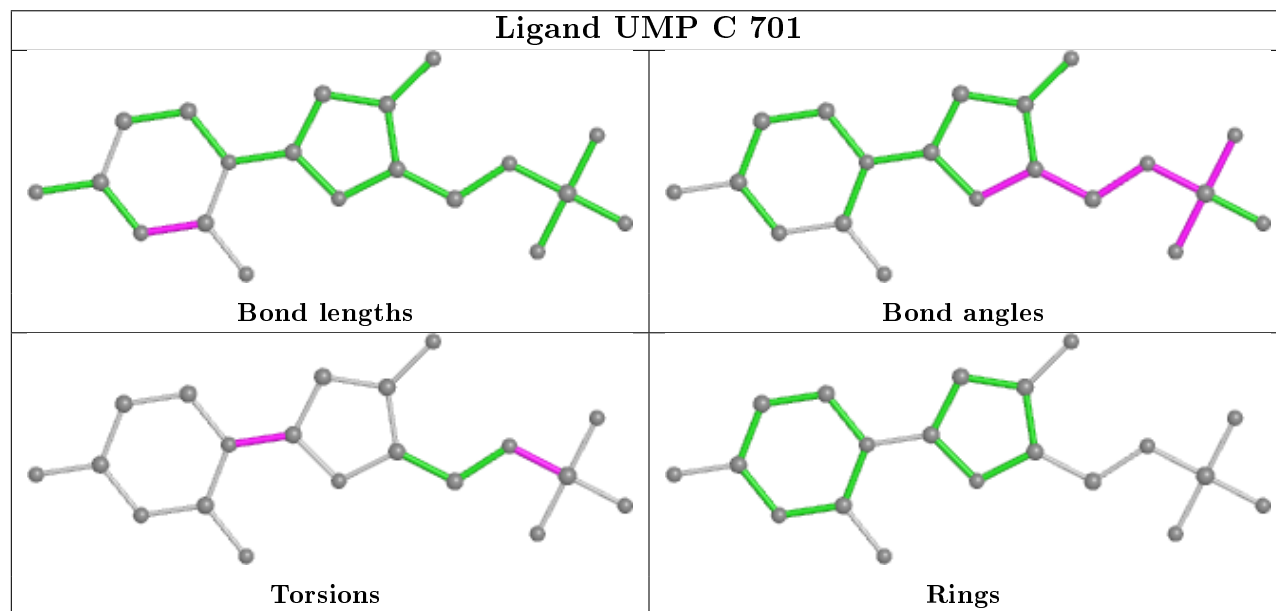
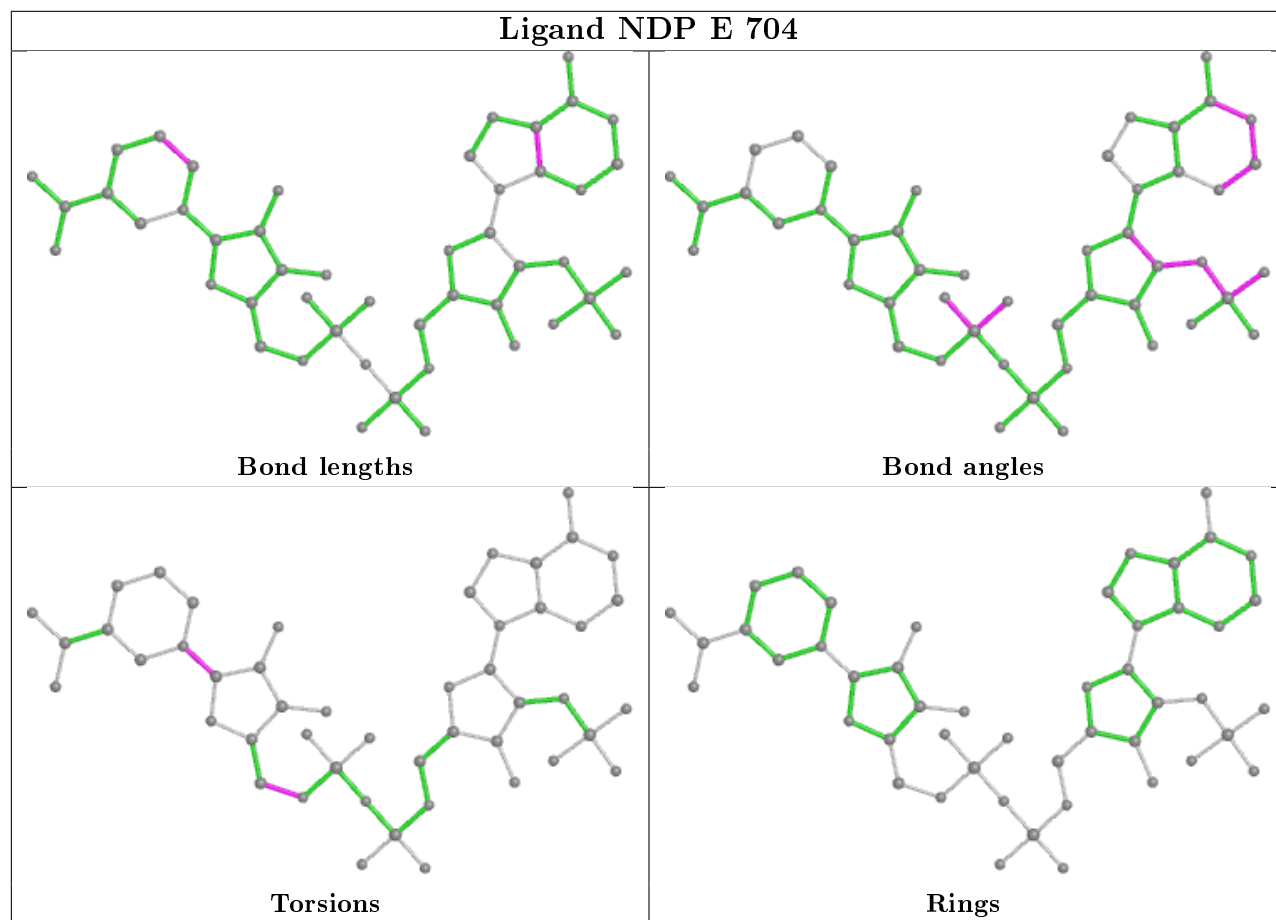
Bond angles

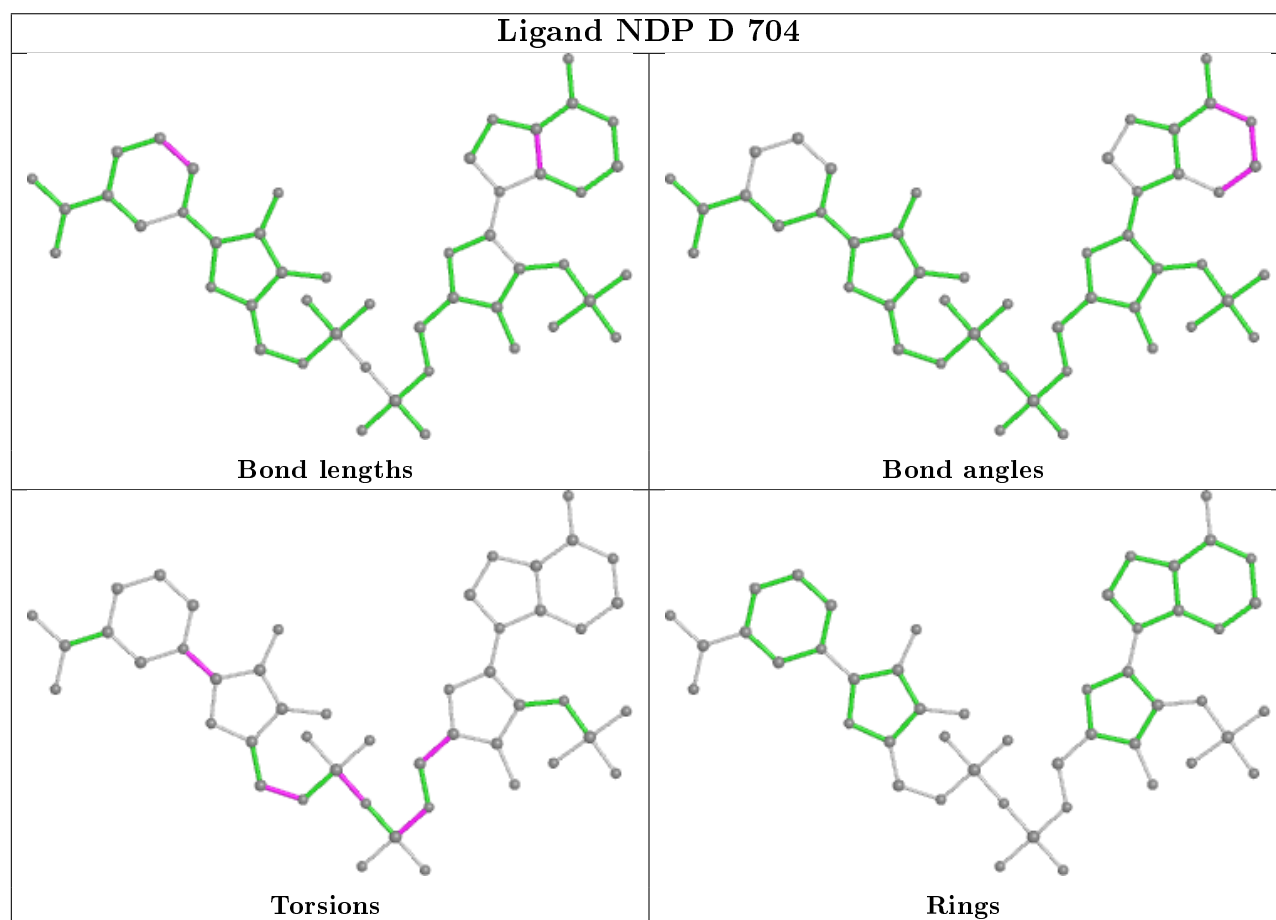
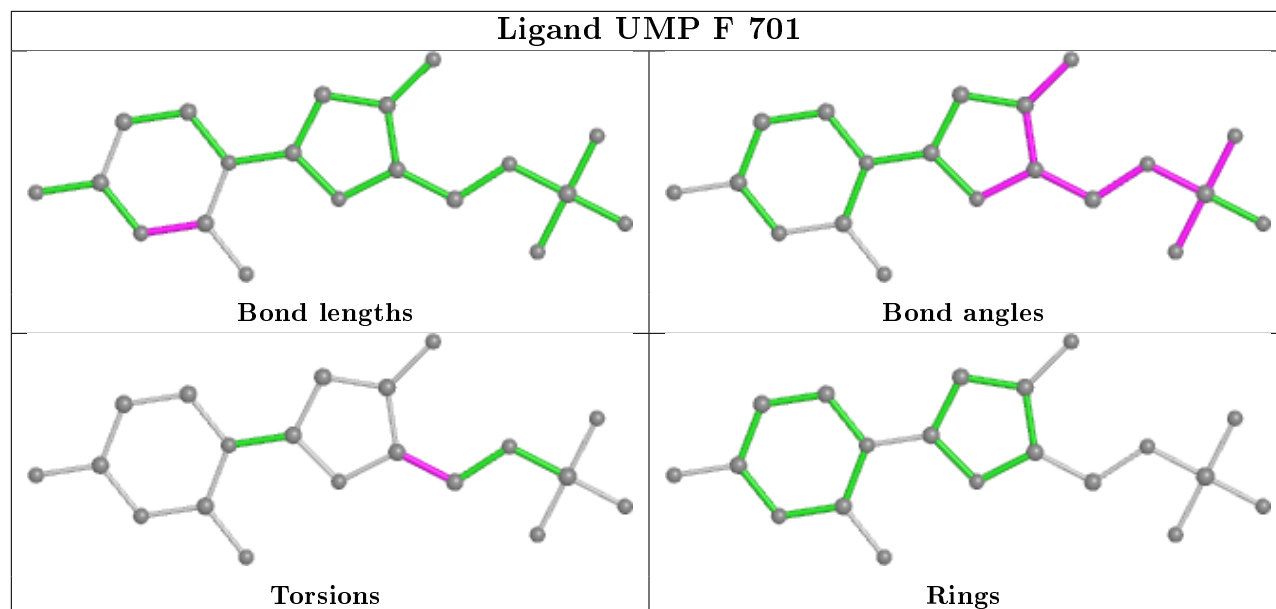


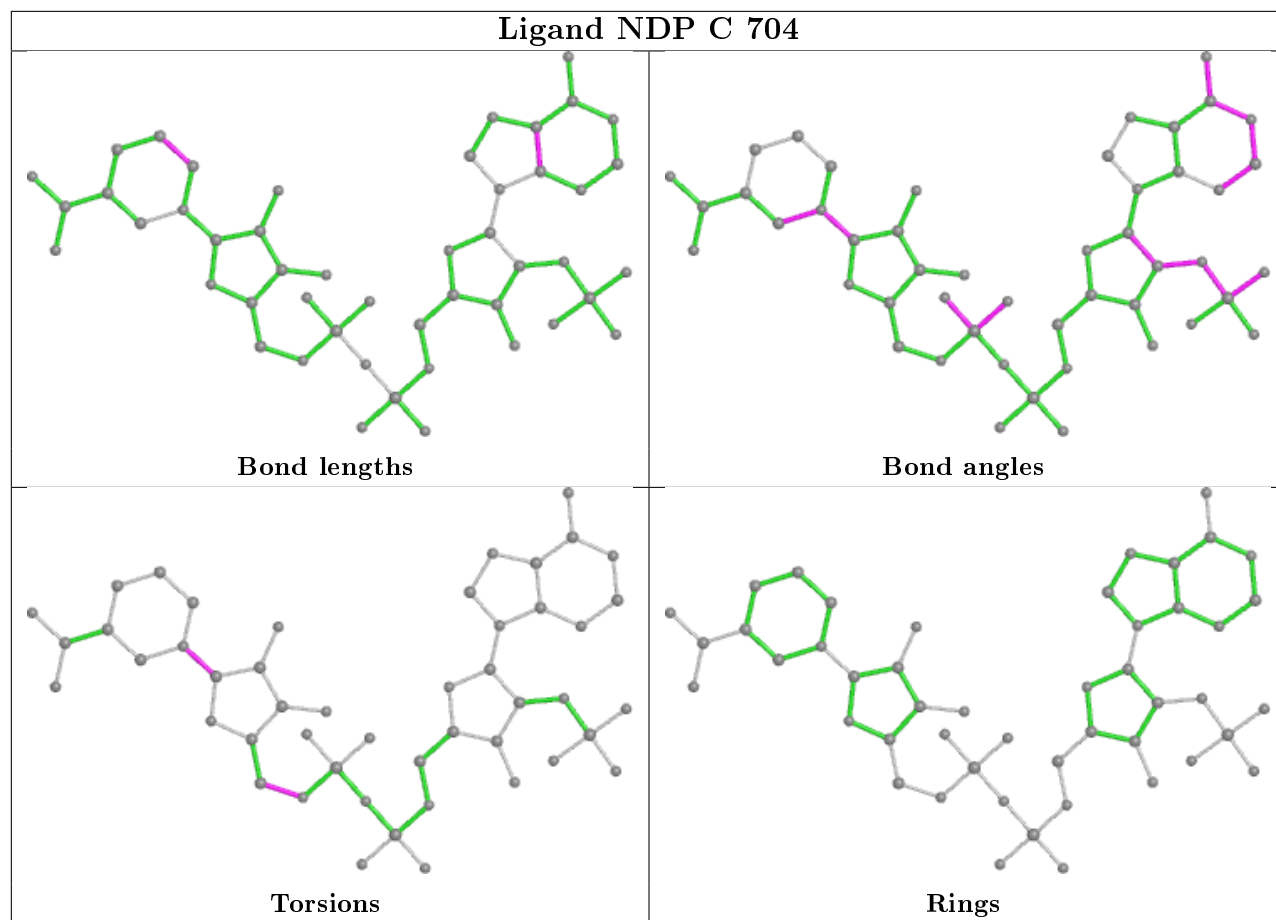
Torsions



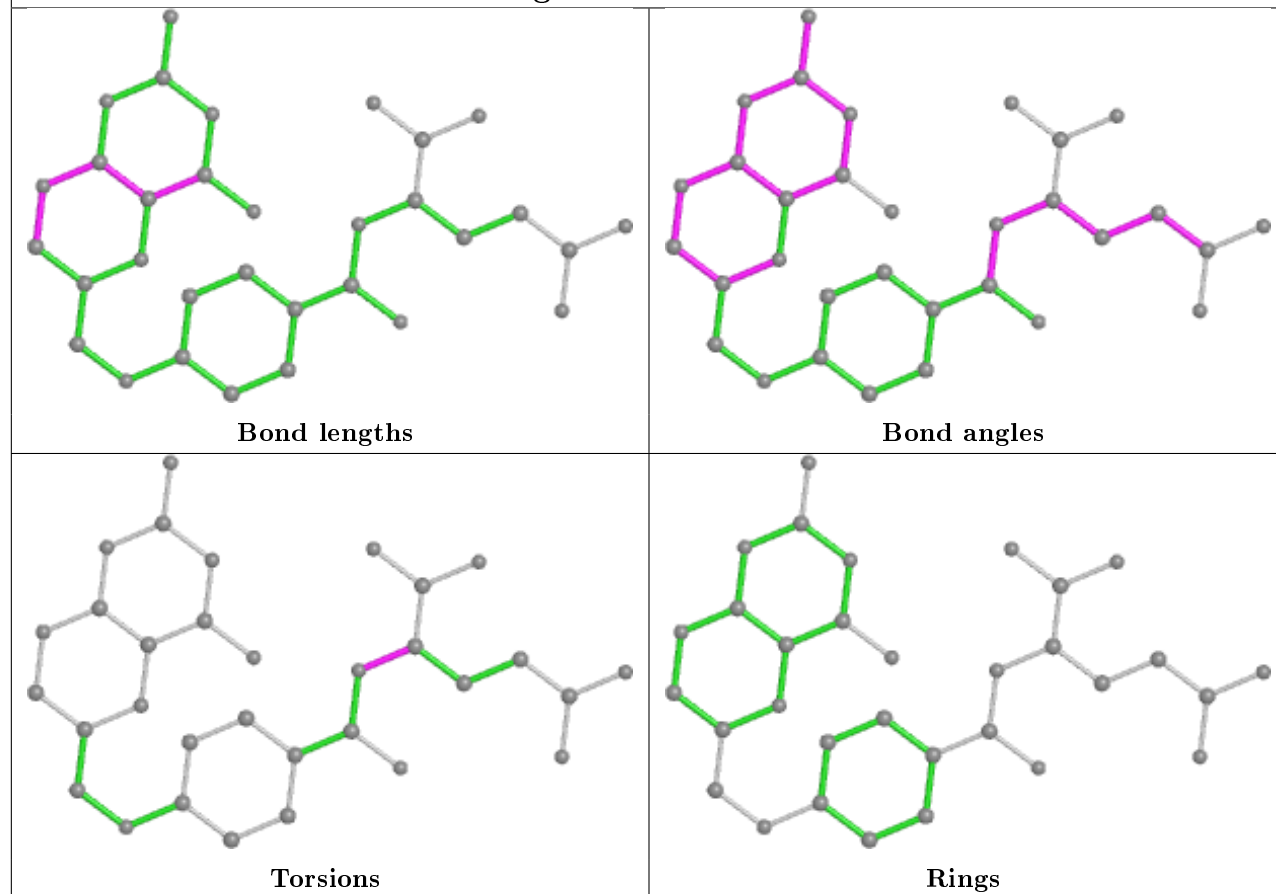
Rings



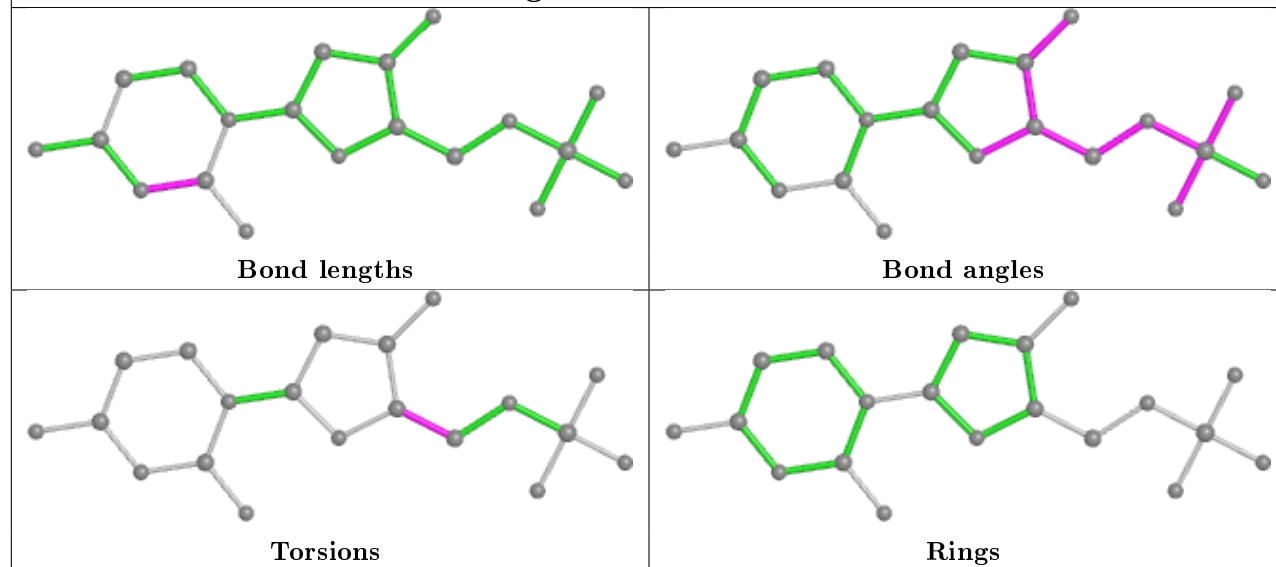




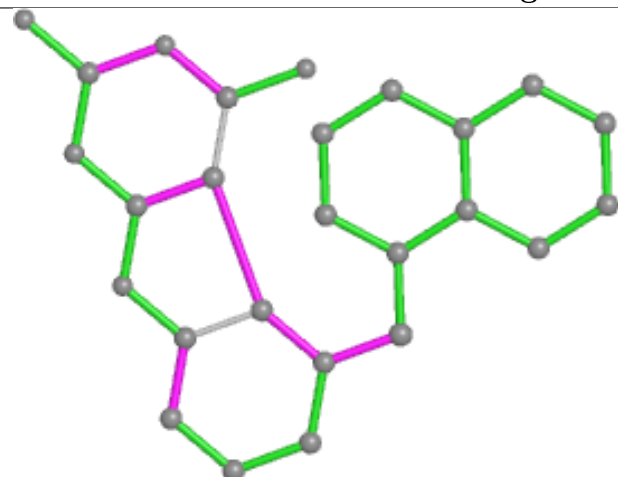
Ligand FOL H 703



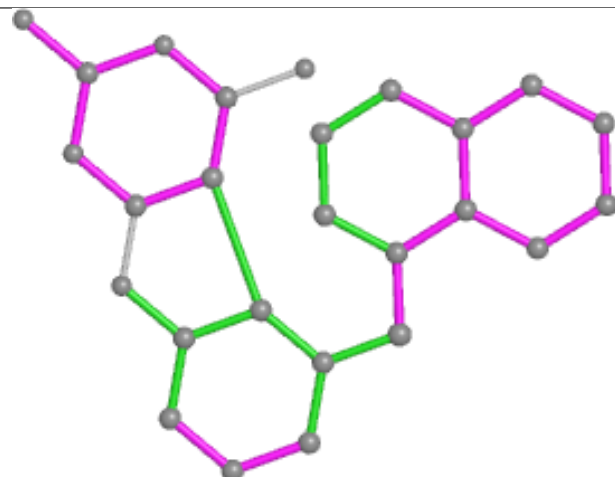
Ligand UMP H 701



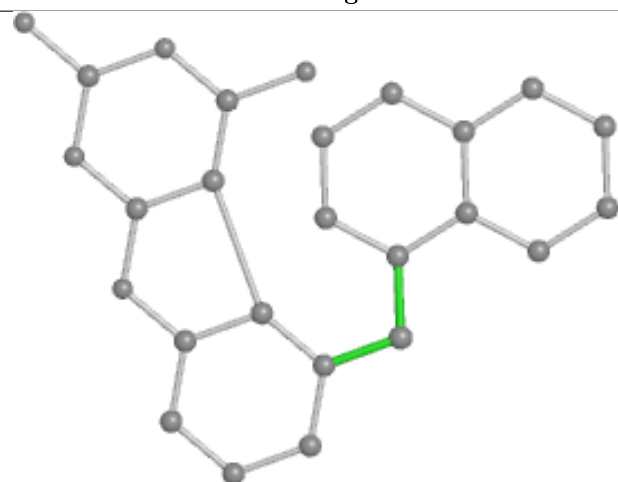
Ligand 1UG E 702



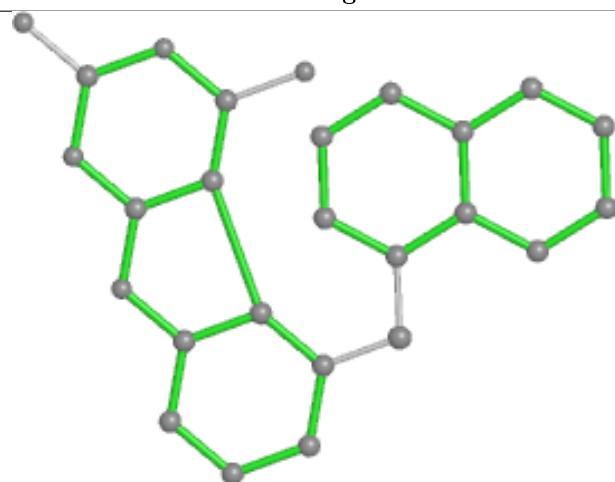
Bond lengths



Bond angles

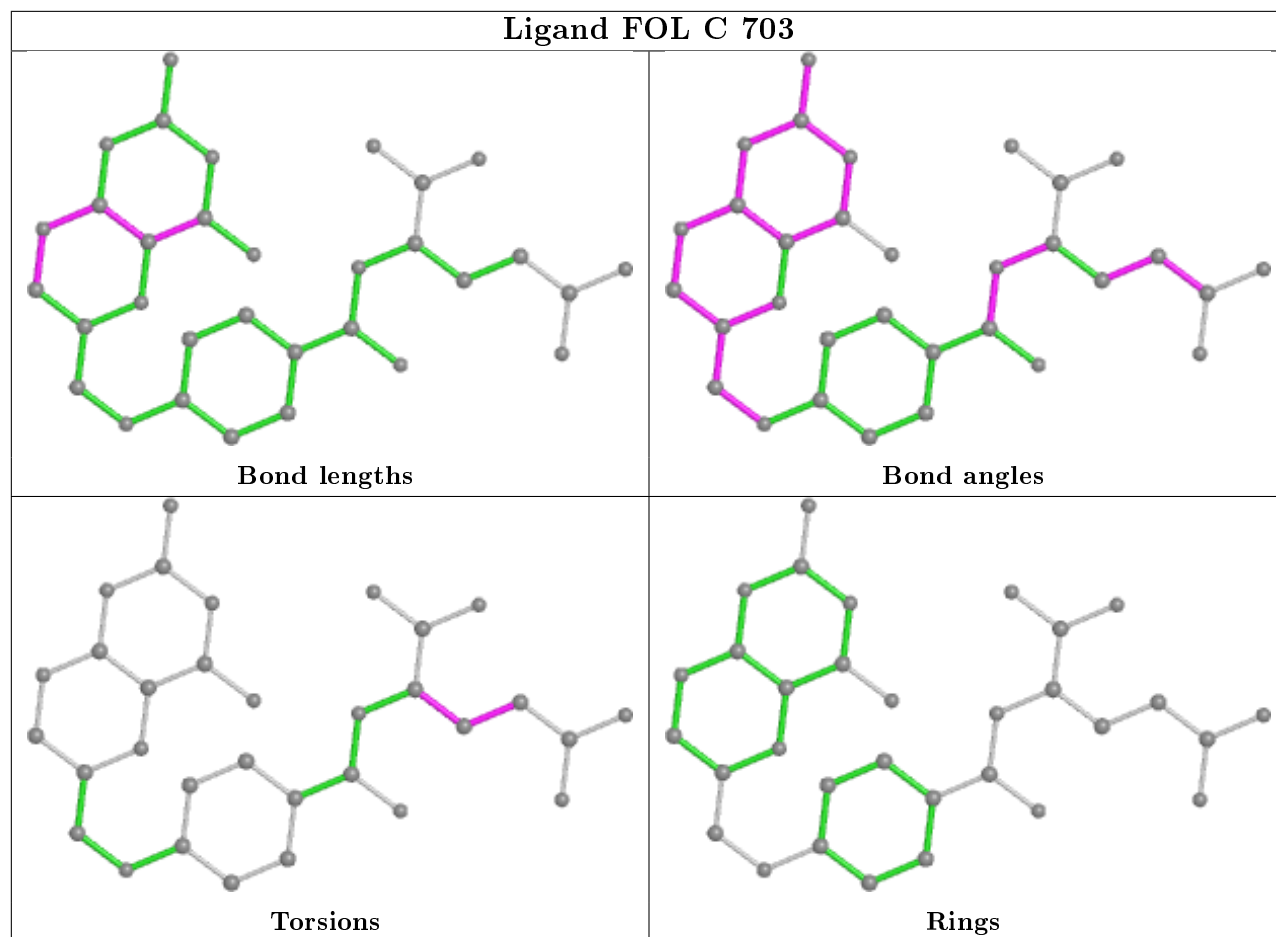


Torsions

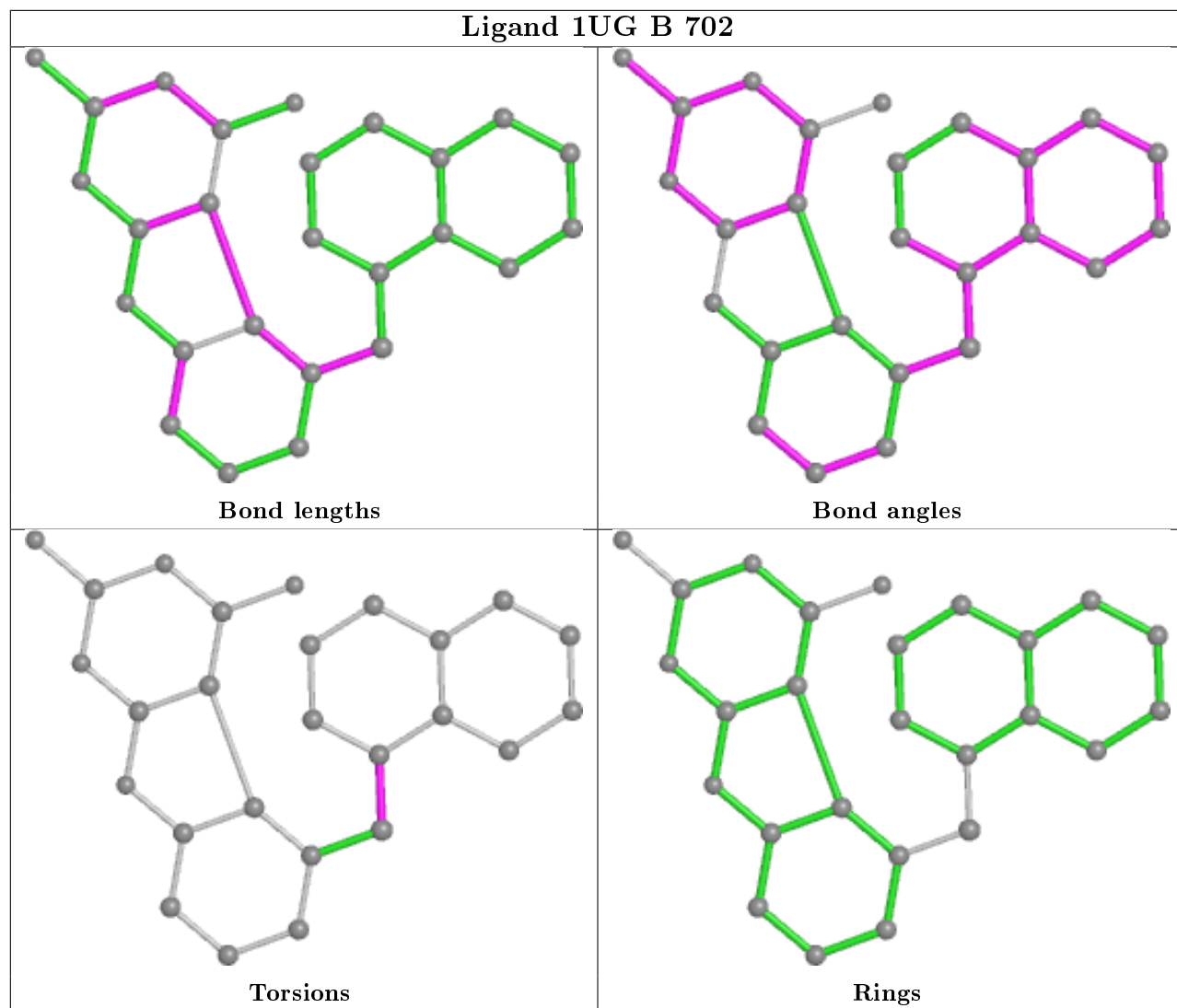


Rings

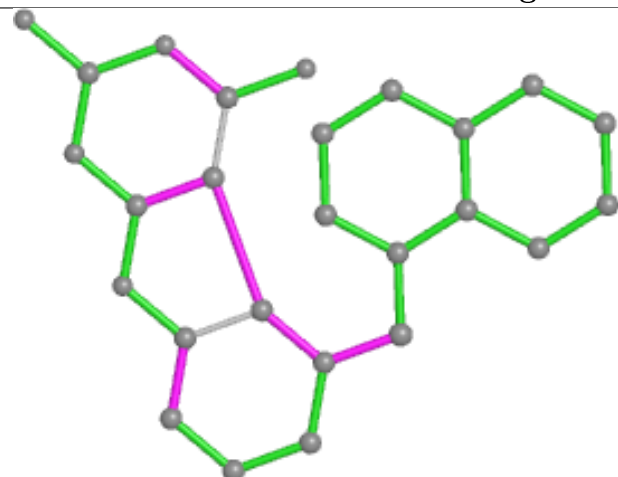
Ligand FOL C 703



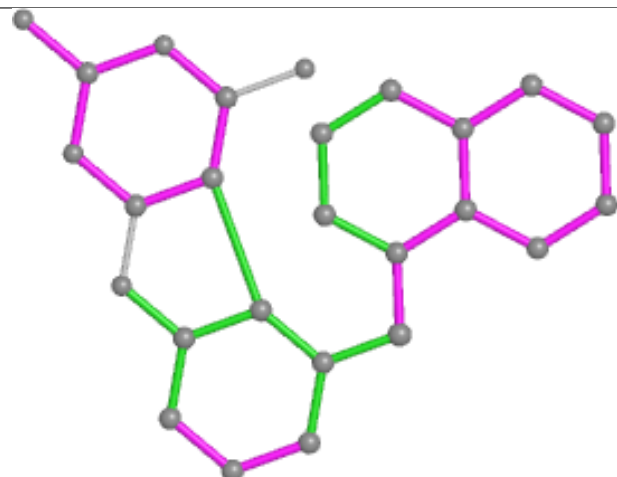
Ligand 1UG B 702



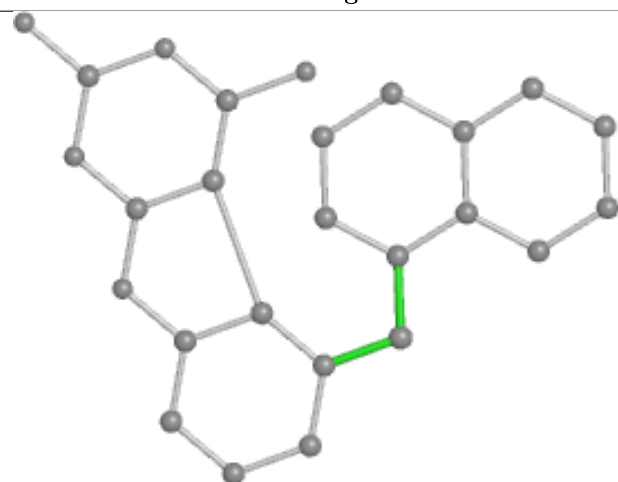
Ligand 1UG C 702



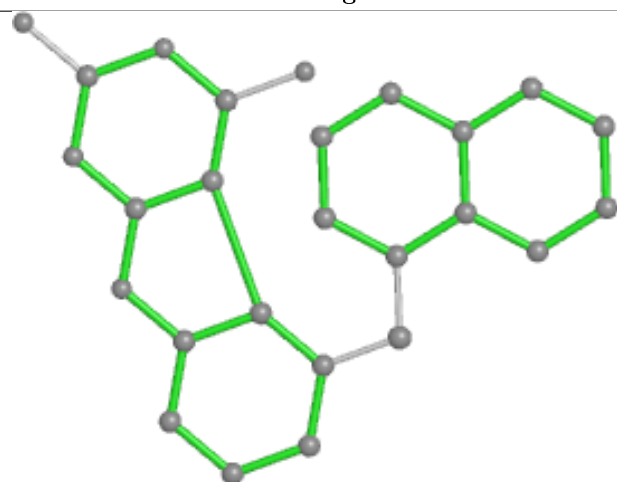
Bond lengths



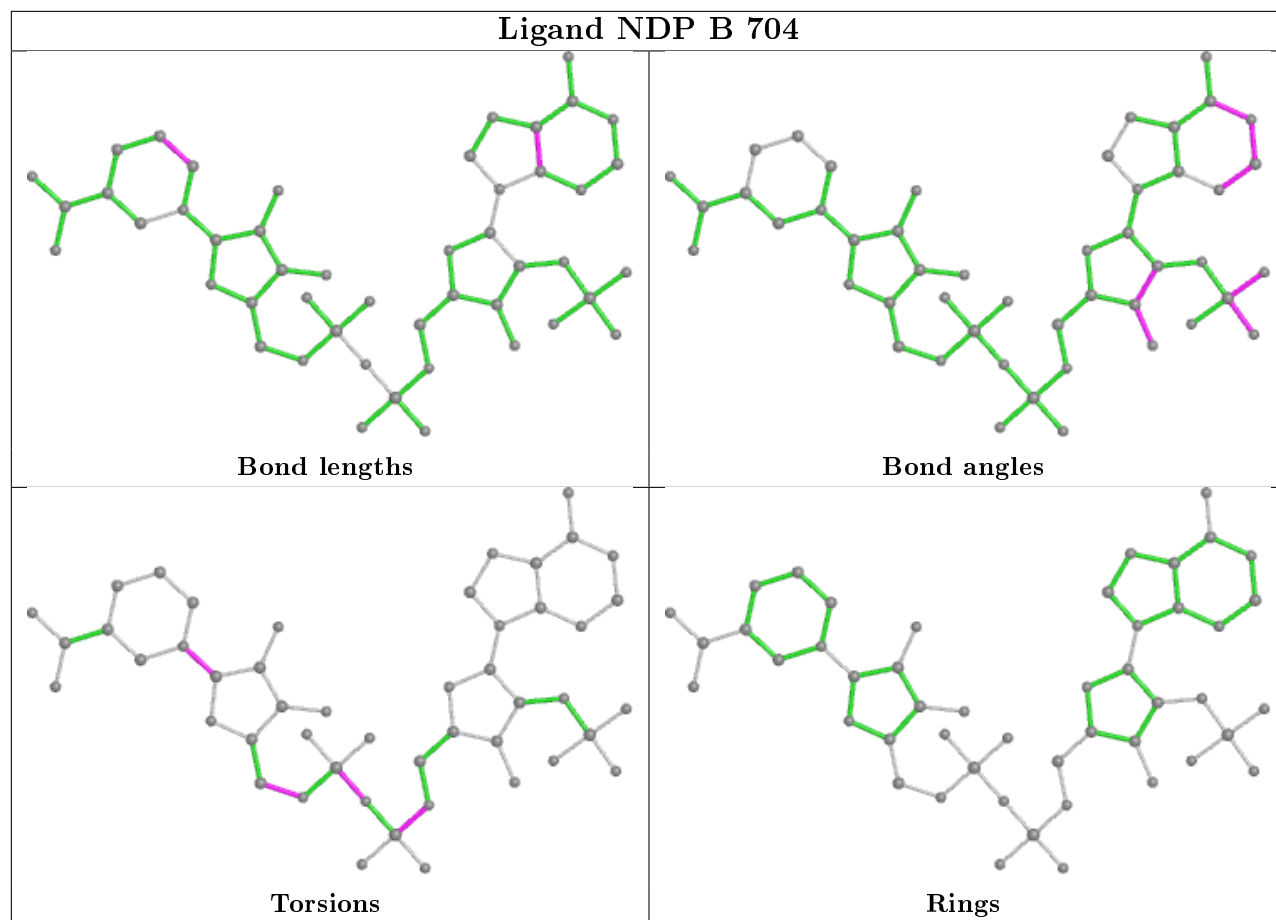
Bond angles



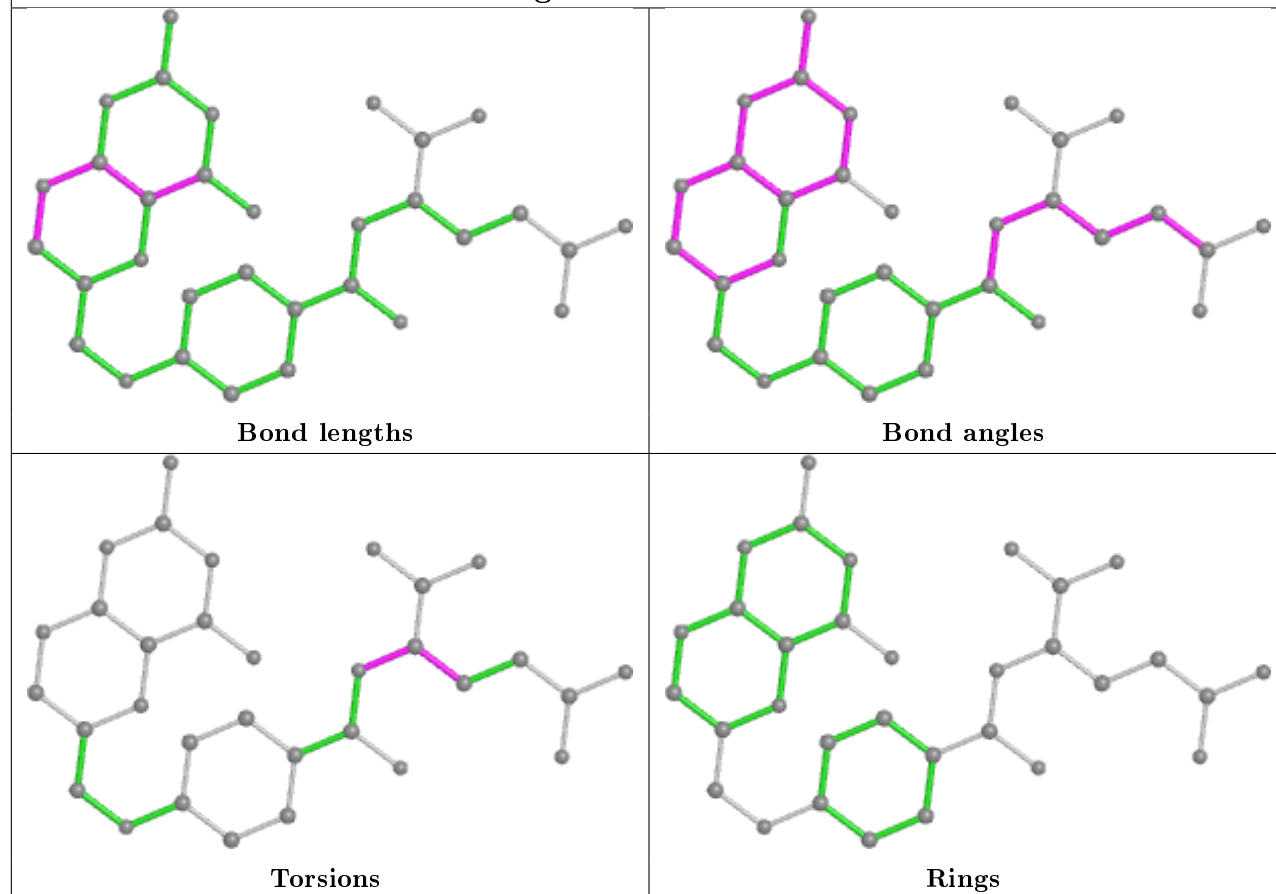
Torsions



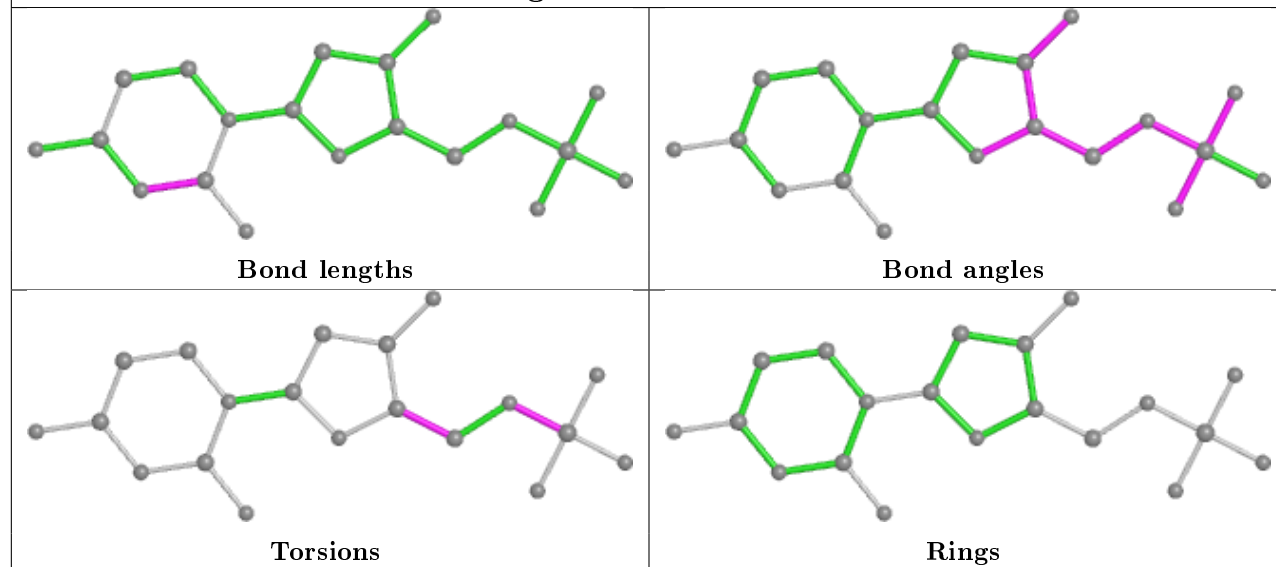
Rings

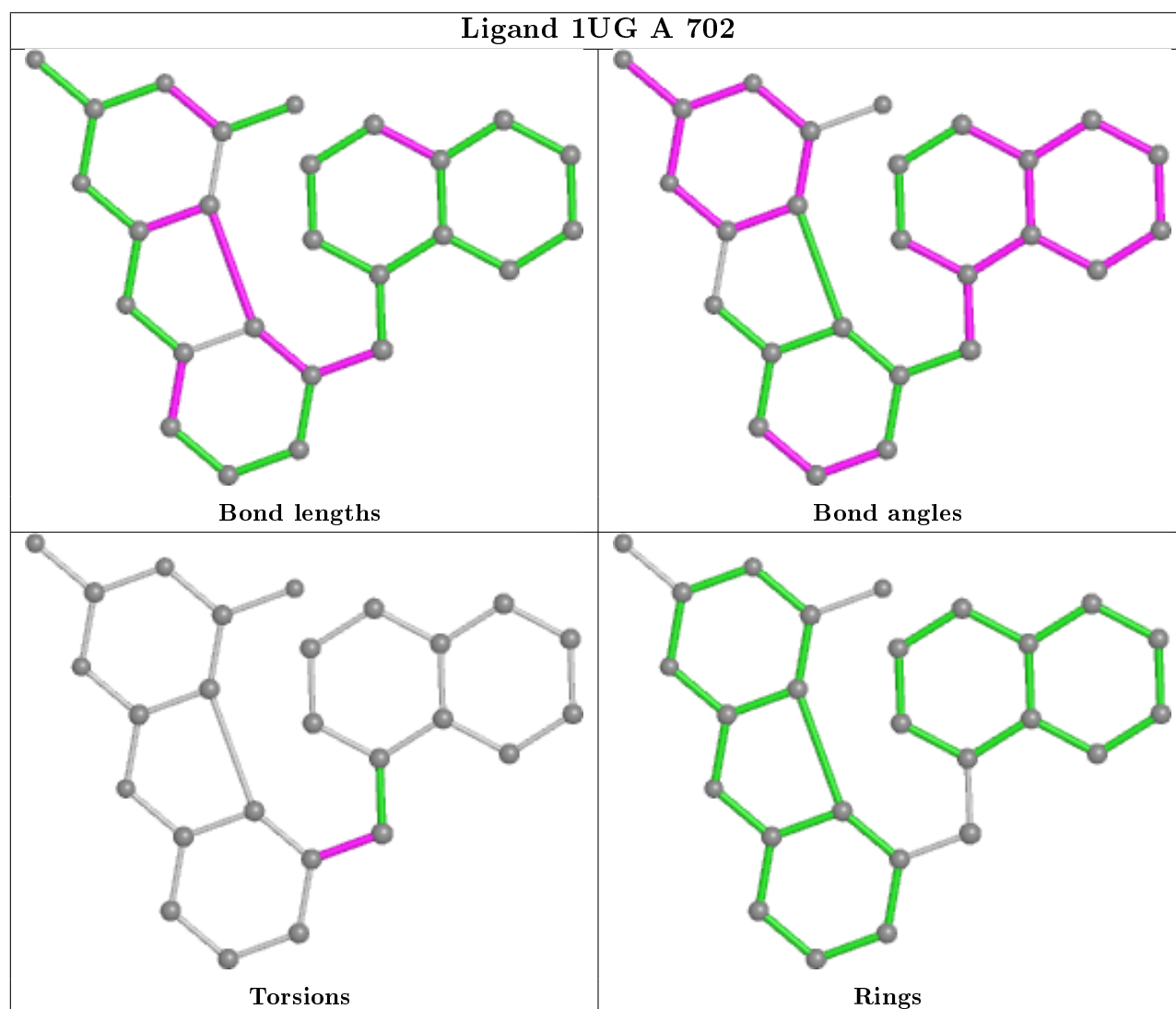
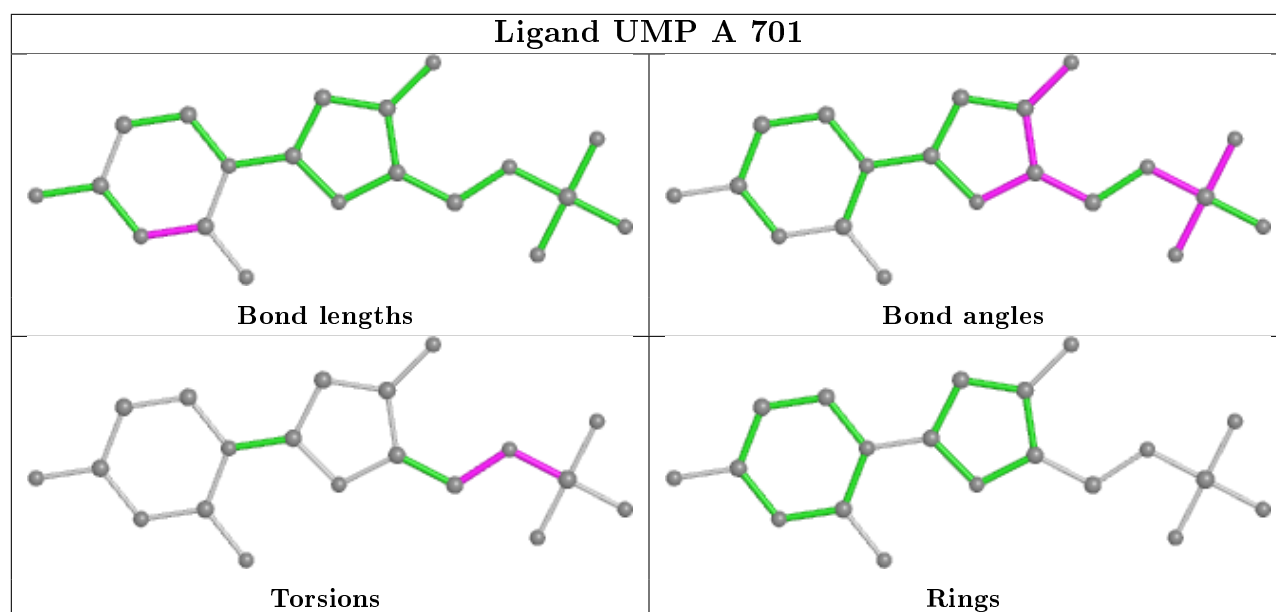


Ligand FOL D 703

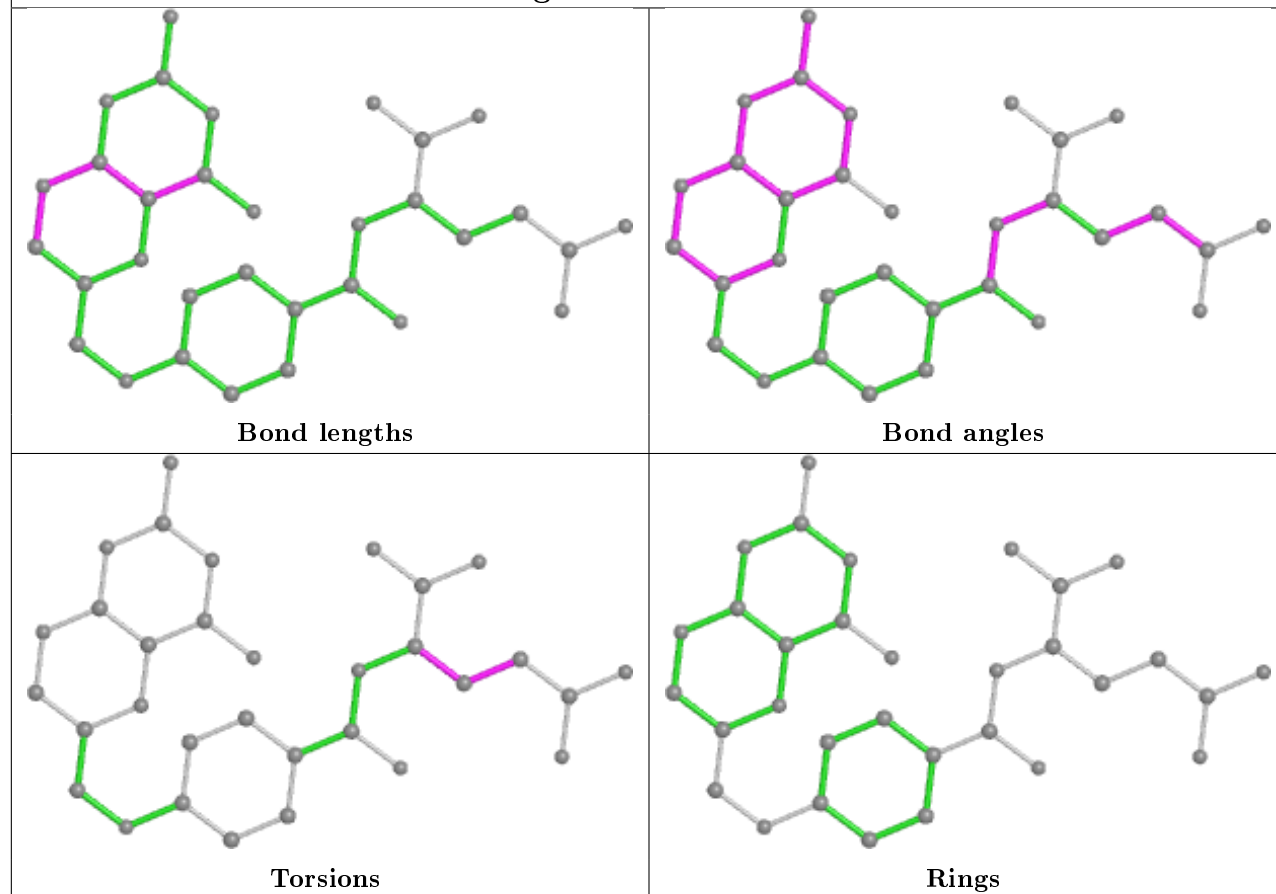


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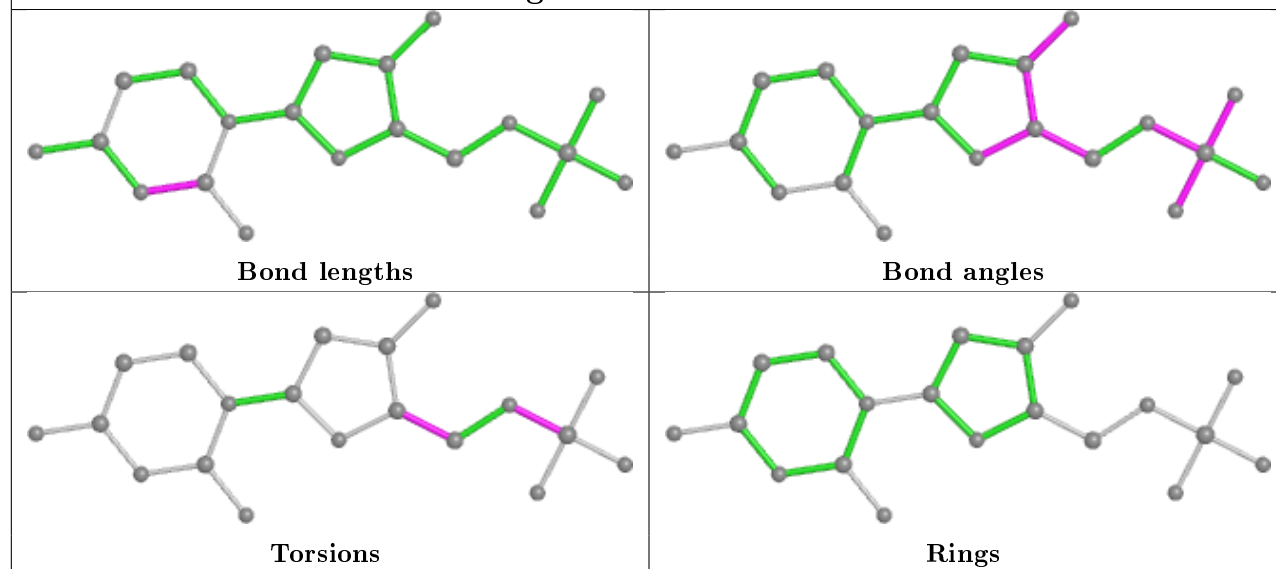


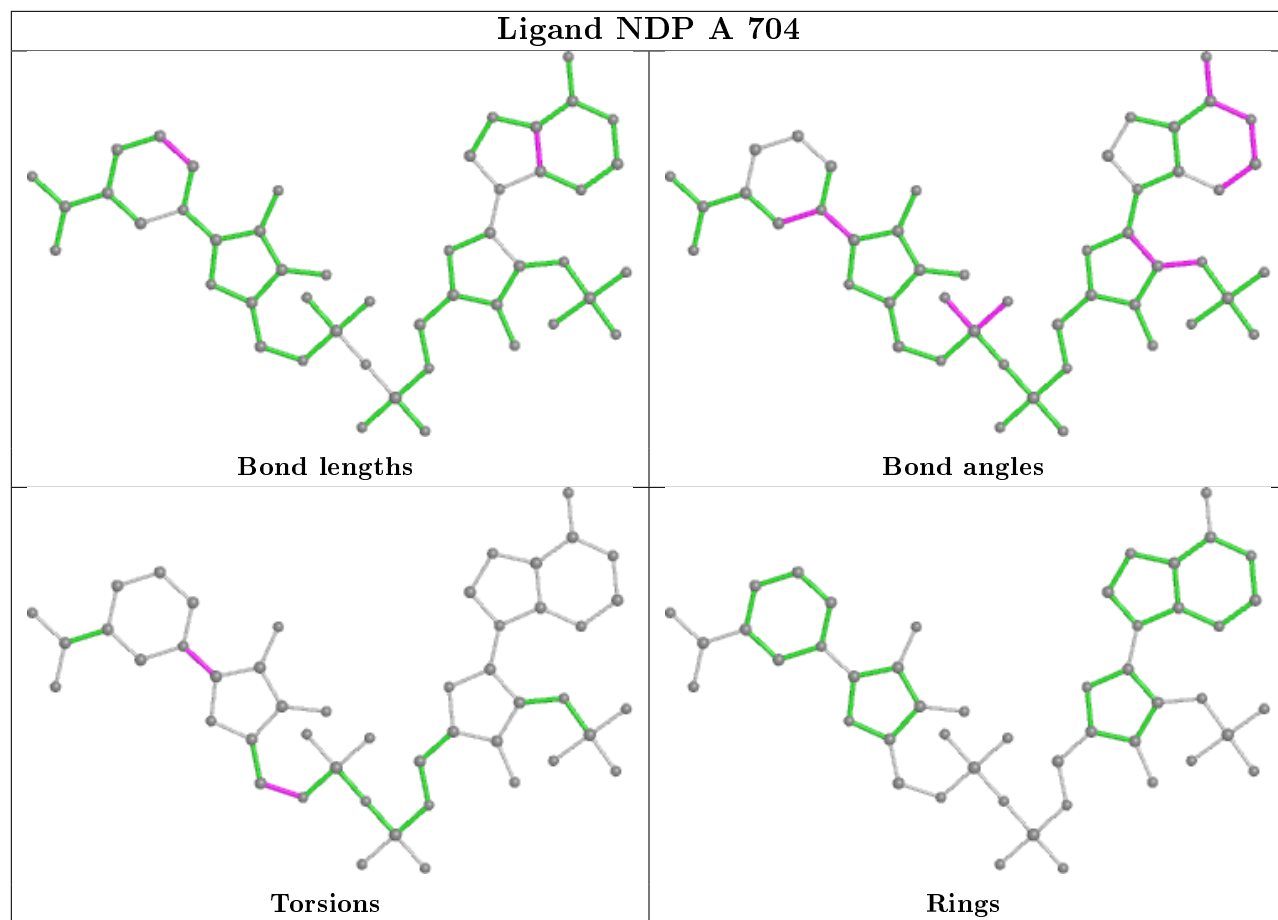


Ligand FOL G 703

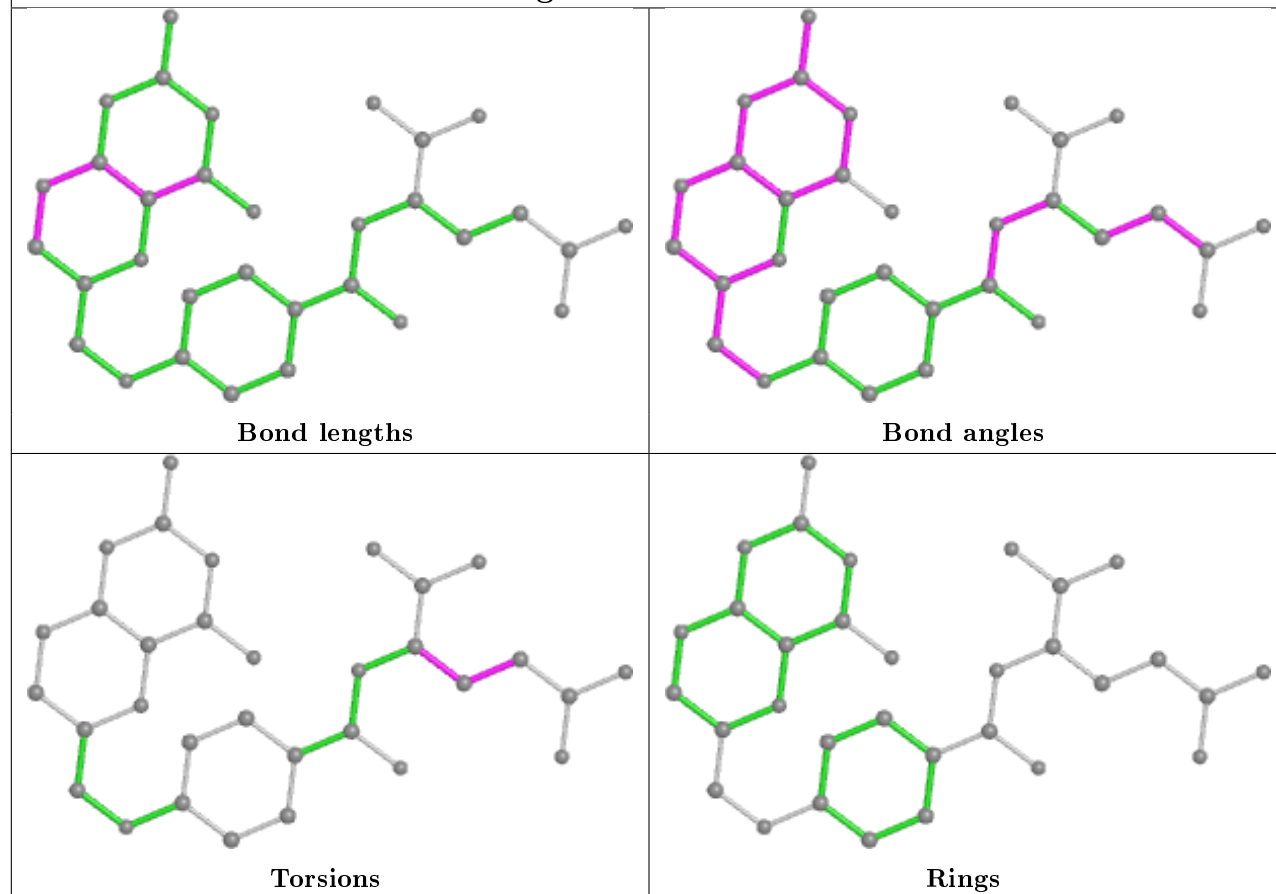


Ligand UMP D 701

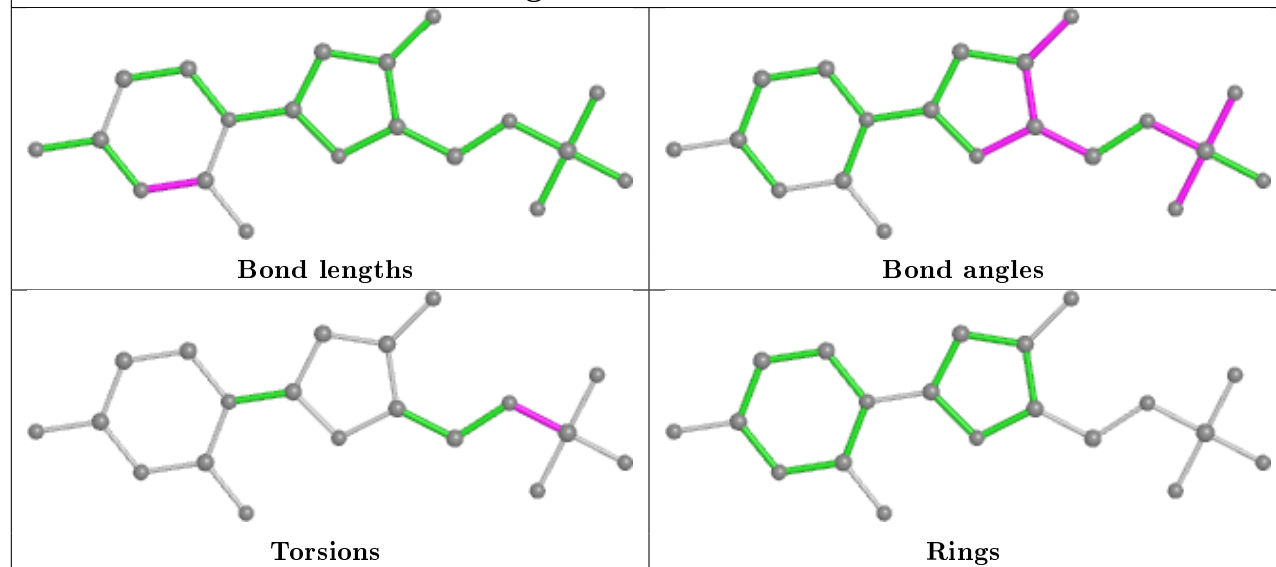


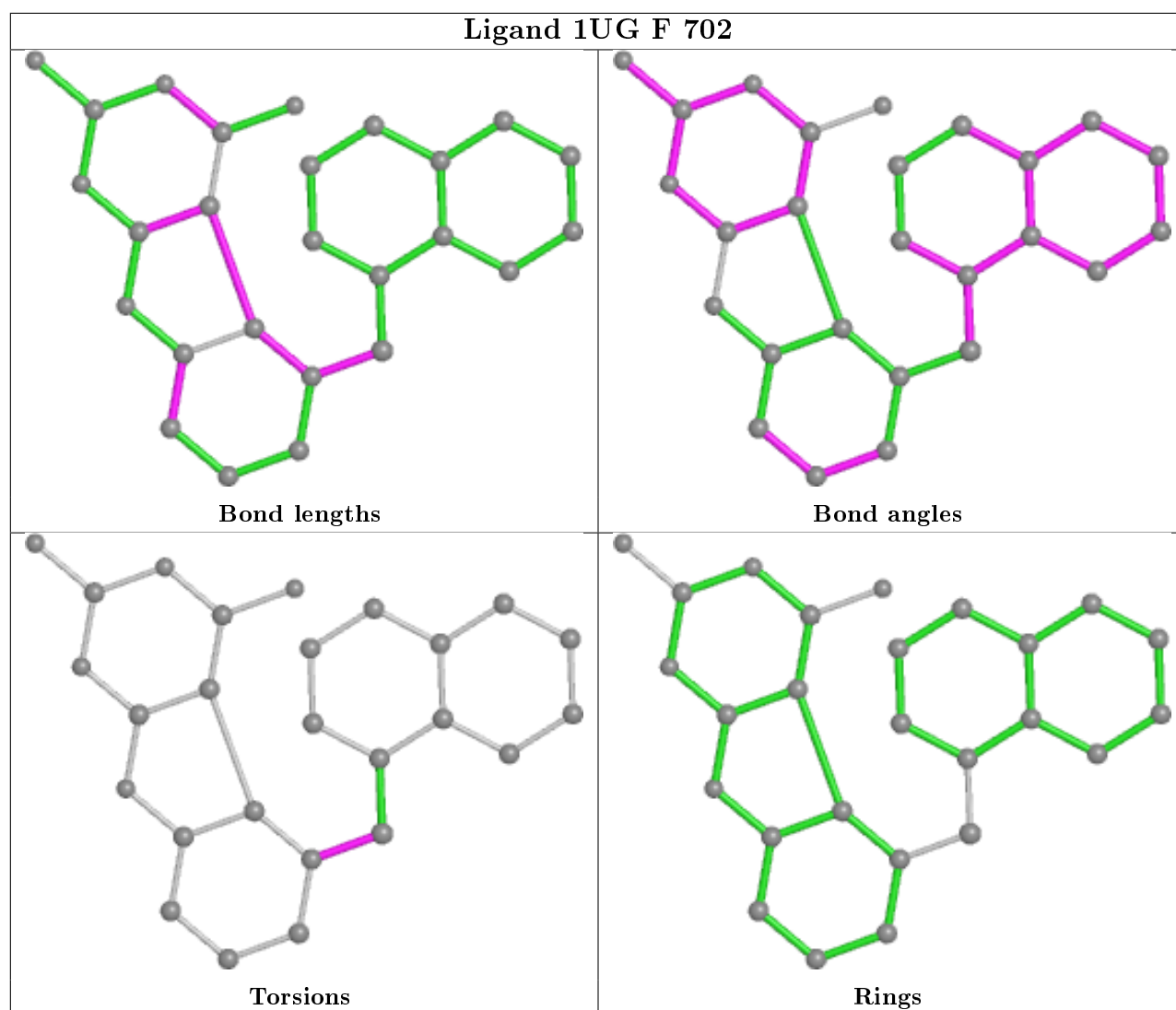


Ligand FOL E 703



Ligand UMP G 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.28	6 (1%) 79 77	13, 30, 69, 99	0
1	B	491/566 (86%)	-0.27	0 100 100	14, 32, 77, 93	0
1	C	510/566 (90%)	-0.26	7 (1%) 75 74	11, 31, 70, 100	0
1	D	491/566 (86%)	-0.20	1 (0%) 95 95	13, 32, 77, 96	0
1	E	510/566 (90%)	-0.28	6 (1%) 79 77	12, 30, 68, 98	0
1	F	491/566 (86%)	-0.23	1 (0%) 95 95	13, 32, 76, 98	0
1	G	510/566 (90%)	-0.27	5 (0%) 82 82	14, 31, 71, 104	0
1	H	491/566 (86%)	-0.25	1 (0%) 95 95	14, 33, 76, 96	0
All	All	4004/4528 (88%)	-0.25	27 (0%) 87 88	11, 31, 74, 104	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	TRP	3.7
1	G	294	LEU	3.6
1	E	296	TRP	3.5
1	C	297	MET	3.2
1	A	297	MET	2.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

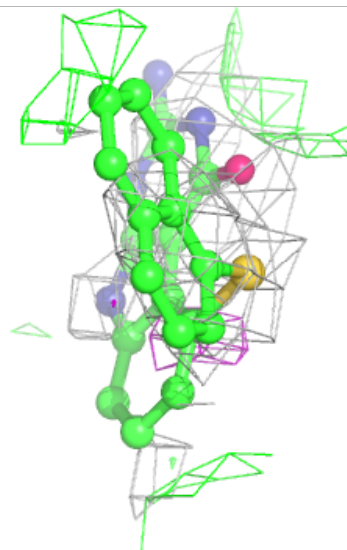
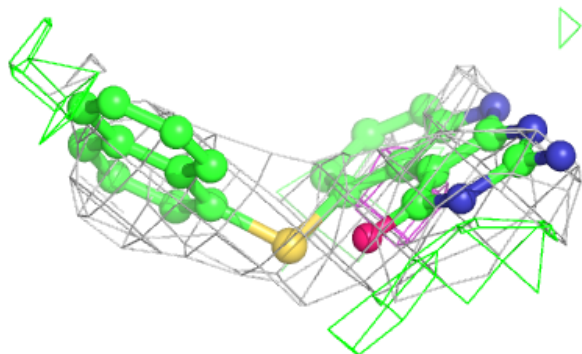
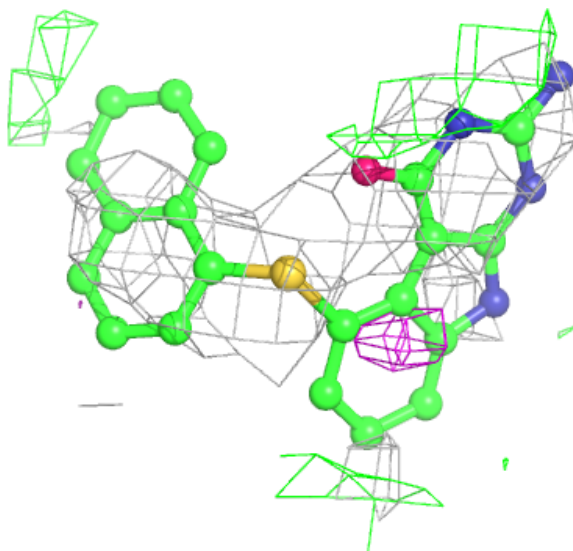
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	1UG	C	702	26/26	0.78	0.50	96,114,132,133	0
3	1UG	H	702	26/26	0.81	0.38	65,82,104,105	0
3	1UG	B	702	26/26	0.82	0.42	64,89,110,111	0
3	1UG	D	702	26/26	0.83	0.40	66,83,105,106	0
3	1UG	F	702	26/26	0.84	0.41	71,86,107,110	0
3	1UG	G	702	26/26	0.86	0.36	69,105,114,116	0
3	1UG	E	702	26/26	0.87	0.36	75,101,115,117	0
3	1UG	A	702	26/26	0.88	0.35	72,99,113,115	0
4	FOL	H	703	32/32	0.89	0.40	33,60,88,93	0
4	FOL	B	703	32/32	0.89	0.40	33,60,87,93	0
4	FOL	F	703	32/32	0.89	0.42	36,63,87,91	0
4	FOL	A	703	32/32	0.91	0.34	24,45,67,89	0
4	FOL	D	703	32/32	0.91	0.39	34,59,86,91	0
4	FOL	G	703	32/32	0.92	0.33	26,41,68,86	0
4	FOL	E	703	32/32	0.92	0.34	24,45,71,90	0
4	FOL	C	703	32/32	0.92	0.35	26,48,68,95	0
5	NDP	B	704	48/48	0.94	0.22	35,69,105,110	0
5	NDP	D	704	48/48	0.95	0.21	34,65,100,106	0
5	NDP	H	704	48/48	0.95	0.23	35,63,99,108	0
5	NDP	F	704	48/48	0.95	0.21	30,65,105,108	0
2	UMP	H	701	20/20	0.96	0.28	24,46,68,70	0
2	UMP	D	701	20/20	0.96	0.27	25,46,67,73	0
2	UMP	B	701	20/20	0.96	0.24	26,47,70,71	0
2	UMP	F	701	20/20	0.96	0.26	26,43,68,70	0
2	UMP	A	701	20/20	0.97	0.18	30,57,70,70	0
2	UMP	C	701	20/20	0.97	0.21	32,62,81,82	0
2	UMP	G	701	20/20	0.97	0.21	35,56,72,72	0
2	UMP	E	701	20/20	0.97	0.22	34,57,75,78	0
5	NDP	A	704	48/48	0.98	0.18	21,34,40,56	0
5	NDP	G	704	48/48	0.98	0.18	21,32,44,56	0
5	NDP	C	704	48/48	0.98	0.17	21,32,43,51	0
5	NDP	E	704	48/48	0.98	0.18	20,33,42,48	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.

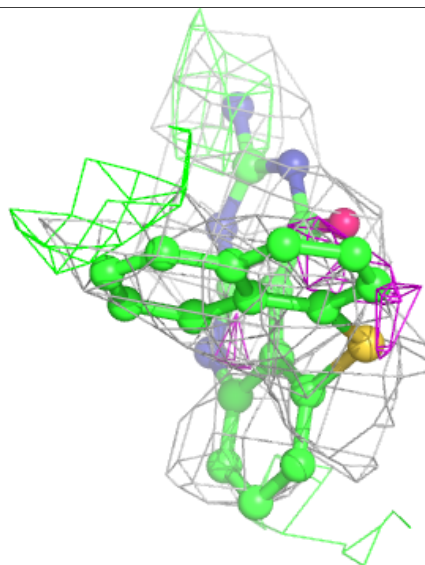
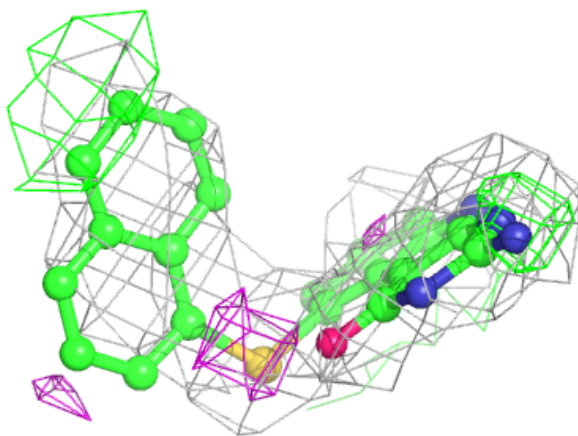
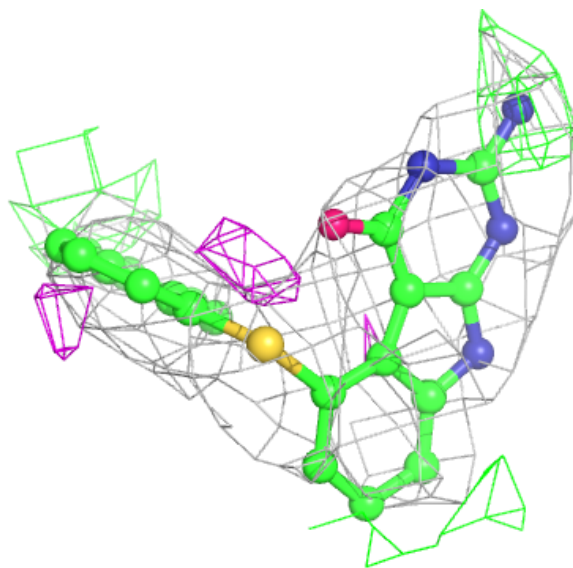
Electron density around 1UG C 702:

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



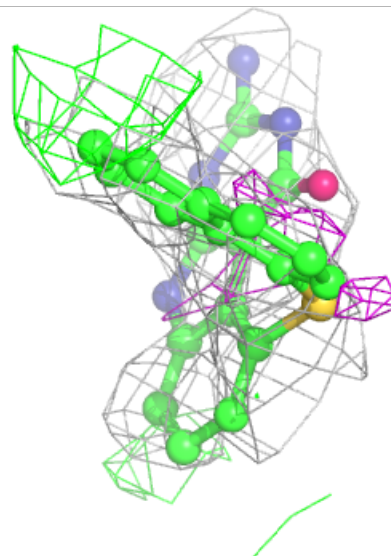
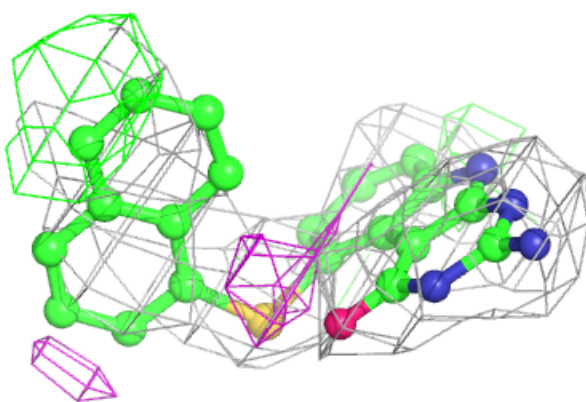
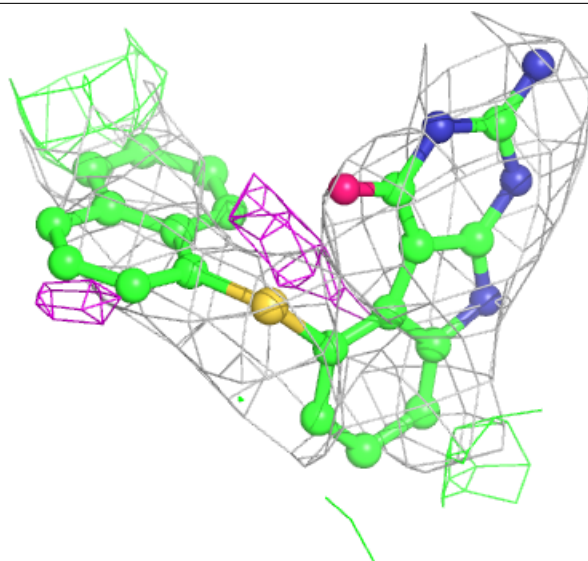
Electron density around 1UG H 702:

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



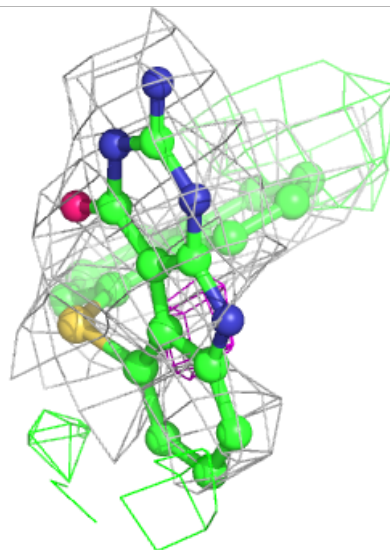
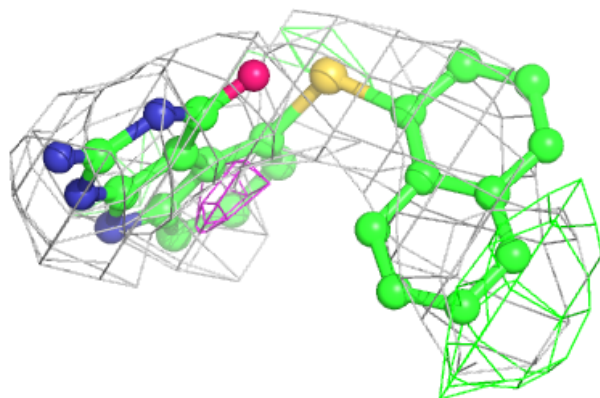
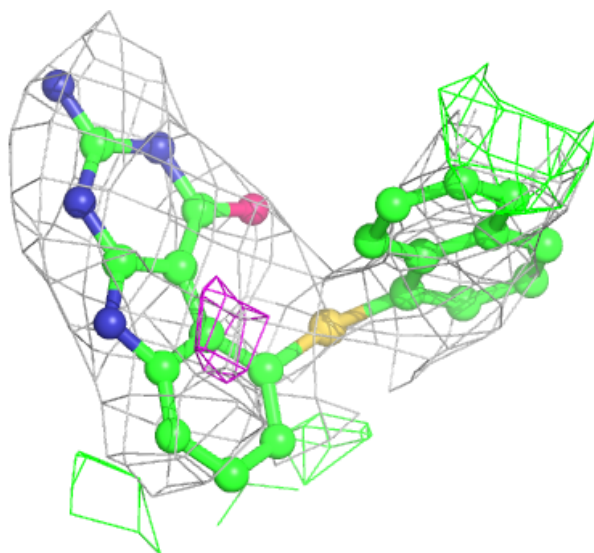
Electron density around 1UG B 702:

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



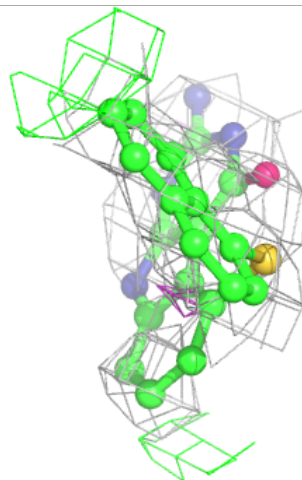
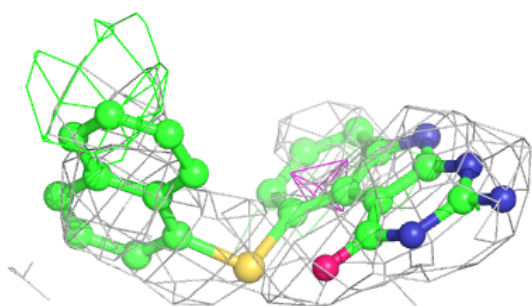
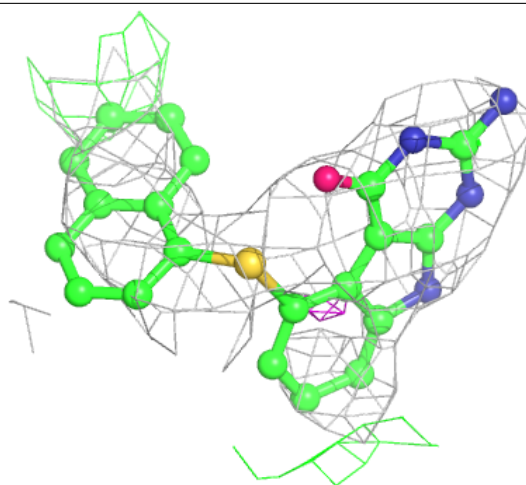
Electron density around 1UG D 702:

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



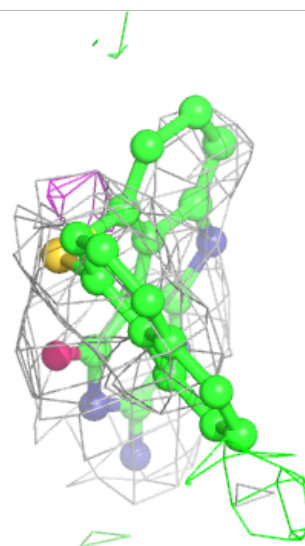
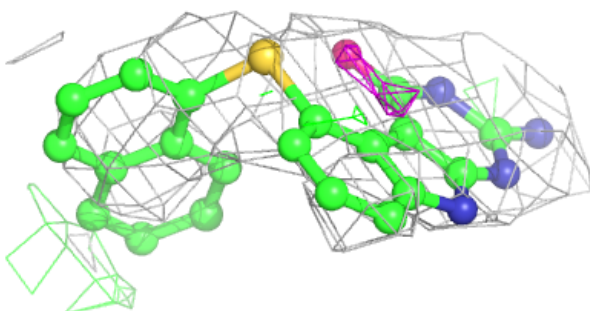
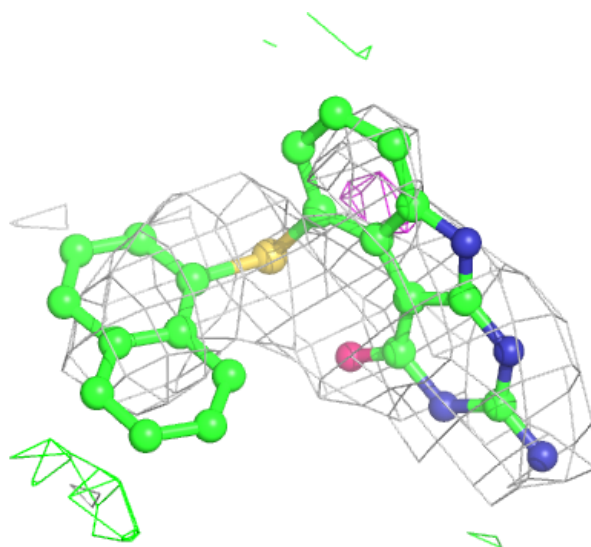
Electron density around 1UG F 702:

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



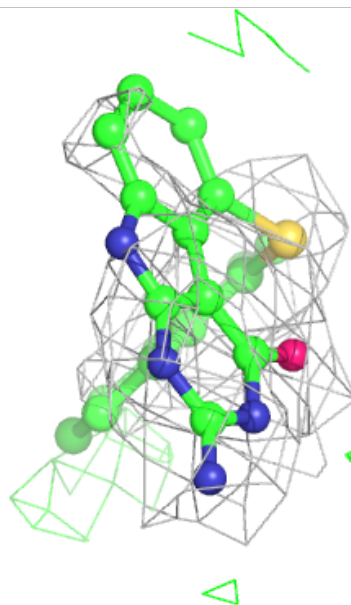
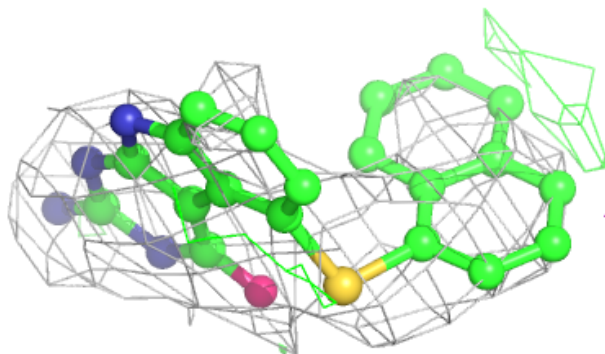
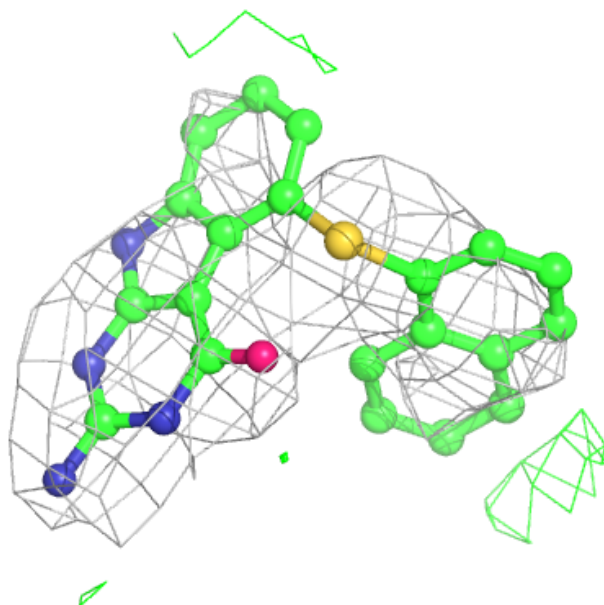
Electron density around 1UG G 702:

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and green (positive)



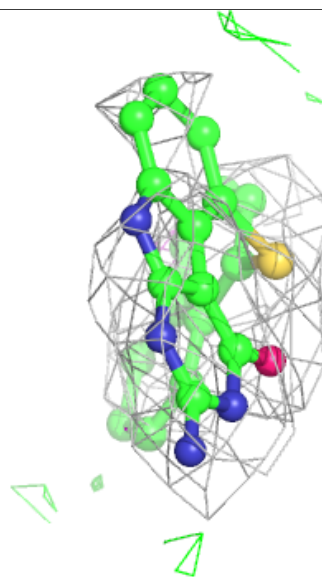
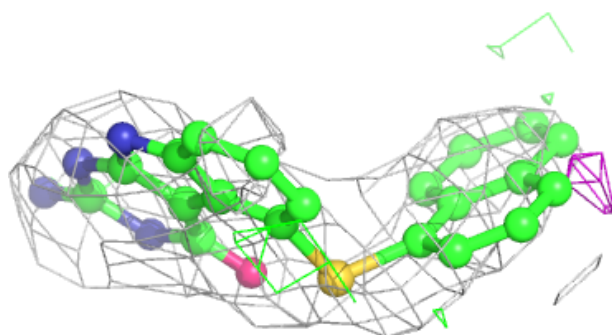
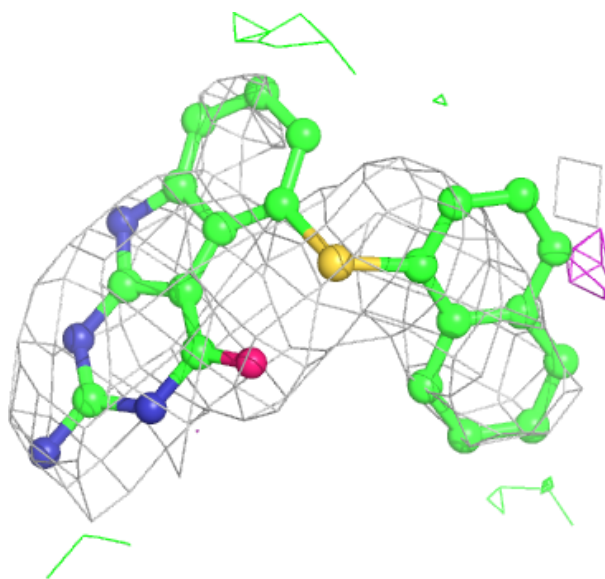
Electron density around 1UG E 702:

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



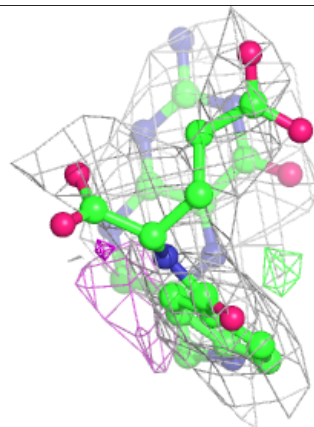
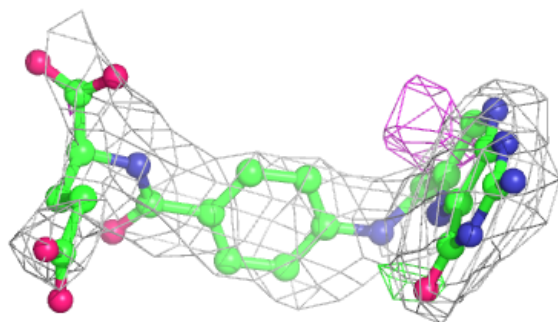
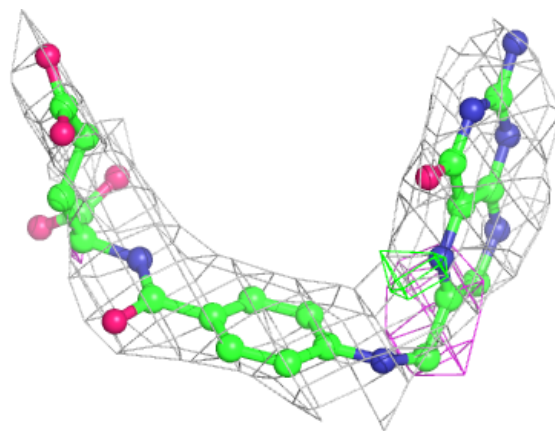
Electron density around 1UG A 702:

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

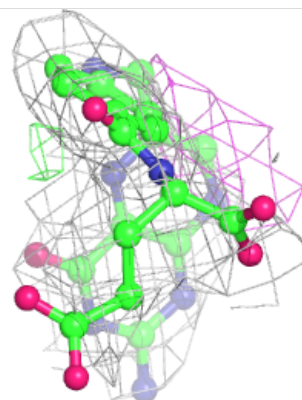
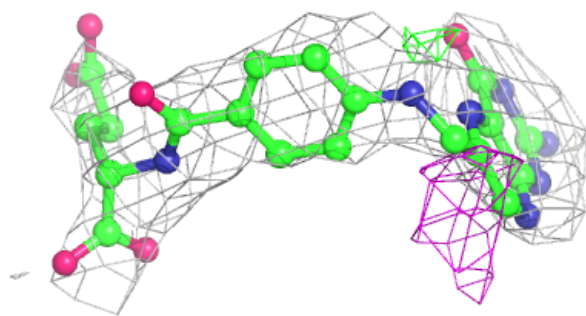
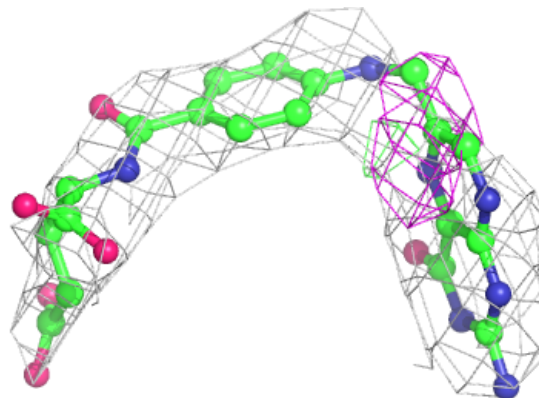


Electron density around FOL H 703:

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

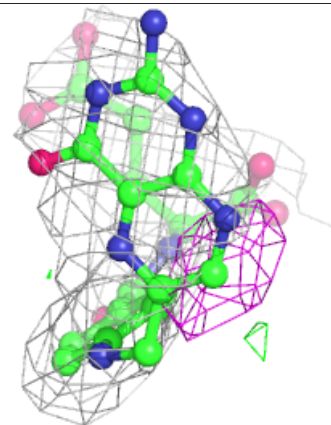
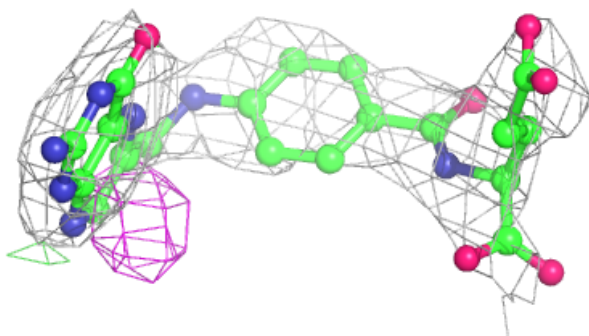
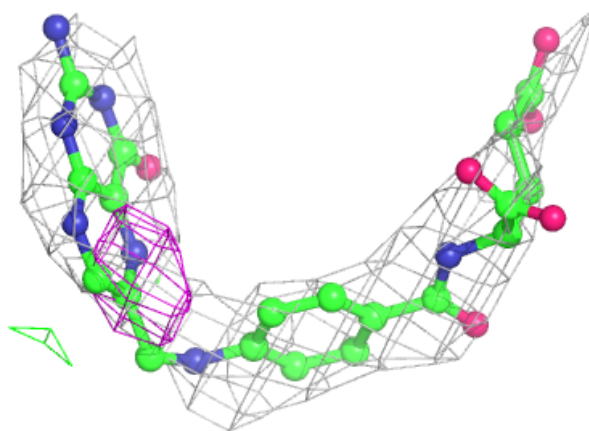
**Electron density around FOL B 703:**

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and green (positive)

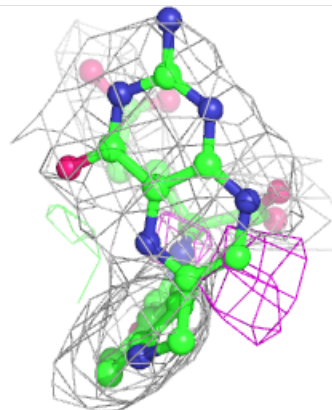
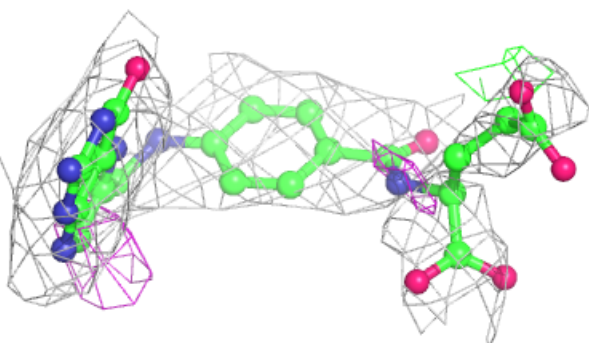
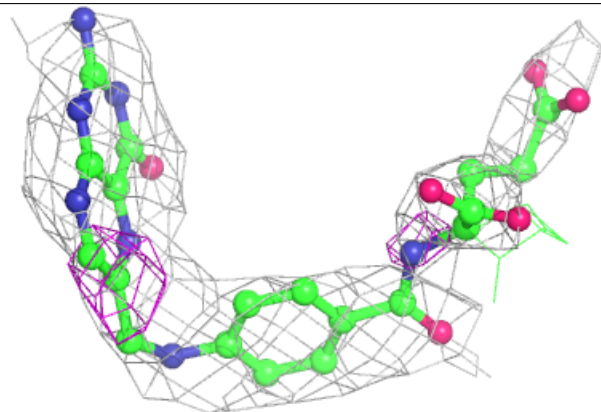


Electron density around FOL F 703:

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and green (positive)

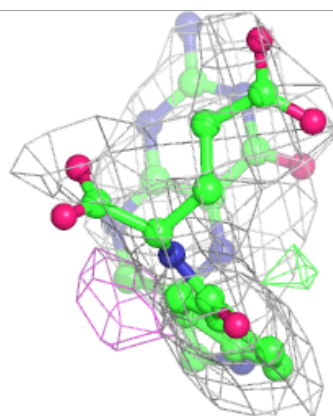
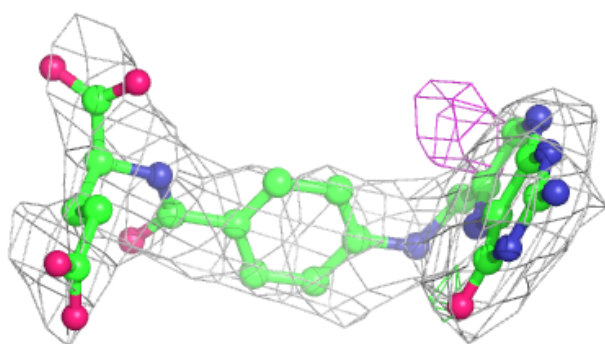
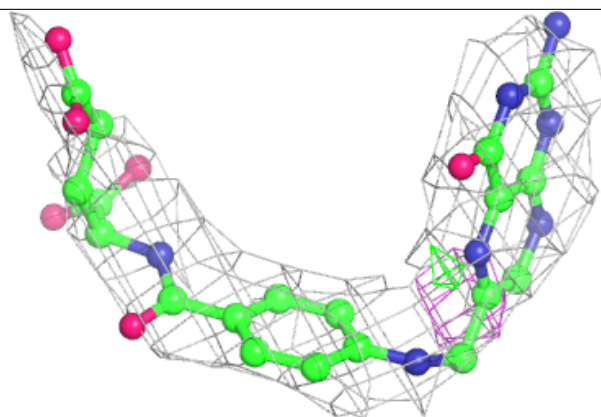
**Electron density around FOL A 703:**

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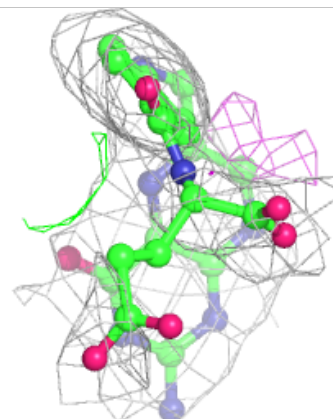
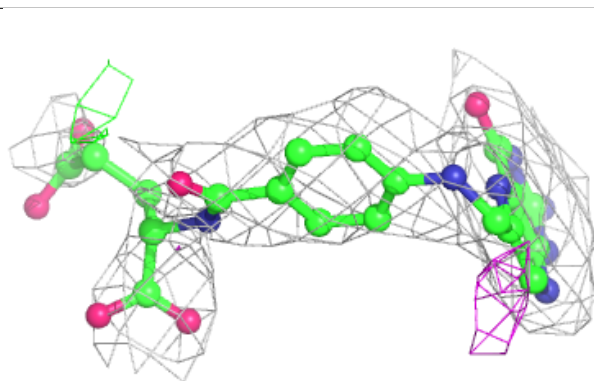
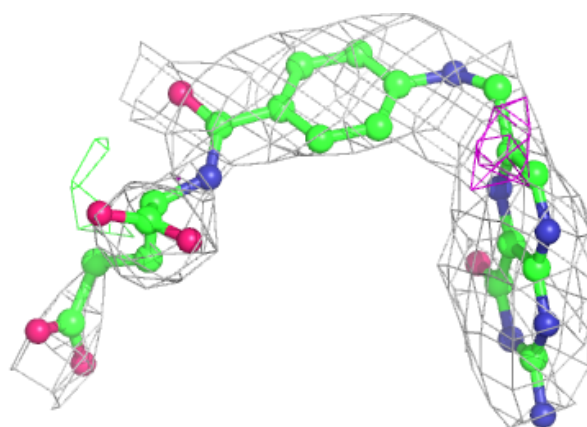


Electron density around FOL D 703:

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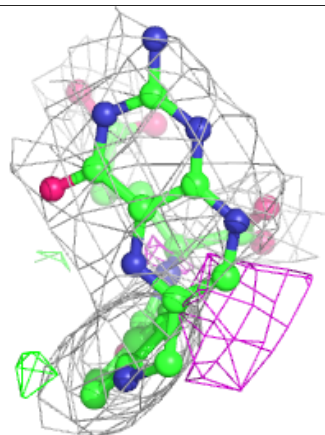
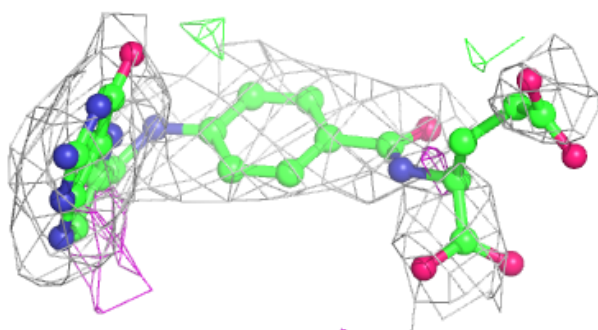
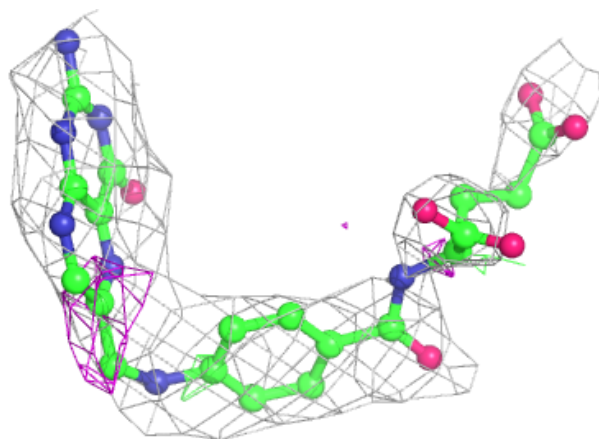
**Electron density around FOL G 703:**

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



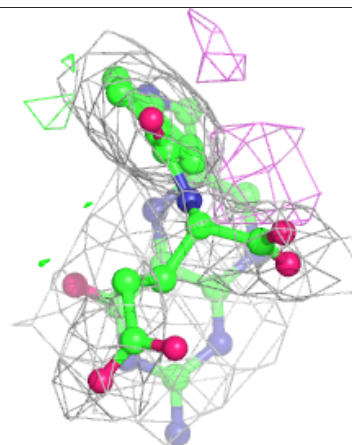
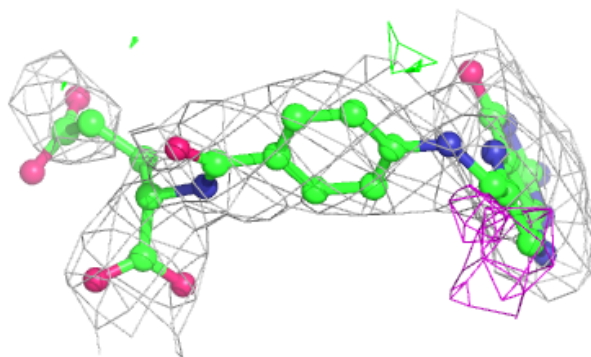
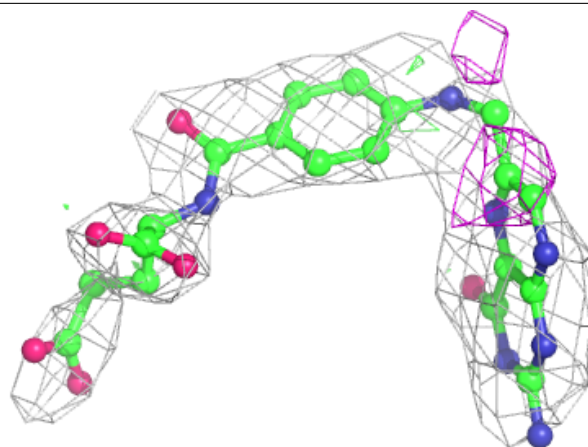
Electron density around FOL E 703:

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and green (positive)

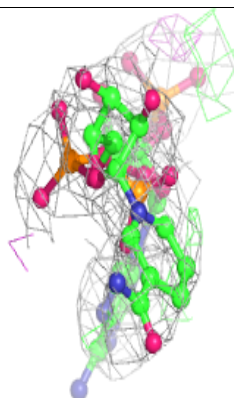
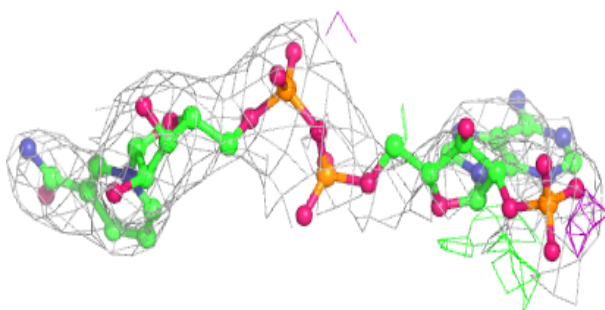
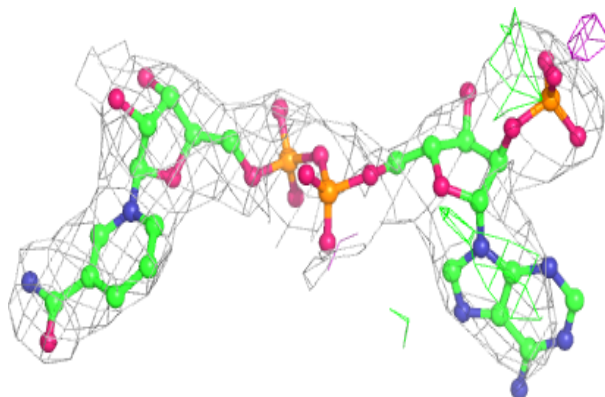


Electron density around FOL C 703:

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and green (positive)

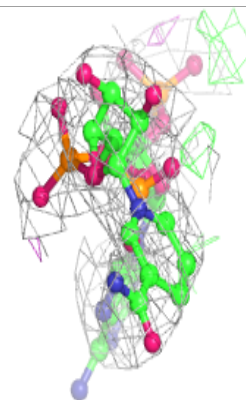
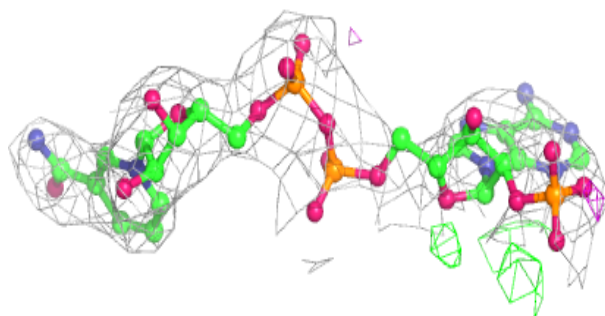
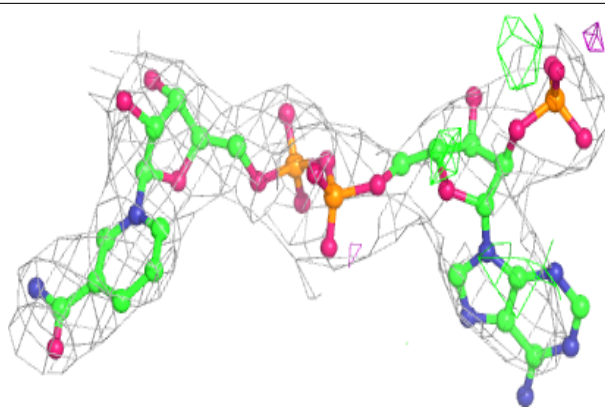
**Electron density around NDP B 704:**

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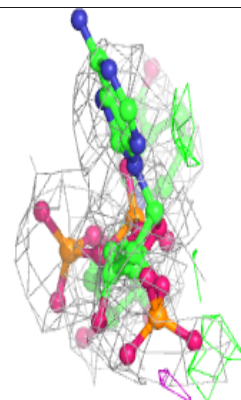
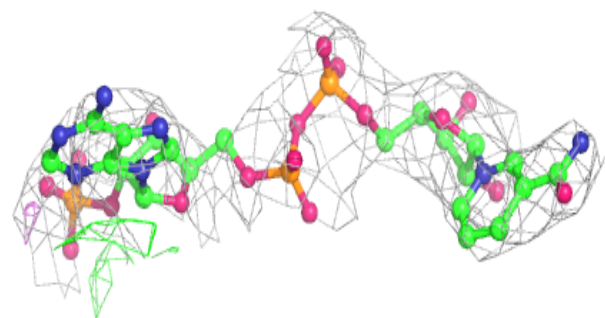
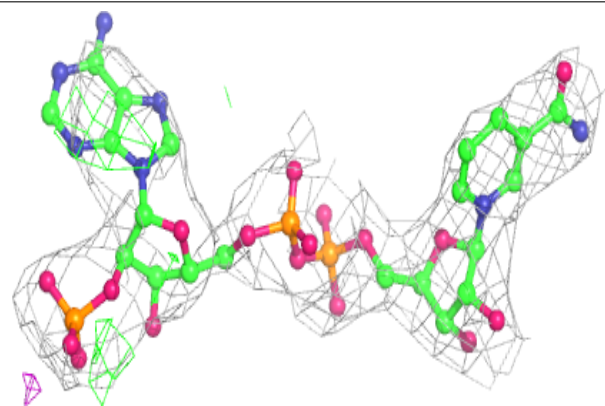


Electron density around NDP D 704:

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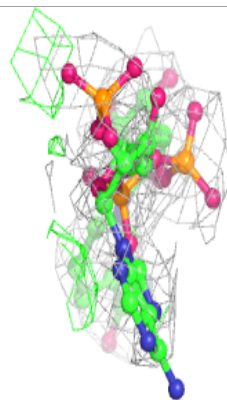
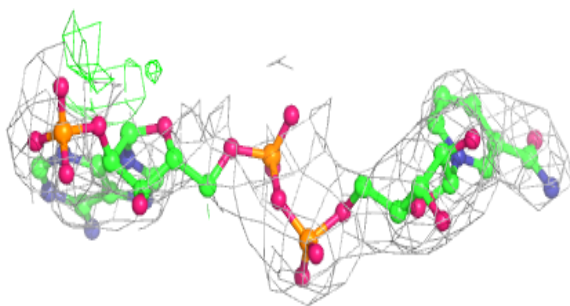
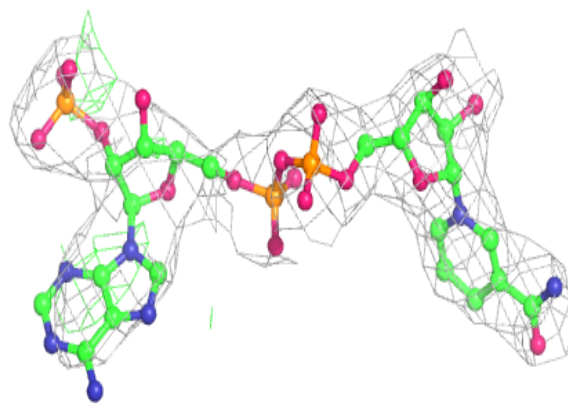
**Electron density around NDP H 704:**

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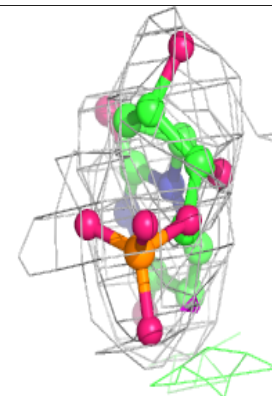
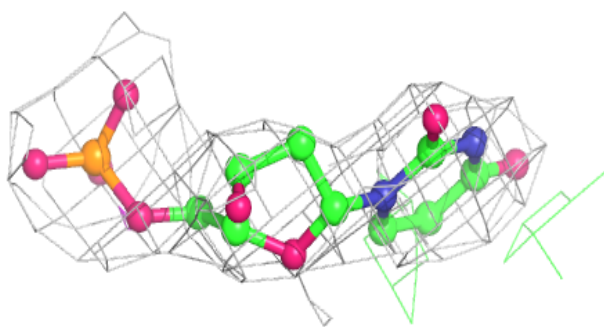
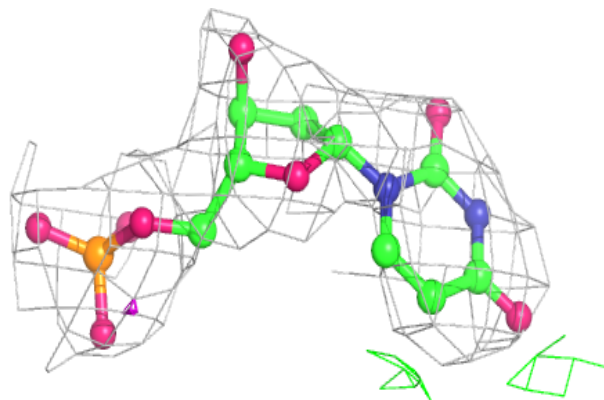


Electron density around NDP F 704:

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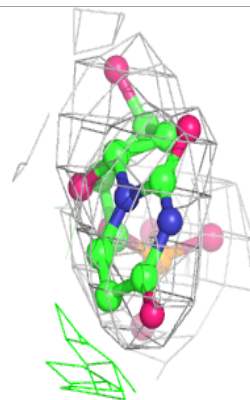
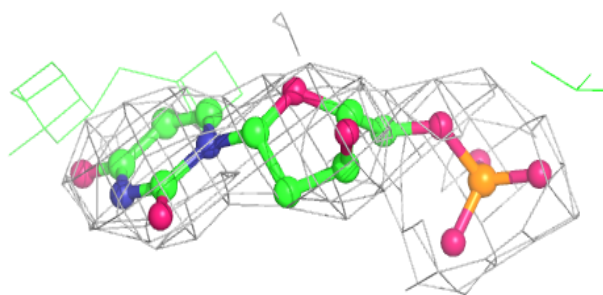
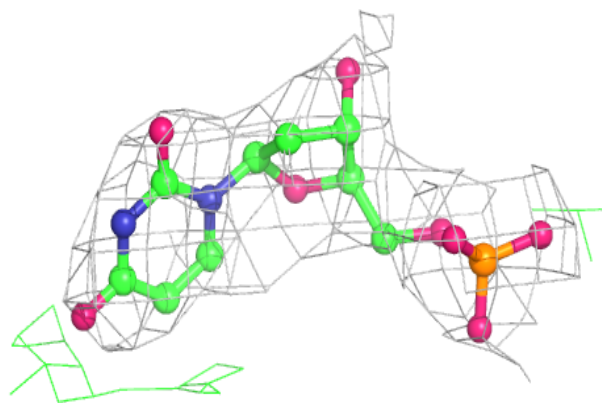
**Electron density around UMP H 701:**

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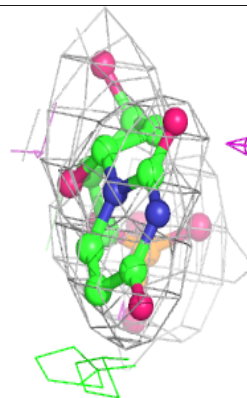
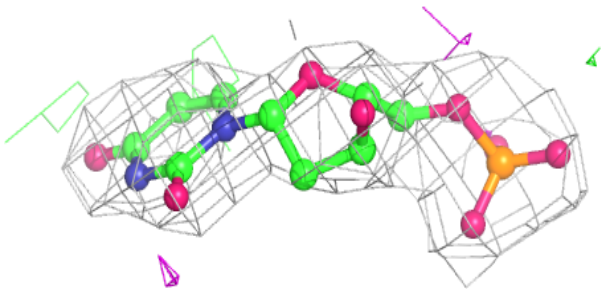
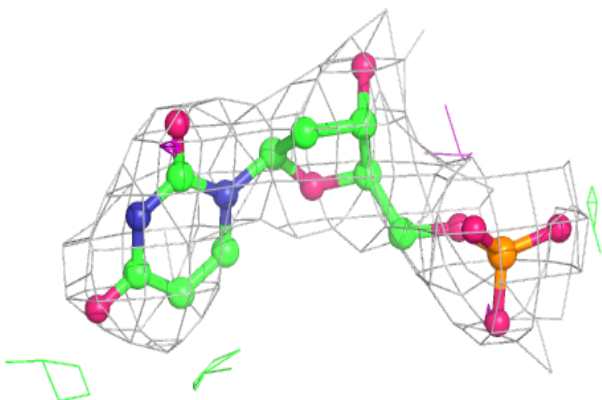


Electron density around UMP D 701:

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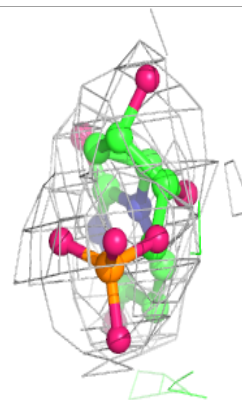
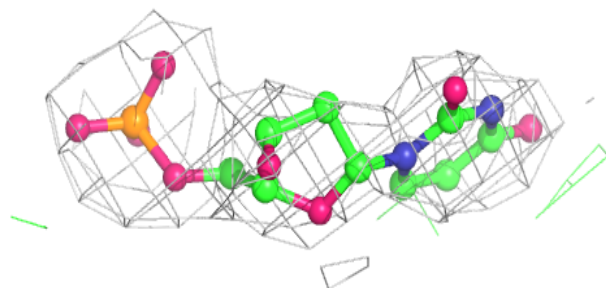
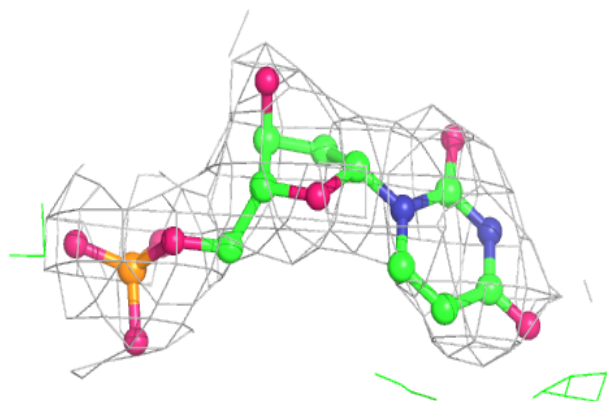
**Electron density around UMP B 701:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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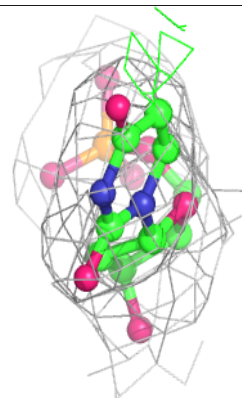
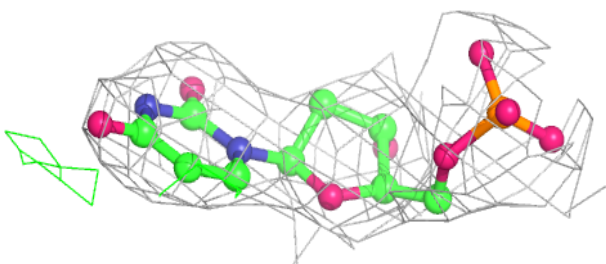
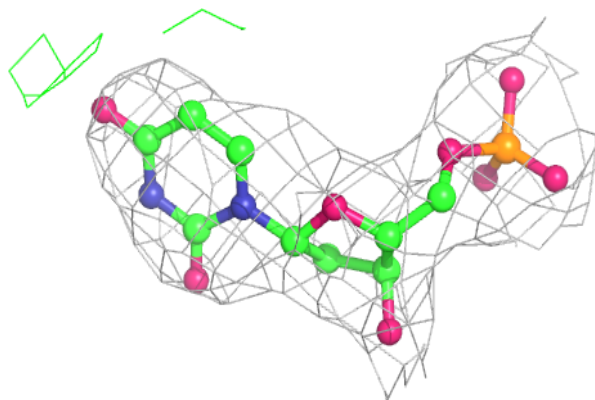


Electron density around UMP F 701:

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

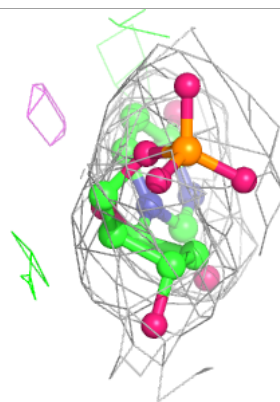
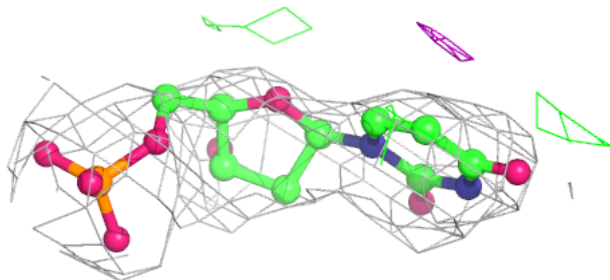
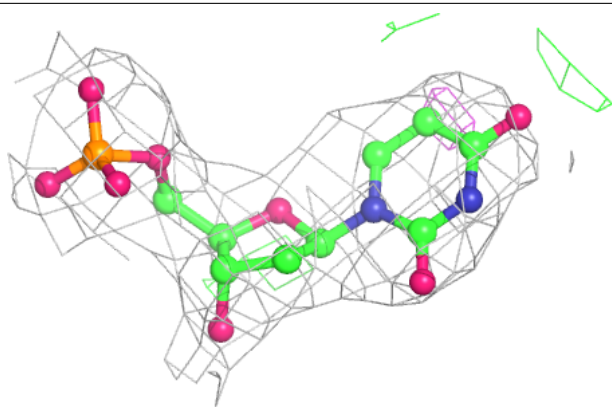
**Electron density around UMP A 701:**

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

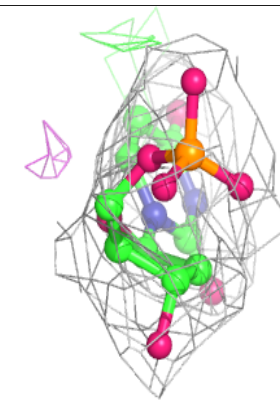
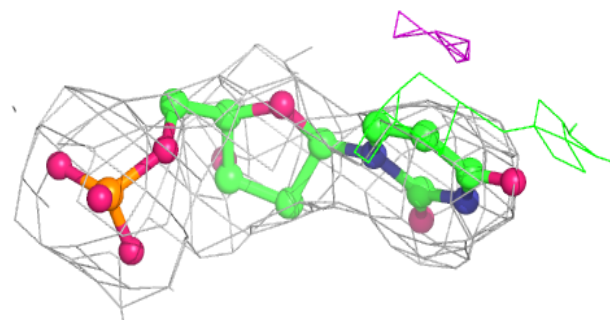
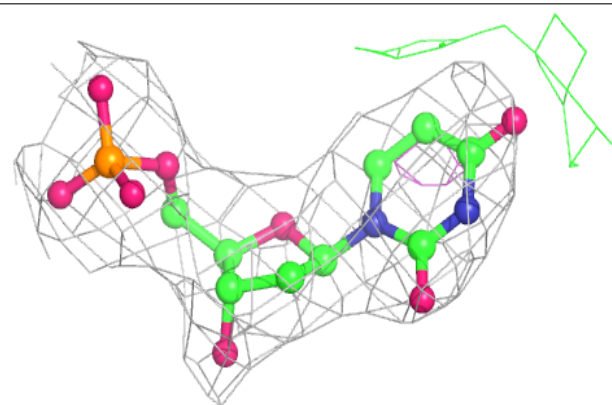


Electron density around UMP C 701:

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

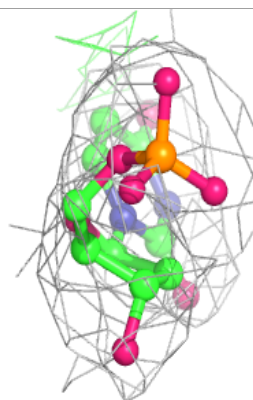
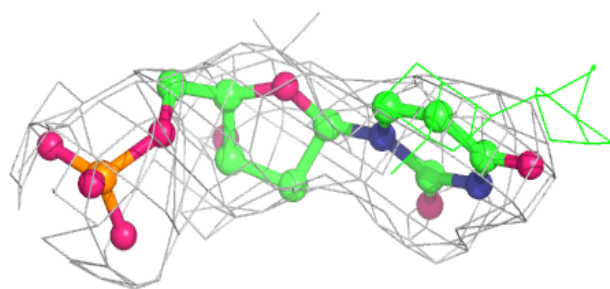
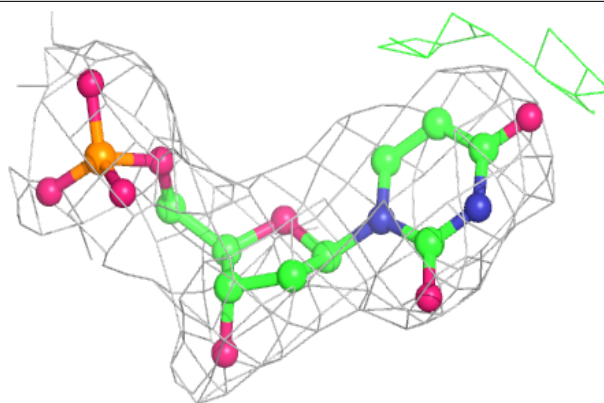
**Electron density around UMP G 701:**

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

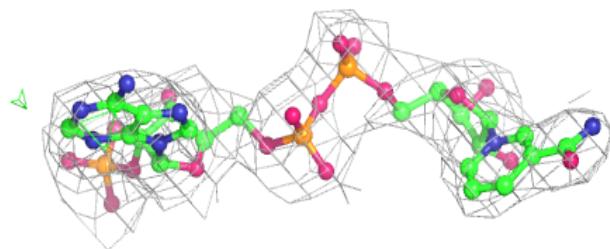
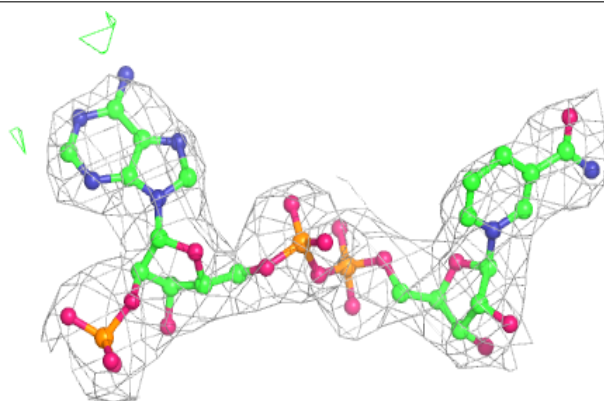


Electron density around UMP E 701:

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

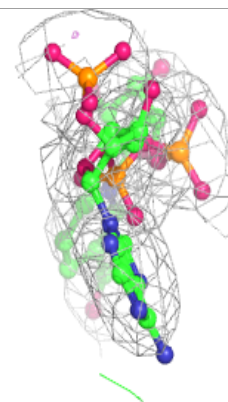
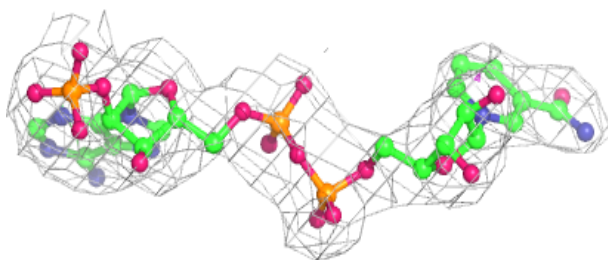
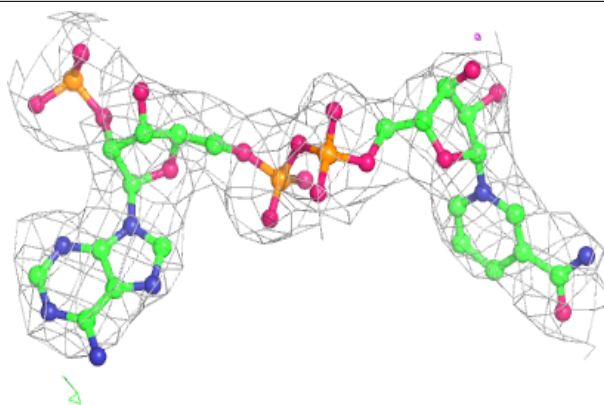
**Electron density around NDP A 704:**

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

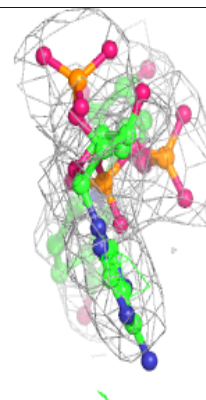
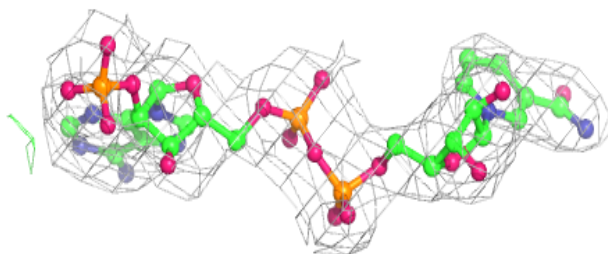
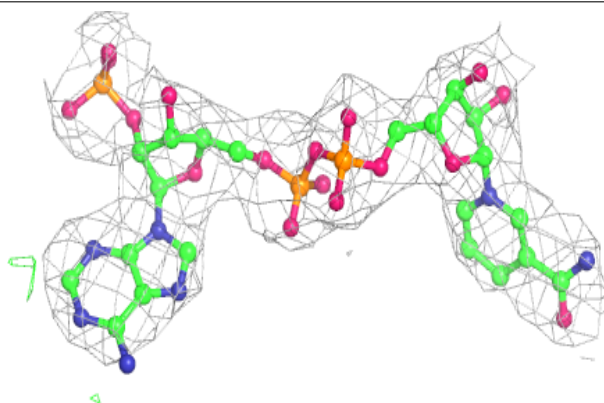


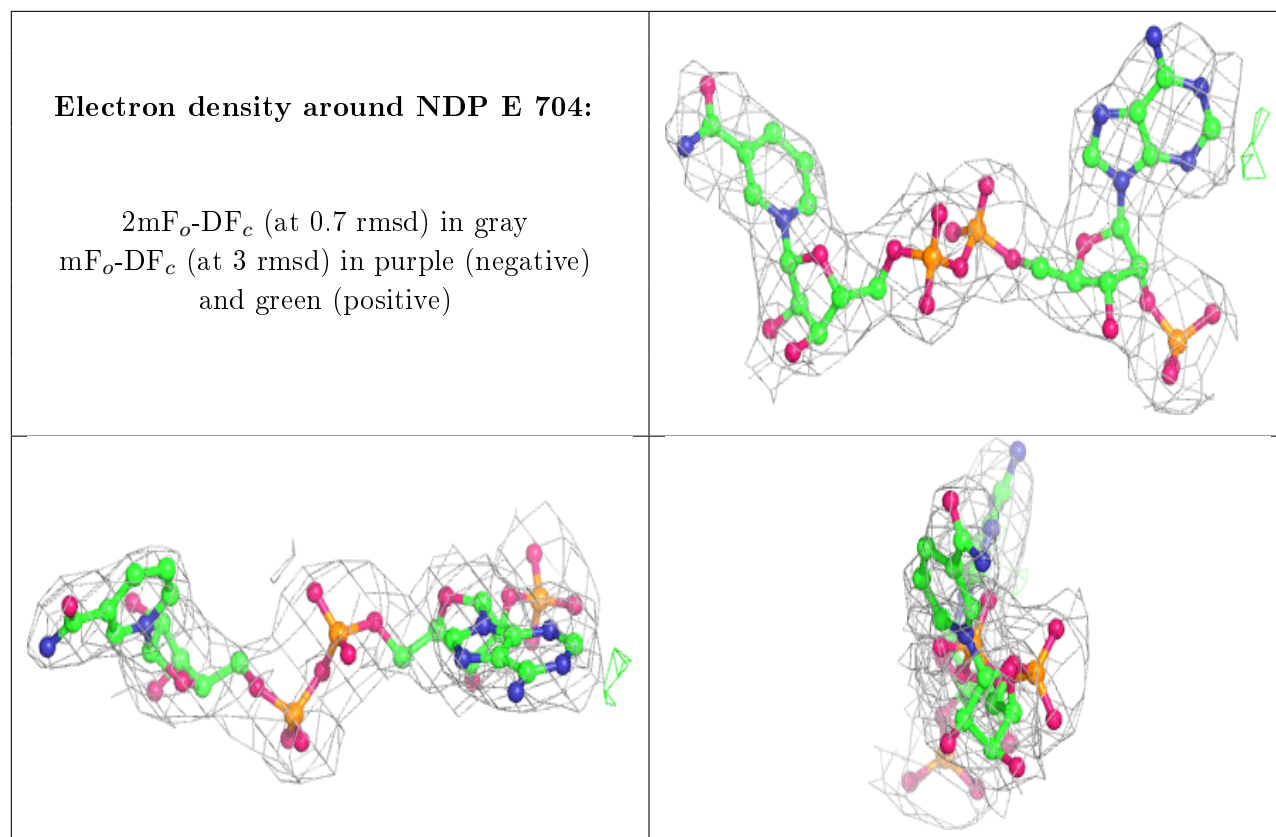
Electron density around NDP G 704:

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

**Electron density around NDP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.