



wwPDB EM Validation Summary Report ⓘ

May 26, 2025 – 01:54 AM EDT

PDB ID : 6UA4 / pdb_00006ua4
EMDB ID : EMD-20705
Title : Human IMPDH2 treated with ATP, IMP, NAD⁺, and 2 mM GTP. Bent (3/4 compressed, 1/4 extended) segment reconstruction.
Authors : Johnson, M.C.; Kollman, J.M.
Deposited on : 2019-09-10
Resolution : 3.65 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

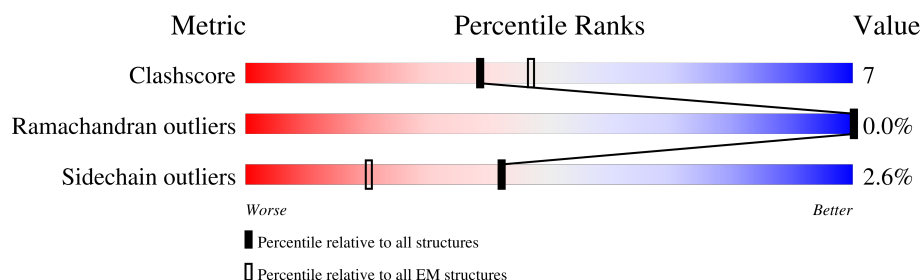
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



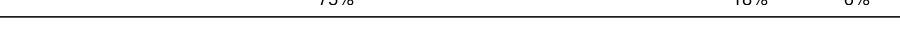


The reported resolution of this entry is 3.65 Å.

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.



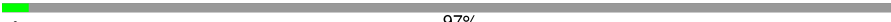
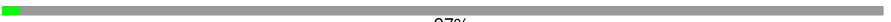






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	
1	B	519	
1	C	519	
1	D	519	
1	E	519	
1	F	519	
1	G	519	
1	H	519	

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Mol	Chain	Length	Quality of chain
1	I	519	 97%
1	J	519	 97%
1	K	519	 97%
1	L	519	 97%
1	M	519	 97%
1	N	519	 97%
1	O	519	 97%
1	P	519	 97%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31726 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	B	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	C	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	D	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	E	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	F	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	G	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	H	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	M	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	N	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	O	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	P	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	I	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	J	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	K	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	L	14	Total	C	N	O	S	0	0
			102	66	14	21	1		

There are 80 discrepancies between the modelled and reference sequences:

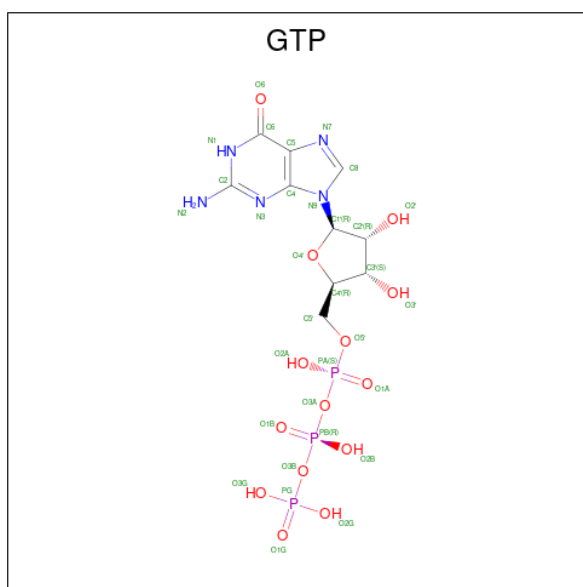
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP P12268
A	-3	GLU	-	expression tag	UNP P12268
A	-2	PHE	-	expression tag	UNP P12268
A	-1	GLU	-	expression tag	UNP P12268
A	0	LEU	-	expression tag	UNP P12268
B	-4	SER	-	expression tag	UNP P12268
B	-3	GLU	-	expression tag	UNP P12268
B	-2	PHE	-	expression tag	UNP P12268
B	-1	GLU	-	expression tag	UNP P12268
B	0	LEU	-	expression tag	UNP P12268
C	-4	SER	-	expression tag	UNP P12268
C	-3	GLU	-	expression tag	UNP P12268
C	-2	PHE	-	expression tag	UNP P12268
C	-1	GLU	-	expression tag	UNP P12268
C	0	LEU	-	expression tag	UNP P12268
D	-4	SER	-	expression tag	UNP P12268
D	-3	GLU	-	expression tag	UNP P12268
D	-2	PHE	-	expression tag	UNP P12268
D	-1	GLU	-	expression tag	UNP P12268
D	0	LEU	-	expression tag	UNP P12268
E	-4	SER	-	expression tag	UNP P12268
E	-3	GLU	-	expression tag	UNP P12268
E	-2	PHE	-	expression tag	UNP P12268
E	-1	GLU	-	expression tag	UNP P12268
E	0	LEU	-	expression tag	UNP P12268
F	-4	SER	-	expression tag	UNP P12268
F	-3	GLU	-	expression tag	UNP P12268
F	-2	PHE	-	expression tag	UNP P12268
F	-1	GLU	-	expression tag	UNP P12268
F	0	LEU	-	expression tag	UNP P12268
G	-4	SER	-	expression tag	UNP P12268
G	-3	GLU	-	expression tag	UNP P12268
G	-2	PHE	-	expression tag	UNP P12268
G	-1	GLU	-	expression tag	UNP P12268
G	0	LEU	-	expression tag	UNP P12268
H	-4	SER	-	expression tag	UNP P12268
H	-3	GLU	-	expression tag	UNP P12268
H	-2	PHE	-	expression tag	UNP P12268
H	-1	GLU	-	expression tag	UNP P12268
H	0	LEU	-	expression tag	UNP P12268
M	-4	SER	-	expression tag	UNP P12268
M	-3	GLU	-	expression tag	UNP P12268
M	-2	PHE	-	expression tag	UNP P12268

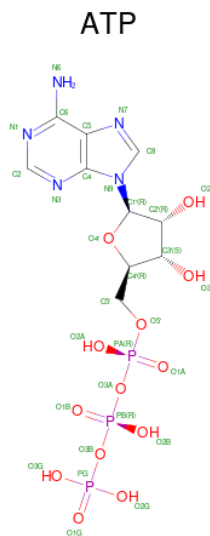
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Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	GLU	-	expression tag	UNP P12268
M	0	LEU	-	expression tag	UNP P12268
N	-4	SER	-	expression tag	UNP P12268
N	-3	GLU	-	expression tag	UNP P12268
N	-2	PHE	-	expression tag	UNP P12268
N	-1	GLU	-	expression tag	UNP P12268
N	0	LEU	-	expression tag	UNP P12268
O	-4	SER	-	expression tag	UNP P12268
O	-3	GLU	-	expression tag	UNP P12268
O	-2	PHE	-	expression tag	UNP P12268
O	-1	GLU	-	expression tag	UNP P12268
O	0	LEU	-	expression tag	UNP P12268
P	-4	SER	-	expression tag	UNP P12268
P	-3	GLU	-	expression tag	UNP P12268
P	-2	PHE	-	expression tag	UNP P12268
P	-1	GLU	-	expression tag	UNP P12268
P	0	LEU	-	expression tag	UNP P12268
I	-4	SER	-	expression tag	UNP P12268
I	-3	GLU	-	expression tag	UNP P12268
I	-2	PHE	-	expression tag	UNP P12268
I	-1	GLU	-	expression tag	UNP P12268
I	0	LEU	-	expression tag	UNP P12268
J	-4	SER	-	expression tag	UNP P12268
J	-3	GLU	-	expression tag	UNP P12268
J	-2	PHE	-	expression tag	UNP P12268
J	-1	GLU	-	expression tag	UNP P12268
J	0	LEU	-	expression tag	UNP P12268
K	-4	SER	-	expression tag	UNP P12268
K	-3	GLU	-	expression tag	UNP P12268
K	-2	PHE	-	expression tag	UNP P12268
K	-1	GLU	-	expression tag	UNP P12268
K	0	LEU	-	expression tag	UNP P12268
L	-4	SER	-	expression tag	UNP P12268
L	-3	GLU	-	expression tag	UNP P12268
L	-2	PHE	-	expression tag	UNP P12268
L	-1	GLU	-	expression tag	UNP P12268
L	0	LEU	-	expression tag	UNP P12268

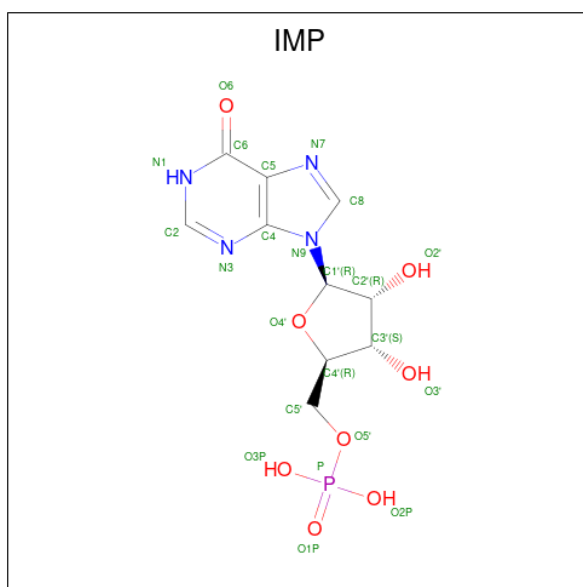
- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).





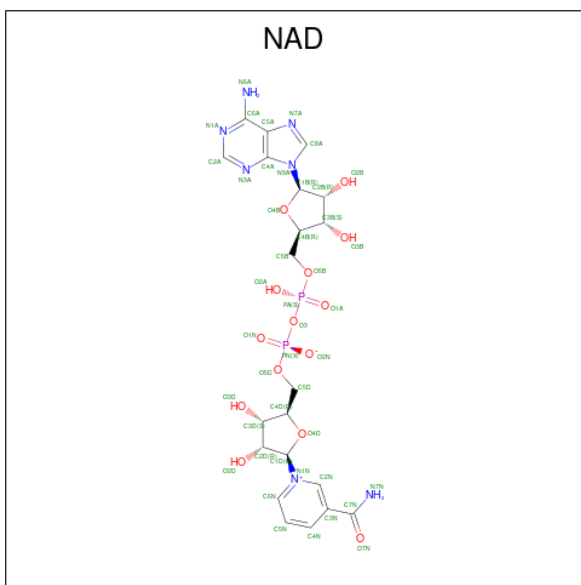
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	H	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is INOSINIC ACID (CCD ID: IMP) (formula: $\text{C}_{10}\text{H}_{13}\text{N}_4\text{O}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	B	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	C	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	D	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	E	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	F	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	G	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	H	1	Total	C	N	O	P	0
			23	10	4	8	1	

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

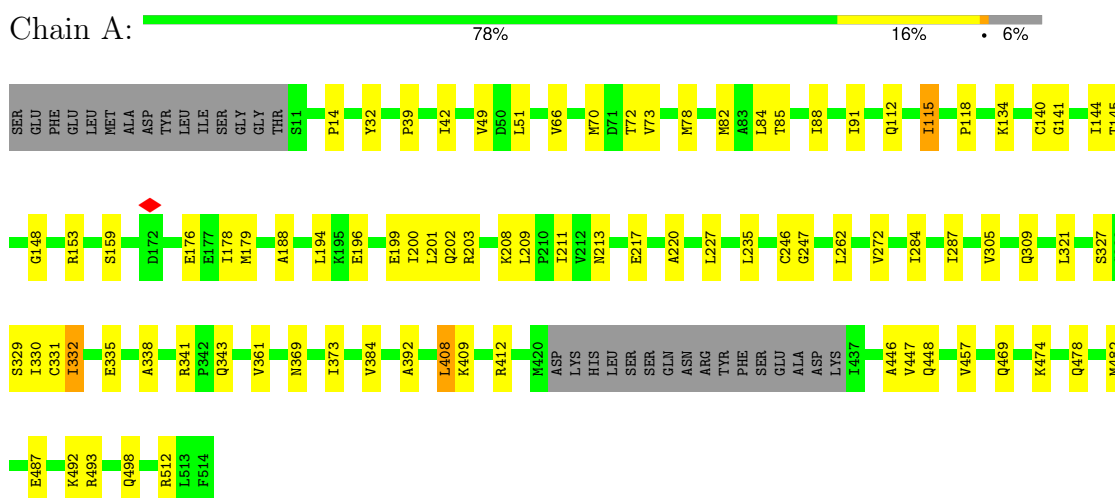


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 44	C 21	N 7	O 14	P 2	0
5	B	1	Total 44	C 21	N 7	O 14	P 2	0
5	C	1	Total 44	C 21	N 7	O 14	P 2	0
5	D	1	Total 44	C 21	N 7	O 14	P 2	0
5	E	1	Total 44	C 21	N 7	O 14	P 2	0
5	F	1	Total 44	C 21	N 7	O 14	P 2	0
5	G	1	Total 44	C 21	N 7	O 14	P 2	0
5	H	1	Total 44	C 21	N 7	O 14	P 2	0

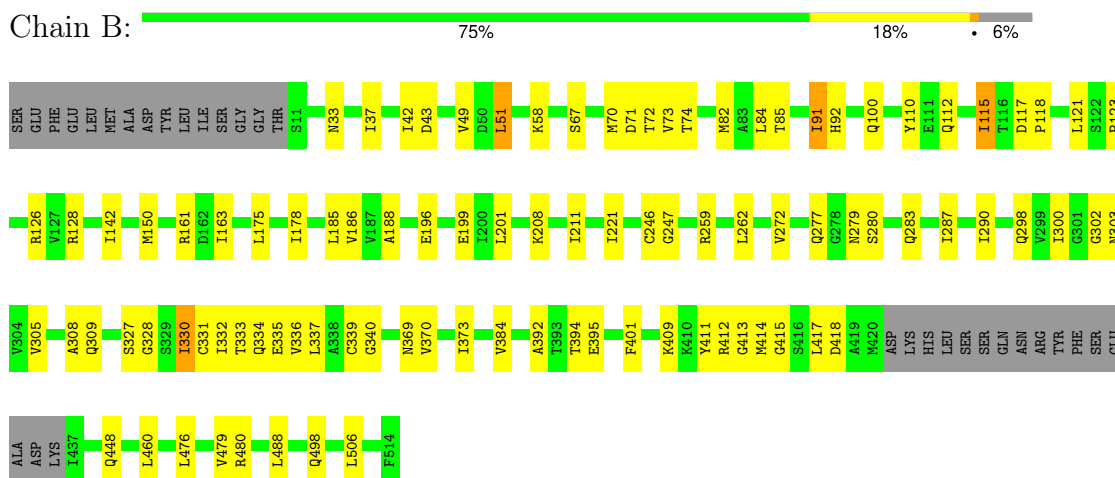
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Inosine-5'-monophosphate dehydrogenase 2

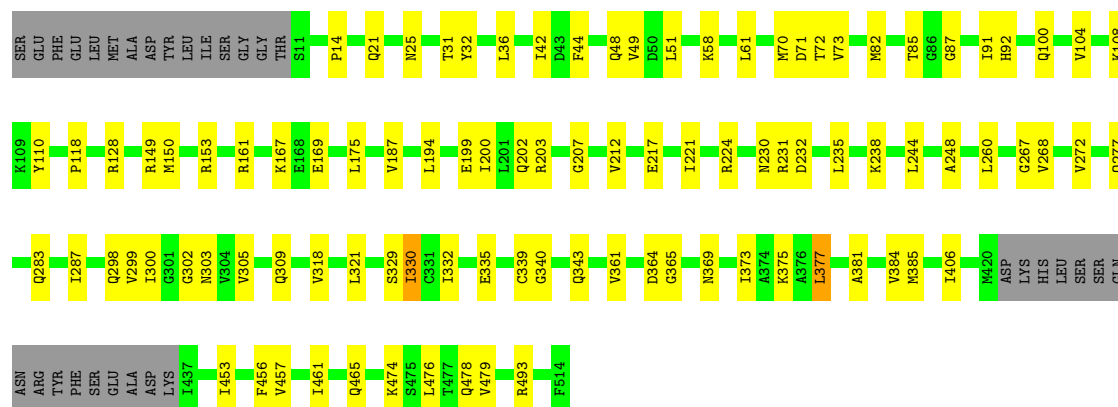


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



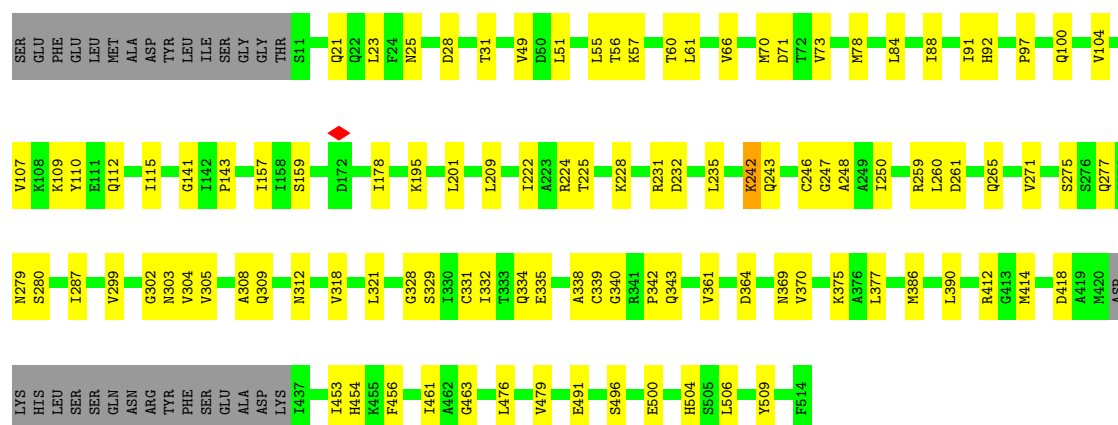
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2





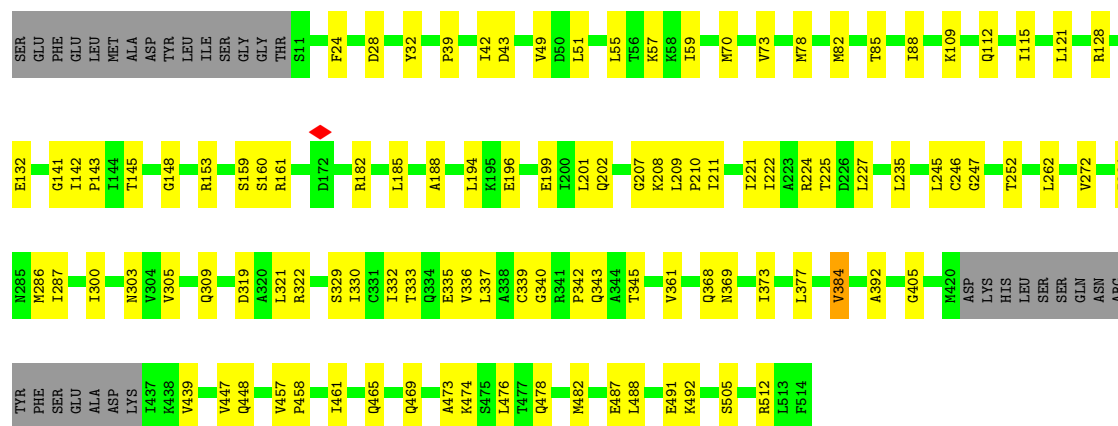
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain D: 74% 20% 6%



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain E: 74% 20% 6%



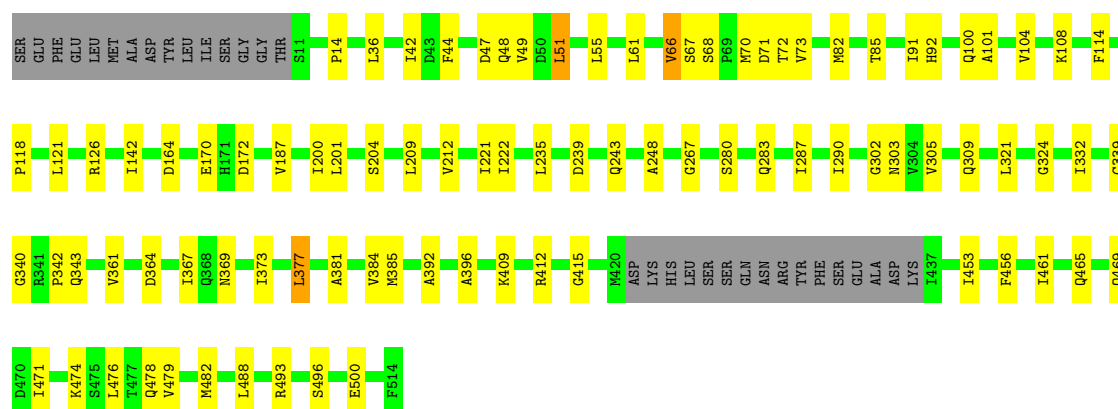
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain F: 75% 18% 6%



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain G: 77% 17% 6%



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain H: 75% 19% 6%

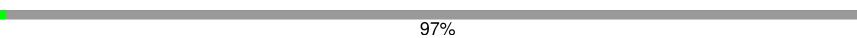


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain M: 97%

ser	gly	ser	gly	val	leu	leu	leu	asp	leu	ser
ser	gly	ser	gly	thr	cys	val	val	arg	val	glu
glu	glu	glu	ile	ala	glu	ile	val	val	ser	phe
leu	leu	asn	glu	ala	ala	ala	pro	arg	ser	glu
phe	phe	tyr	val	ala	ile	ile	ala	val	met	m1
glu	gly	phe	gly	lys	thr	gly	gly	phe	asp	
lys	his	ser	his	asn	thr	thr	ile	glu	thr	
arg	glu	glu	ile	leu	his	thr	leu	ala	val	l5
thr	ala	ala	ile	ala	glu	ile	thr	lys	thr	
ser	ser	asp	lys	asp	asp	lys	lys	ala	glu	p14
ser	ser	lys	ala	ala	asp	glu	arg	ala	asp	
ala	ile	ile	leu	gly	lys	ala	his	gly	asp	
glu	lys	lys	ala	val	tyr	asn	met	gly	leu	
val	val	val	val	asp	arg	glu	phe	ala	thr	
glu	glu	ala	ala	leu	leu	ile	ile	ile	ala	
gly	glu	glu	ala	leu	asp	leu	gly	gly	glu	
gly	gly	gly	arg	leu	leu	glu	ile	ile	met	
val	val	val	val	val	leu	arg	arg	pro	ala	
his	his	ser	val	gly	leu	ser	ile	ile	leu	
ser	ser	gly	met	met	glu	thr	thr	thr	thr	
leu	leu	ala	met	gly	ala	lys	asp	gly	thr	
his	his	val	gly	ser	gly	gly	thr	gly	asp	
ser	ser	glu	ser	leu	asp	val	ile	ile	gly	
tyr	tyr	asp	leu	ser	asp	leu	arg	arg	gly	
glu	glu	lys	leu	leu	val	pro	met	phe	phe	
lys	lys	gly	ala	val	ile	ile	gly	ile	thr	
arg	arg	ser	ala	ile	val	val	ser	ser	his	
leu	leu	ile	thr	thr	leu	asn	arg	asn	asn	
phe	phe	his	thr	thr	asp	glu	leu	leu	asp	
	lys	lys	glu	ser	ser	asp	val	cys	phe	
		val	leu	glu	glu	thr	thr	thr	leu	
		val	pro	leu	glu	glu	ile	pro	ile	
		pro	gly	ala	leu	leu	ile	glu	leu	
		tyr	glu	cys	asn	val	ser	phe	pro	
		leu	tyr	arg	ser	ala	ser	glu	gly	
		ile	phe	gly	ile	ile	arg	ala	ala	
		ala	phe	thr	phe	ile	arg	asn	asn	
		gly	ser	ala	met	thr	phe	arg	thr	
		glu	ile	ala	leu	asp	leu	lys	ala	
		ser	arg	val	ile	leu	lys	val	asp	
		cys	thr	tyr	lys	lys	glu	lys	glu	
		glu	lys	lys	tyr	asn	glu	tyr	asp	
		asp	tyr	ser	lys	arg	his	asp	leu	
		ile	arg	glu	asp	thr	asp	glu	glu	
		gly	thr	glu	asp	tyr	cys	thr	thr	
		ala	gly	tyr	lys	pro	gly	gly	ser	
		lys	met	ala	pro	leu	phe	ile	ala	
		leu	ser	arg	thr	ala	leu	leu	thr	
		thr	leu	phe	leu	glu	glu	thr	lys	
		glu	asp	gly	glu	lys	ile	asp	pro	
		val	ala	val	val	asp	ile	ile	thr	
		arg	ala	pro	val	thr	met	met	val	
		arg	val	val	glu	thr	arg	thr	val	
		glu	thr	glu	thr	ser	glu	asp	lys	
		thr	leu	thr	glu	ser	glu	thr	thr	
		thr	leu	thr	asn	lys	asp	thr	lys	
		met	asn	val	asn	asp	leu	pro	lys	
		met	asn	ile	glu	thr	glu	thr	ile	
		thr	asn	glu	thr	thr	thr	thr	thr	
		tyr	val	thr	val	arg	thr	thr	thr	

- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain N: [illegible]

- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

97%

GLU LEU LYS PHE GLU LYS ARG THR SER SER ALA GLN VAL GLU GLY GLY VAL HIS SER LEU HIS SER SER TYR GLU LYS ARG LEU PHE

- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

97%

LYS HIS LEU SER SER SER GLN ASN ASP ARG TYR PHE SER SER SER GLY ALA ASP LYS ILE ILE VAL VAL GLN GLN GLY VAL VAL SER SER GLY GLY ILE HIS LYS PHE VAL VAL VAL PRO TYR LEU LEU ILE ALA GLY ILE ILE GLN HIS SER CYS GLN ASP ASP GLY GLY LYS SER SER THR GLN VAL ARG ALA

[illegible]

- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain K: 97%

[illegible]

- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain L: 97%

[illegible]

SER	GLY	GLU	LEU	LYS	PHE	GLU	LYS	ARG	THR	SER	ALA	GLN	VAL	GLY	GLN	GLY	VAL	HIS	SER	LEU	HIS	TYR	SER	GLY	GLY	ARG	LEU	PHE	SER	GLY	GLU	TYR	LEU	PHE	PHE	SER	ASP	ILE	GLN	HIS	SER	CYS	GLN	ASP	ILE	GLY	ARG	LYS	LYS	THR	THR	LEU	SER	GLY	MET	GLY	ASP	LYS	HIS	LEU
SER	GLY	GLU	LEU	LYS	PHE	GLU	LYS	ARG	THR	SER	ALA	GLN	VAL	GLY	GLN	GLY	VAL	HIS	SER	LEU	HIS	TYR	SER	GLY	GLY	ARG	LEU	PHE		PRO	VAL	PHE	LYS	HIS	ILE	SER	GLY	GLN	HIS	SER	CYS	GLN	ASP	ILE	GLY	ARG	LYS	LYS	THR	THR	LEU	SER	GLY	MET	GLY	ASP	LYS	HIS	LEU	
SER	GLY	GLU	LEU	LYS	PHE	GLU	LYS	ARG	THR	SER	ALA	GLN	VAL	GLY	GLN	GLY	VAL	HIS	SER	LEU	HIS	TYR	SER	GLY	GLY	ARG	LEU	PHE		PRO	VAL	PHE	LYS	HIS	ILE	SER	GLY	GLN	HIS	SER	CYS	GLN	ASP	ILE	GLY	ARG	LYS	LYS	THR	THR	LEU	SER	GLY	MET	GLY	ASP	LYS	HIS	LEU	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	31726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	115.642	Depositor
Minimum map value	-69.181	Depositor
Average map value	0.074	Depositor
Map value standard deviation	2.929	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

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: ATP, GTP, IMP, NAD

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	0.39	0/3766	0.72	0/5078
1	B	0.42	0/3766	0.73	1/5078 (0.0%)
1	C	0.39	0/3766	0.73	0/5078
1	D	0.37	0/3766	0.70	0/5078
1	E	0.38	0/3766	0.70	0/5078
1	F	0.43	1/3766 (0.0%)	0.73	1/5078 (0.0%)
1	G	0.38	0/3766	0.71	0/5078
1	H	0.36	0/3766	0.70	0/5078
1	I	0.36	0/104	0.94	0/141
1	J	0.27	0/104	0.92	0/141
1	K	0.26	0/104	0.90	0/141
1	L	0.26	0/104	0.98	0/141
1	M	0.36	0/104	0.93	0/141
1	N	0.26	0/104	0.90	0/141
1	O	0.36	0/104	0.86	0/141
1	P	0.33	0/104	1.08	2/141 (1.4%)
All	All	0.39	1/30960 (0.0%)	0.72	4/41752 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	J	0	1
1	L	0	1
1	N	0	1
1	P	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	417	LEU	CA-C	-5.44	1.45	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	111	GLU	N-CA-C	5.56	119.31	112.03
1	B	110	TYR	N-CA-CB	-5.30	108.13	114.17
1	P	11	SER	CA-C-N	-5.12	114.29	122.17
1	P	11	SER	C-N-CA	-5.12	114.29	122.17

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	110	TYR	Peptide
1	J	11	SER	Peptide
1	L	11	SER	Peptide
1	N	11	SER	Peptide
1	P	10	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3710	0	3766	51	0
1	B	3710	0	3766	64	0
1	C	3710	0	3766	55	0
1	D	3710	0	3766	63	0
1	E	3710	0	3766	71	0
1	F	3710	0	3766	64	0
1	G	3710	0	3766	57	0
1	H	3710	0	3766	68	0
1	I	102	0	99	0	0
1	J	102	0	99	1	0
1	K	102	0	99	1	0
1	L	102	0	99	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	102	0	99	1	0
1	N	102	0	99	0	0
1	O	102	0	99	1	0
1	P	102	0	99	0	0
2	A	64	0	22	2	0
2	B	64	0	24	2	0
2	D	64	0	21	2	0
2	E	64	0	23	3	0
2	F	64	0	23	0	0
2	H	64	0	23	1	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
3	C	62	0	24	1	0
3	D	31	0	12	0	0
3	E	31	0	12	4	0
3	F	31	0	12	3	0
3	G	62	0	24	0	0
3	H	31	0	12	0	0
4	A	23	0	11	1	0
4	B	23	0	11	2	0
4	C	23	0	11	1	0
4	D	23	0	11	2	0
4	E	23	0	11	1	0
4	F	23	0	11	2	0
4	G	23	0	11	2	0
4	H	23	0	11	2	0
5	A	44	0	24	0	0
5	B	44	0	24	3	0
5	C	44	0	24	1	0
5	D	44	0	24	1	0
5	E	44	0	24	2	0
5	F	44	0	24	2	0
5	G	44	0	24	2	0
5	H	44	0	24	2	0
All	All	31726	0	31456	448	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 448 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:G:67:SER:HB3	1:G:82:MET:HE1	1.66	0.77
1:E:305:VAL:H	1:E:309:GLN:HE21	1.34	0.75
1:E:474:LYS:H	1:E:478:GLN:HE21	1.31	0.75
1:C:305:VAL:H	1:C:309:GLN:HE21	1.36	0.72
1:B:305:VAL:H	1:B:309:GLN:HE21	1.38	0.71

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 PDB entries followed by that with respect to all EM entries.

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	484/519 (93%)	447 (92%)	37 (8%)	0	100	100
1	B	484/519 (93%)	453 (94%)	31 (6%)	0	100	100
1	C	484/519 (93%)	454 (94%)	29 (6%)	1 (0%)	44	72
1	D	484/519 (93%)	451 (93%)	33 (7%)	0	100	100
1	E	484/519 (93%)	447 (92%)	37 (8%)	0	100	100
1	F	484/519 (93%)	450 (93%)	34 (7%)	0	100	100
1	G	484/519 (93%)	449 (93%)	35 (7%)	0	100	100
1	H	484/519 (93%)	453 (94%)	31 (6%)	0	100	100
1	I	12/519 (2%)	6 (50%)	6 (50%)	0	100	100
1	J	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	K	12/519 (2%)	9 (75%)	3 (25%)	0	100	100
1	L	12/519 (2%)	5 (42%)	7 (58%)	0	100	100
1	M	12/519 (2%)	6 (50%)	6 (50%)	0	100	100
1	N	12/519 (2%)	6 (50%)	6 (50%)	0	100	100
1	O	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	P	12/519 (2%)	8 (67%)	4 (33%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3968/8304 (48%)	3658 (92%)	309 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	110	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	398/425 (94%)	383 (96%)	15 (4%)	28	53
1	B	398/425 (94%)	387 (97%)	11 (3%)	38	59
1	C	398/425 (94%)	389 (98%)	9 (2%)	45	64
1	D	398/425 (94%)	387 (97%)	11 (3%)	38	59
1	E	398/425 (94%)	390 (98%)	8 (2%)	50	68
1	F	398/425 (94%)	386 (97%)	12 (3%)	36	58
1	G	398/425 (94%)	388 (98%)	10 (2%)	42	61
1	H	398/425 (94%)	390 (98%)	8 (2%)	50	68
1	I	11/425 (3%)	11 (100%)	0	100	100
1	J	11/425 (3%)	11 (100%)	0	100	100
1	K	11/425 (3%)	11 (100%)	0	100	100
1	L	11/425 (3%)	11 (100%)	0	100	100
1	M	11/425 (3%)	11 (100%)	0	100	100
1	N	11/425 (3%)	11 (100%)	0	100	100
1	O	11/425 (3%)	11 (100%)	0	100	100
1	P	11/425 (3%)	10 (91%)	1 (9%)	7	29
All	All	3272/6800 (48%)	3187 (97%)	85 (3%)	42	60

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	163	ILE
1	G	287	ILE
1	F	185	LEU
1	F	384	VAL
1	G	471	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	441	GLN
1	H	92	HIS
1	H	498	GLN
1	C	343	GLN
1	C	312	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

38 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	ATP	C	601	-	28,33,33	3.48	14 (50%)	34,52,52	3.74	5 (14%)
5	NAD	C	604	-	42,48,48	3.64	17 (40%)	50,73,73	2.59	6 (12%)
2	GTP	F	601	-	29,34,34	4.25	18 (62%)	35,54,54	1.93	5 (14%)
5	NAD	G	604	-	42,48,48	3.67	17 (40%)	50,73,73	2.69	8 (16%)
4	IMP	F	604	-	21,25,25	2.76	7 (33%)	22,38,38	1.66	6 (27%)
5	NAD	D	605	-	42,48,48	3.68	18 (42%)	50,73,73	2.64	7 (14%)
2	GTP	E	601	-	29,34,34	4.18	18 (62%)	35,54,54	1.64	5 (14%)
3	ATP	G	601	-	28,33,33	3.45	14 (50%)	34,52,52	3.79	6 (17%)
3	ATP	D	603	-	28,33,33	3.57	14 (50%)	34,52,52	3.74	5 (14%)
4	IMP	C	603	-	21,25,25	2.75	7 (33%)	22,38,38	1.66	6 (27%)
2	GTP	A	601	-	29,34,34	4.18	17 (58%)	35,54,54	1.58	6 (17%)
2	GTP	H	602	-	29,34,34	4.32	17 (58%)	35,54,54	1.44	5 (14%)
5	NAD	A	605	-	42,48,48	3.64	17 (40%)	50,73,73	2.57	7 (14%)
4	IMP	D	604	-	21,25,25	2.79	7 (33%)	22,38,38	1.58	5 (22%)
5	NAD	B	605	-	42,48,48	3.66	18 (42%)	50,73,73	2.67	8 (16%)
2	GTP	H	601	-	29,34,34	4.29	17 (58%)	35,54,54	1.52	5 (14%)
3	ATP	B	603	-	28,33,33	3.39	14 (50%)	34,52,52	3.75	6 (17%)
2	GTP	F	602	-	29,34,34	4.31	18 (62%)	35,54,54	1.50	6 (17%)
2	GTP	A	602	-	29,34,34	4.27	18 (62%)	35,54,54	2.00	6 (17%)
3	ATP	C	602	-	28,33,33	3.49	14 (50%)	34,52,52	3.73	5 (14%)
3	ATP	A	603	-	28,33,33	3.36	14 (50%)	34,52,52	3.71	5 (14%)
5	NAD	E	605	-	42,48,48	3.67	17 (40%)	50,73,73	2.60	8 (16%)
3	ATP	G	602	-	28,33,33	3.51	14 (50%)	34,52,52	3.74	5 (14%)
3	ATP	E	603	-	28,33,33	3.40	14 (50%)	34,52,52	3.73	5 (14%)
4	IMP	G	603	-	21,25,25	2.70	7 (33%)	22,38,38	1.62	6 (27%)
2	GTP	E	602	-	29,34,34	4.29	18 (62%)	35,54,54	1.72	4 (11%)
5	NAD	H	605	-	42,48,48	3.68	17 (40%)	50,73,73	2.68	7 (14%)
2	GTP	B	601	-	29,34,34	4.17	17 (58%)	35,54,54	1.68	5 (14%)
2	GTP	D	601	-	29,34,34	4.32	17 (58%)	35,54,54	1.57	7 (20%)
4	IMP	B	604	-	21,25,25	2.74	7 (33%)	22,38,38	1.71	5 (22%)
3	ATP	H	603	-	28,33,33	3.47	14 (50%)	34,52,52	3.70	5 (14%)
2	GTP	B	602	-	29,34,34	4.27	17 (58%)	35,54,54	1.49	5 (14%)
2	GTP	D	602	-	29,34,34	4.29	17 (58%)	35,54,54	1.43	5 (14%)
4	IMP	A	604	-	21,25,25	2.69	7 (33%)	22,38,38	1.64	5 (22%)
4	IMP	E	604	-	21,25,25	2.69	7 (33%)	22,38,38	1.64	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAD	F	605	-	42,48,48	3.65	18 (42%)	50,73,73	2.60	7 (14%)
3	ATP	F	603	-	28,33,33	3.47	14 (50%)	34,52,52	3.77	5 (14%)
4	IMP	H	604	-	21,25,25	2.75	7 (33%)	22,38,38	1.75	5 (22%)

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	ATP	C	601	-	-	2/18/38/38	0/3/3/3
5	NAD	C	604	-	-	8/26/62/62	0/5/5/5
2	GTP	F	601	-	-	6/18/38/38	0/3/3/3
5	NAD	G	604	-	-	8/26/62/62	0/5/5/5
4	IMP	F	604	-	-	3/6/26/26	0/3/3/3
5	NAD	D	605	-	-	9/26/62/62	0/5/5/5
2	GTP	E	601	-	-	7/18/38/38	0/3/3/3
3	ATP	G	601	-	-	5/18/38/38	0/3/3/3
3	ATP	D	603	-	-	10/18/38/38	0/3/3/3
4	IMP	C	603	-	-	5/6/26/26	0/3/3/3
2	GTP	A	601	-	-	6/18/38/38	0/3/3/3
2	GTP	H	602	-	-	3/18/38/38	0/3/3/3
5	NAD	A	605	-	-	4/26/62/62	0/5/5/5
4	IMP	D	604	-	-	0/6/26/26	0/3/3/3
5	NAD	B	605	-	-	15/26/62/62	0/5/5/5
2	GTP	H	601	-	-	5/18/38/38	0/3/3/3
3	ATP	B	603	-	-	7/18/38/38	0/3/3/3
2	GTP	F	602	-	-	3/18/38/38	0/3/3/3
2	GTP	A	602	-	-	3/18/38/38	0/3/3/3
3	ATP	C	602	-	-	3/18/38/38	0/3/3/3
3	ATP	A	603	-	-	5/18/38/38	0/3/3/3
5	NAD	E	605	-	-	11/26/62/62	0/5/5/5
3	ATP	G	602	-	-	7/18/38/38	0/3/3/3
3	ATP	E	603	-	-	6/18/38/38	0/3/3/3
4	IMP	G	603	-	-	5/6/26/26	0/3/3/3
2	GTP	E	602	-	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	H	605	-	-	11/26/62/62	0/5/5/5
2	GTP	B	601	-	-	3/18/38/38	0/3/3/3
2	GTP	D	601	-	-	5/18/38/38	0/3/3/3
4	IMP	B	604	-	-	2/6/26/26	0/3/3/3
3	ATP	H	603	-	-	0/18/38/38	0/3/3/3
2	GTP	B	602	-	-	1/18/38/38	0/3/3/3
2	GTP	D	602	-	-	6/18/38/38	0/3/3/3
4	IMP	A	604	-	-	1/6/26/26	0/3/3/3
4	IMP	E	604	-	-	5/6/26/26	0/3/3/3
5	NAD	F	605	-	-	9/26/62/62	0/5/5/5
3	ATP	F	603	-	-	2/18/38/38	0/3/3/3
4	IMP	H	604	-	-	0/6/26/26	0/3/3/3

The worst 5 of 544 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GTP	C2'-C3'	-11.05	1.23	1.53
2	F	601	GTP	C2'-C3'	-10.97	1.23	1.53
2	E	601	GTP	C2'-C3'	-10.95	1.23	1.53
2	A	601	GTP	C2'-C3'	-10.93	1.23	1.53
2	F	602	GTP	C2'-C3'	-10.91	1.23	1.53

The worst 5 of 217 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	603	ATP	C5-C6-N6	14.52	142.42	120.31
3	B	603	ATP	C5-C6-N6	14.51	142.41	120.31
3	D	603	ATP	C5-C6-N6	14.47	142.35	120.31
3	A	603	ATP	C5-C6-N6	14.47	142.35	120.31
3	F	603	ATP	C5-C6-N6	14.46	142.34	120.31

There are no chirality outliers.

5 of 198 torsion outliers are listed below:

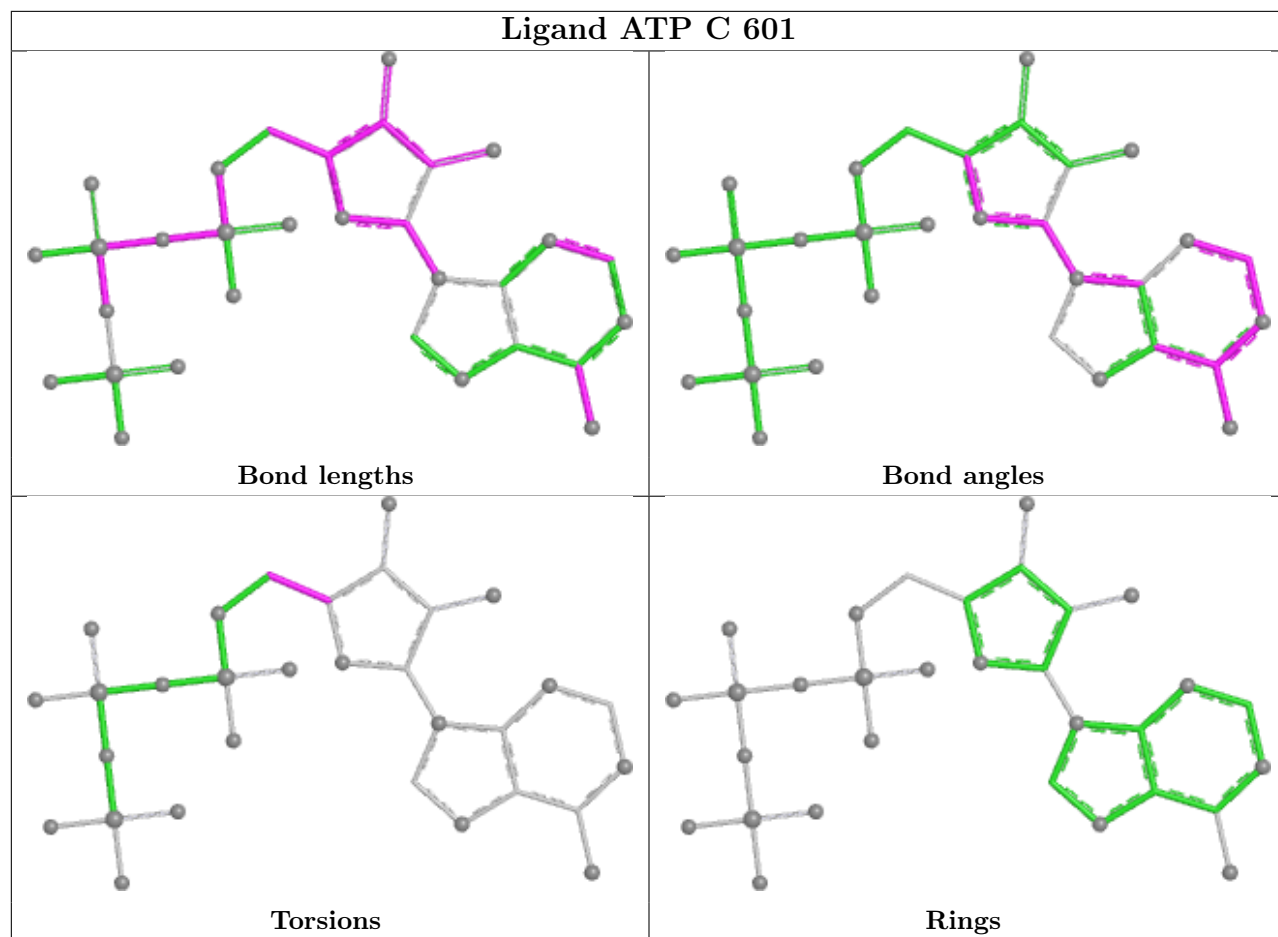
Mol	Chain	Res	Type	Atoms
2	A	601	GTP	PB-O3B-PG-O2G
2	A	601	GTP	PB-O3B-PG-O3G
2	D	601	GTP	PB-O3B-PG-O2G
2	D	601	GTP	PB-O3B-PG-O3G
2	D	601	GTP	C5'-O5'-PA-O1A

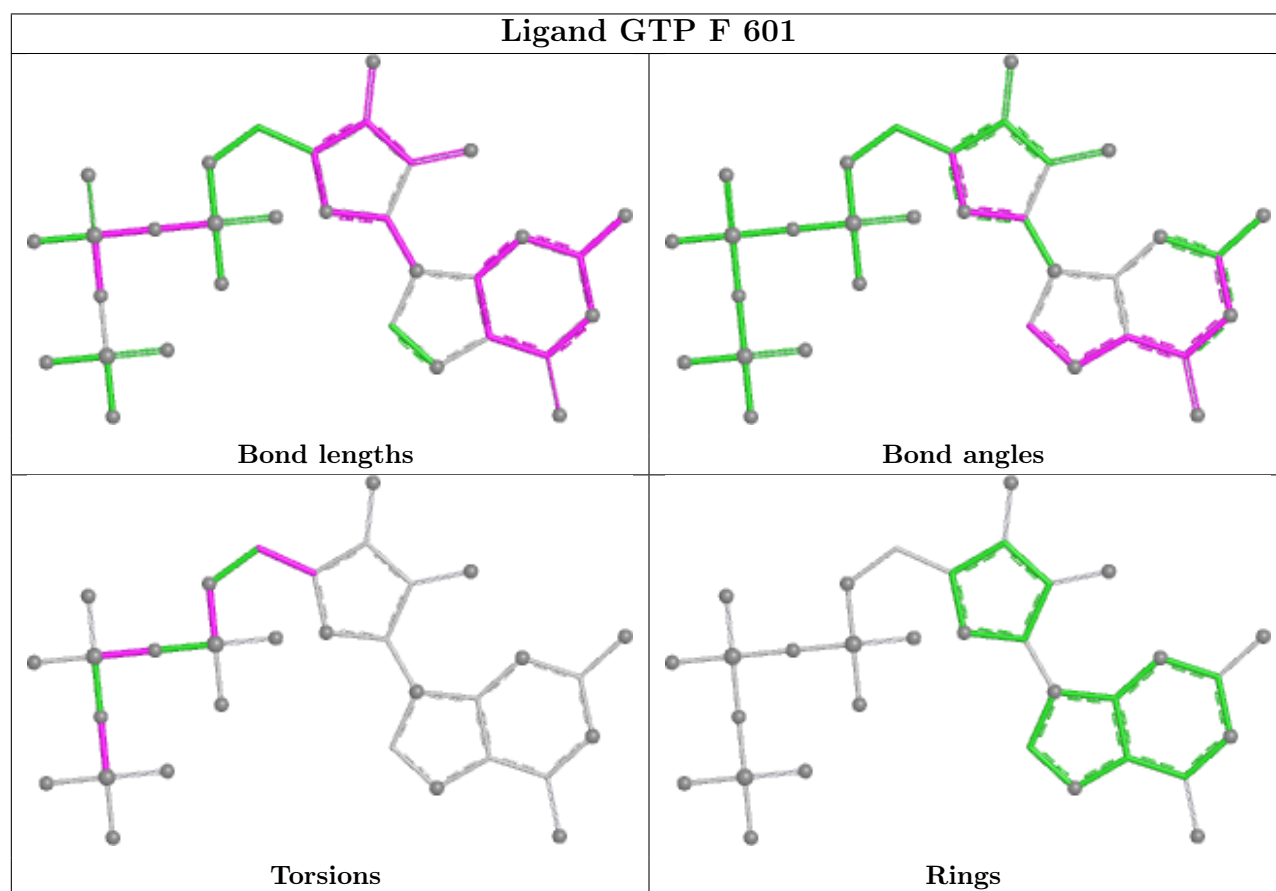
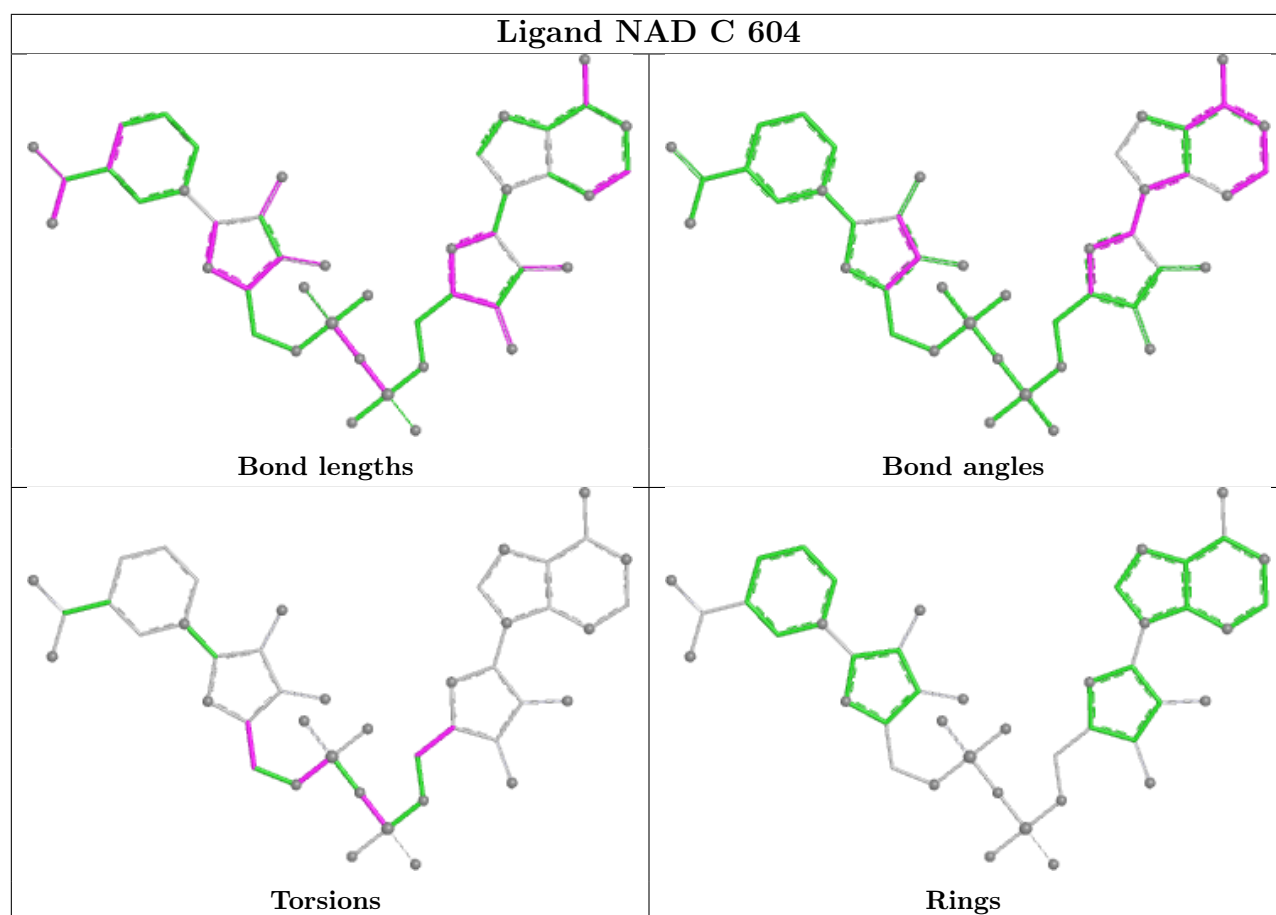
There are no ring outliers.

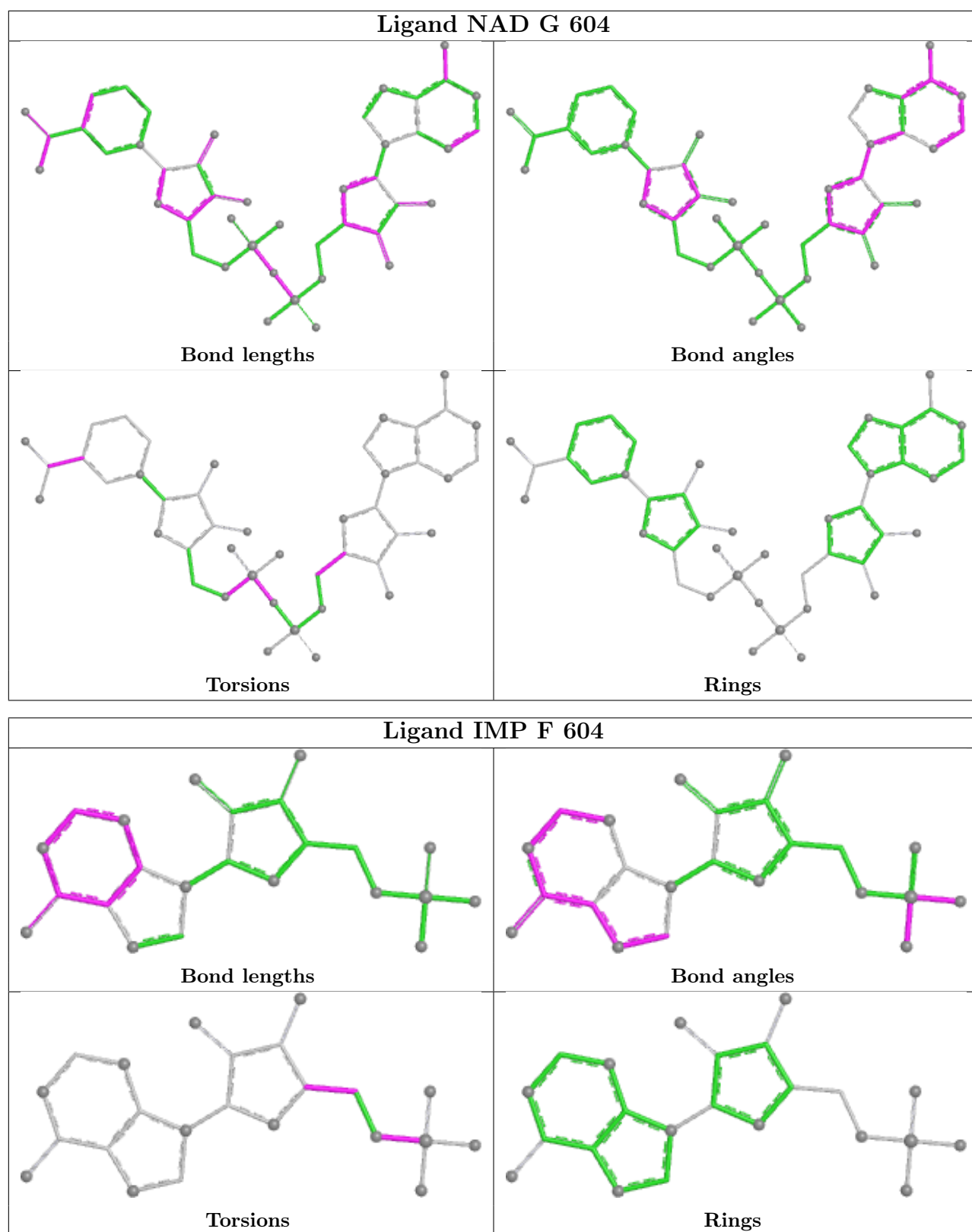
27 monomers are involved in 47 short contacts:

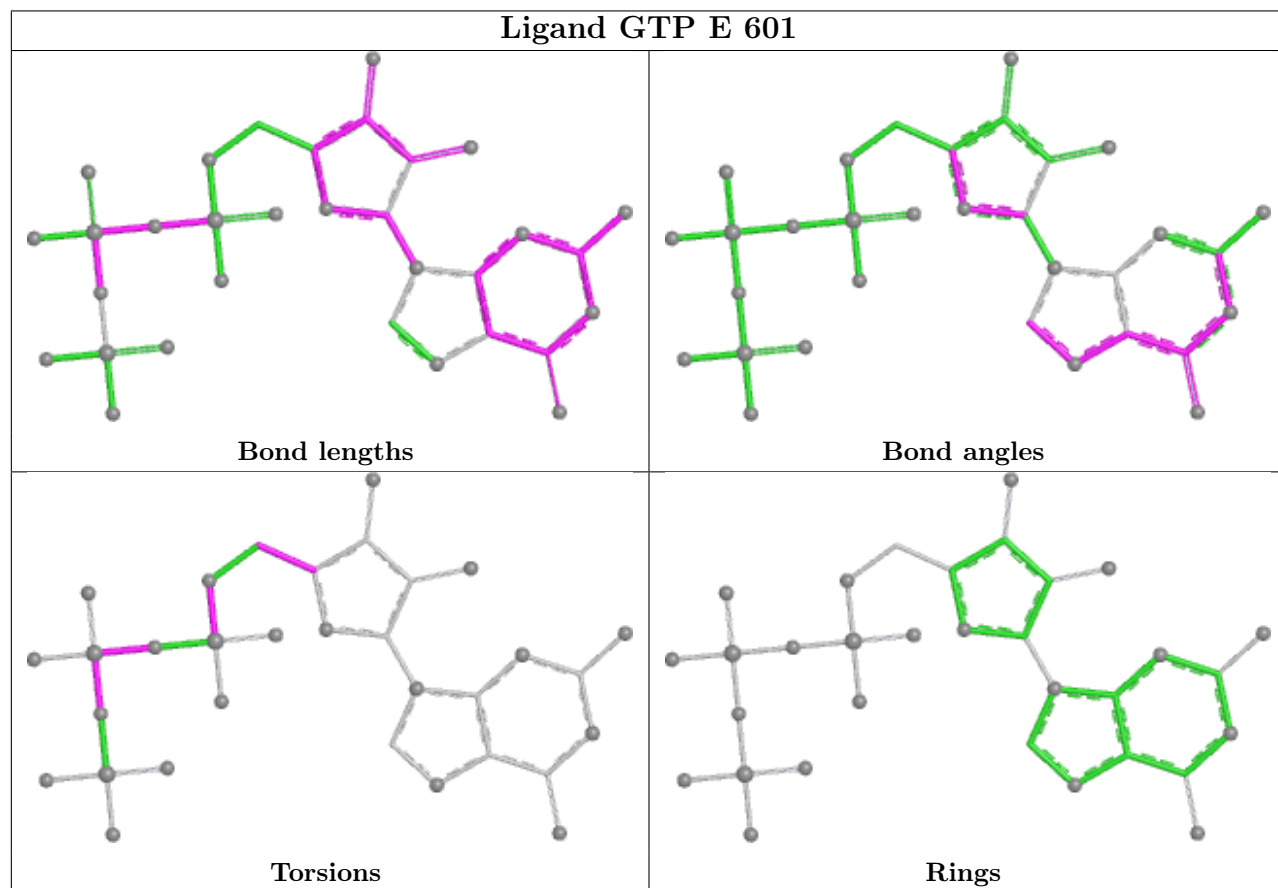
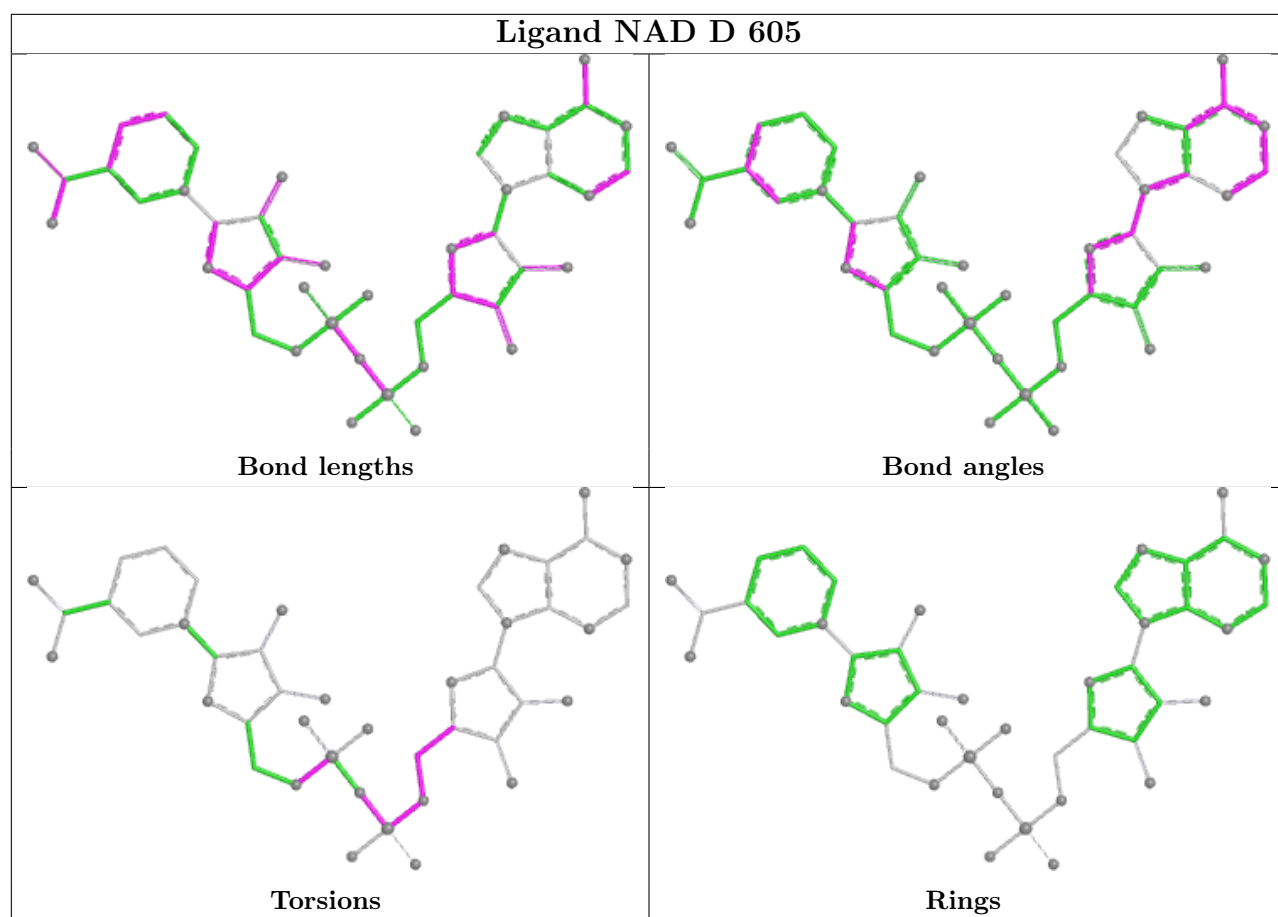
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	ATP	1	0
5	C	604	NAD	1	0
5	G	604	NAD	2	0
4	F	604	IMP	2	0
5	D	605	NAD	1	0
2	E	601	GTP	1	0
4	C	603	IMP	1	0
2	H	602	GTP	1	0
4	D	604	IMP	2	0
5	B	605	NAD	3	0
3	B	603	ATP	2	0
2	A	602	GTP	2	0
3	A	603	ATP	1	0
5	E	605	NAD	2	0
3	E	603	ATP	4	0
4	G	603	IMP	2	0
2	E	602	GTP	2	0
5	H	605	NAD	2	0
2	B	601	GTP	1	0
4	B	604	IMP	2	0
2	B	602	GTP	1	0
2	D	602	GTP	2	0
4	A	604	IMP	1	0
4	E	604	IMP	1	0
5	F	605	NAD	2	0
3	F	603	ATP	3	0
4	H	604	IMP	2	0

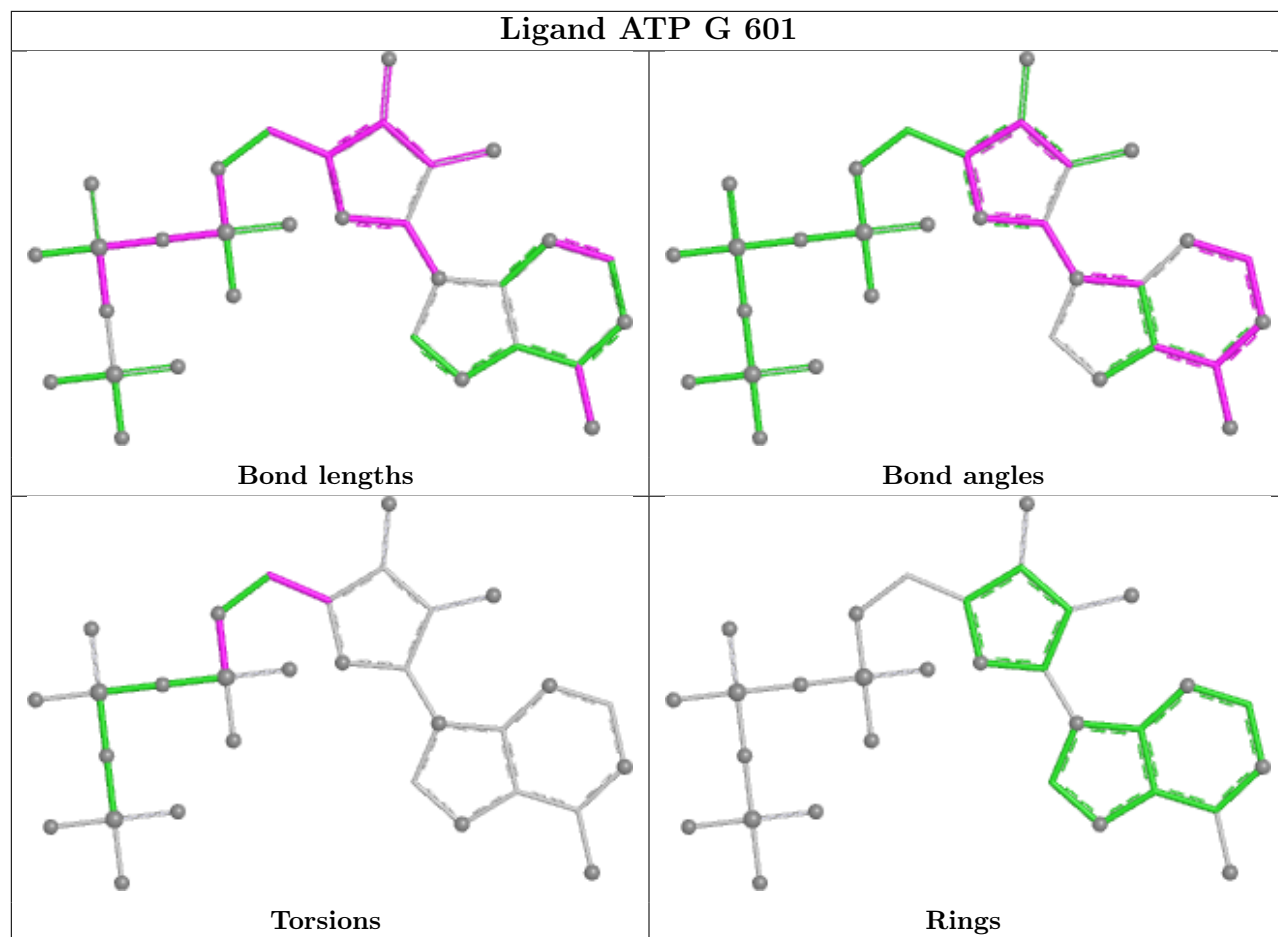
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



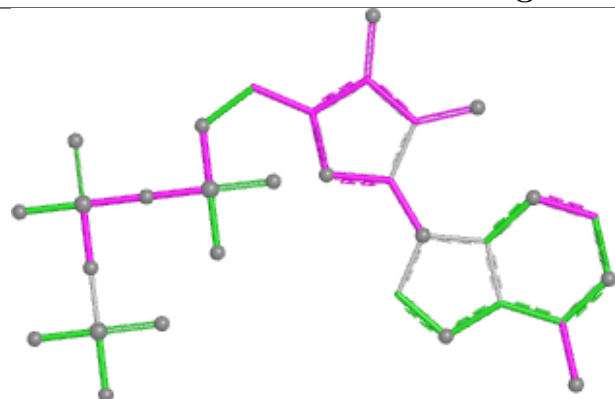




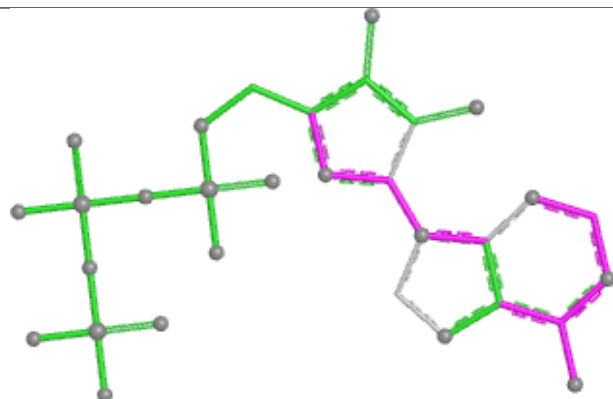




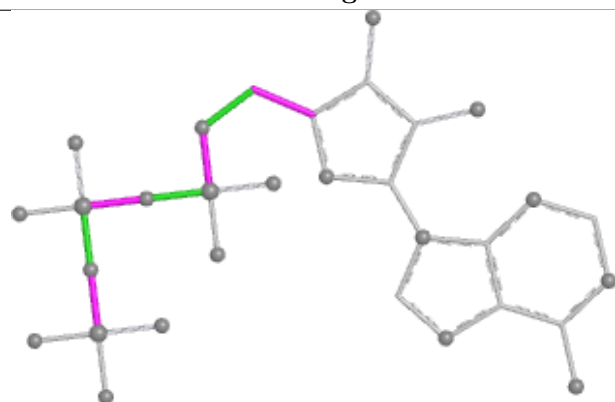
Ligand ATP D 603



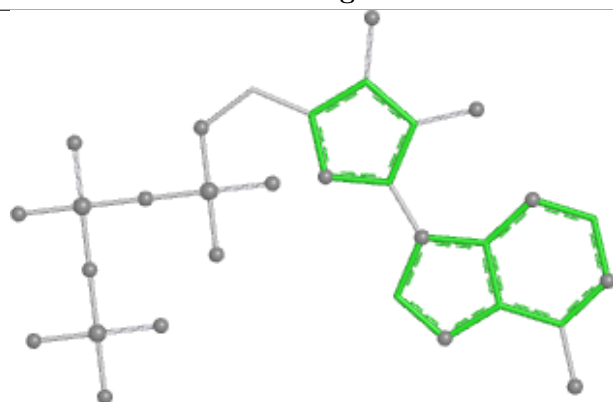
Bond lengths



Bond angles

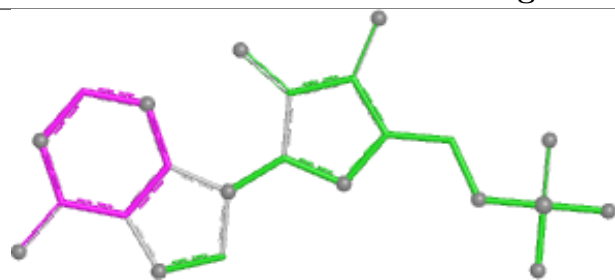


Torsions

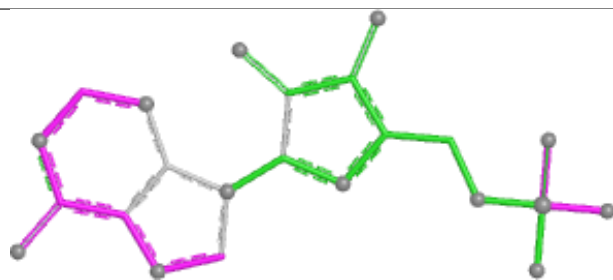


Rings

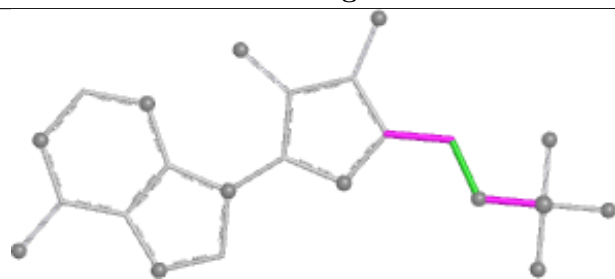
Ligand IMP C 603



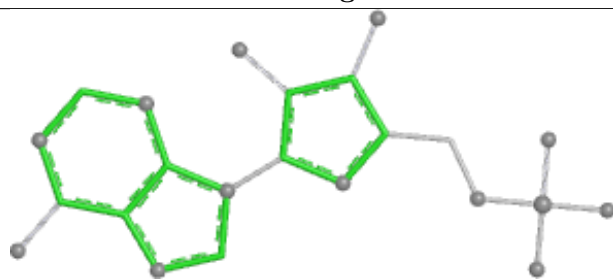
Bond lengths



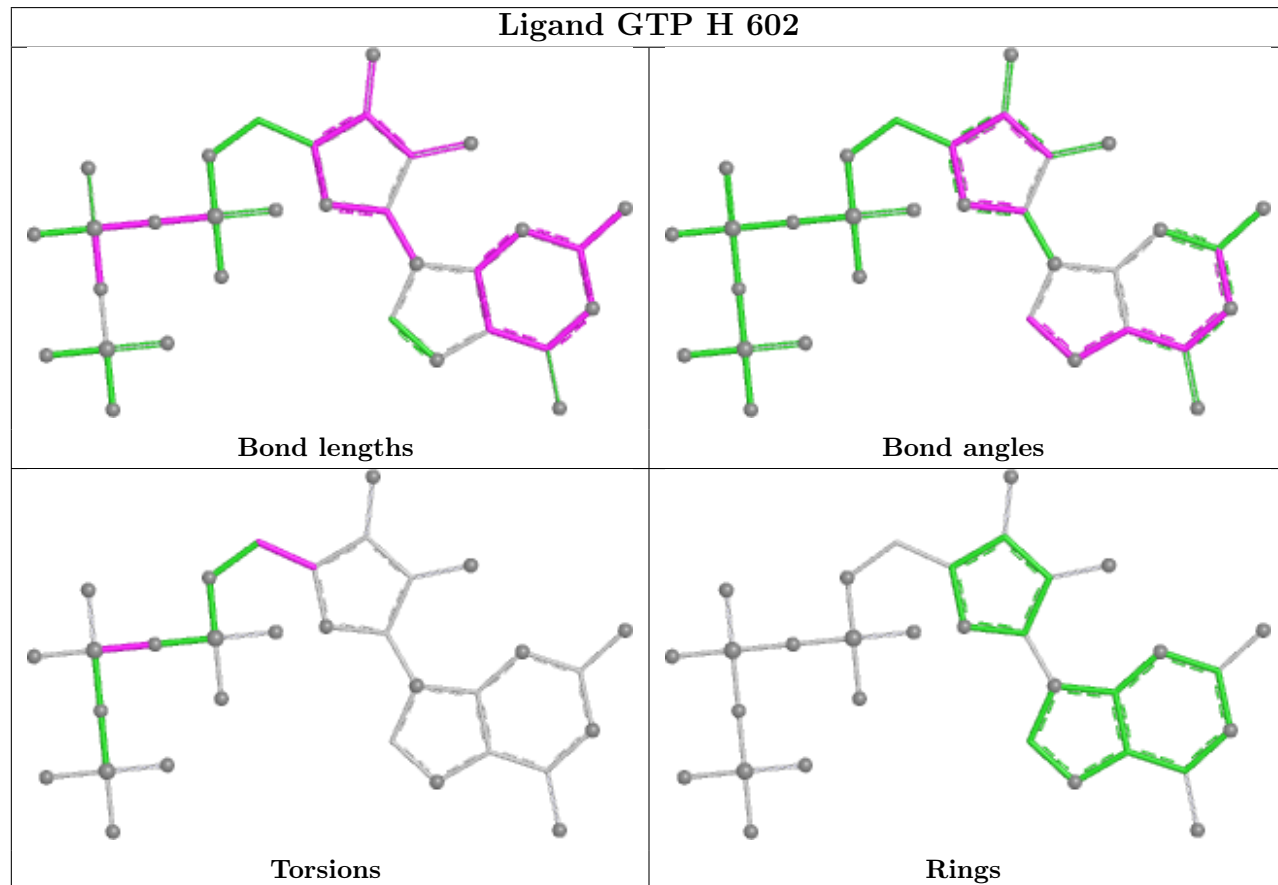
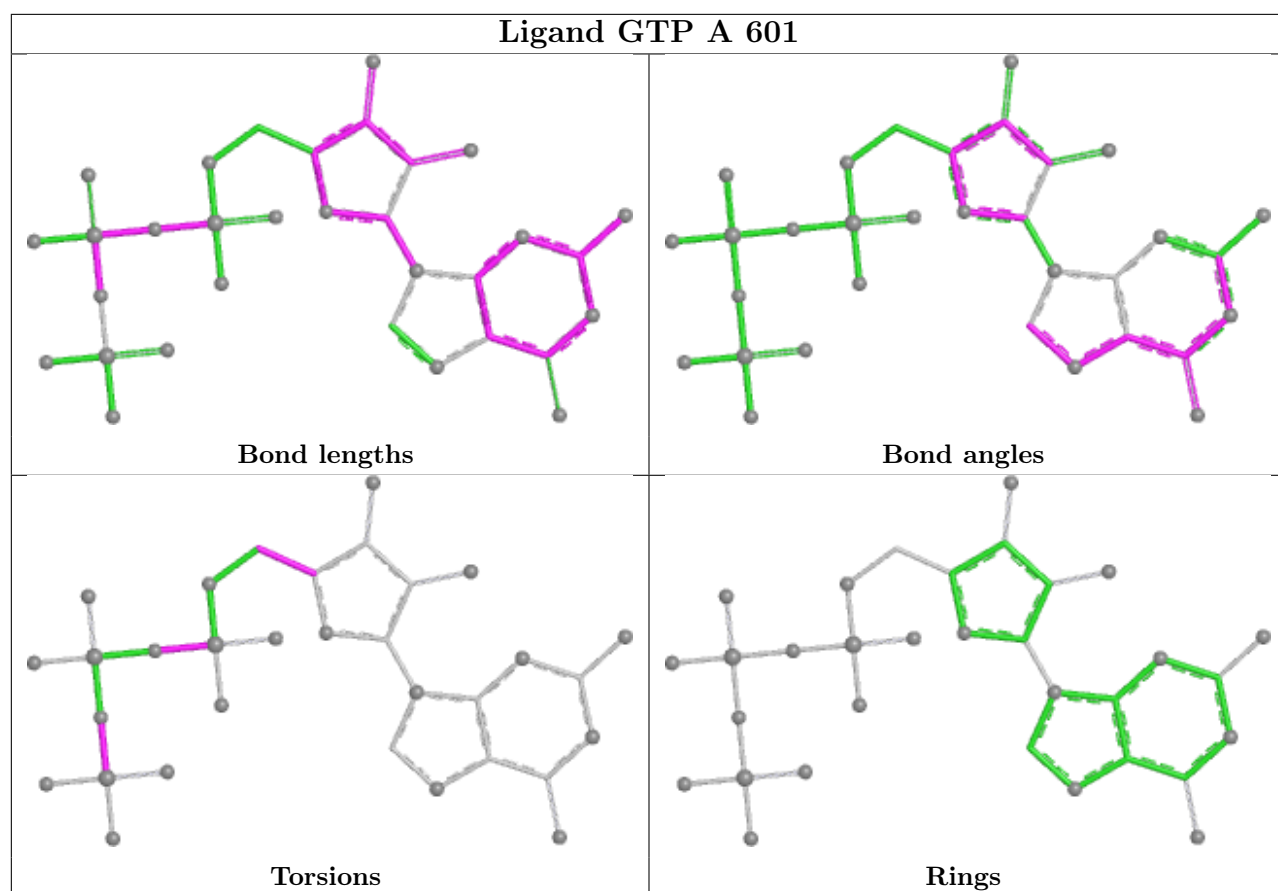
Bond angles

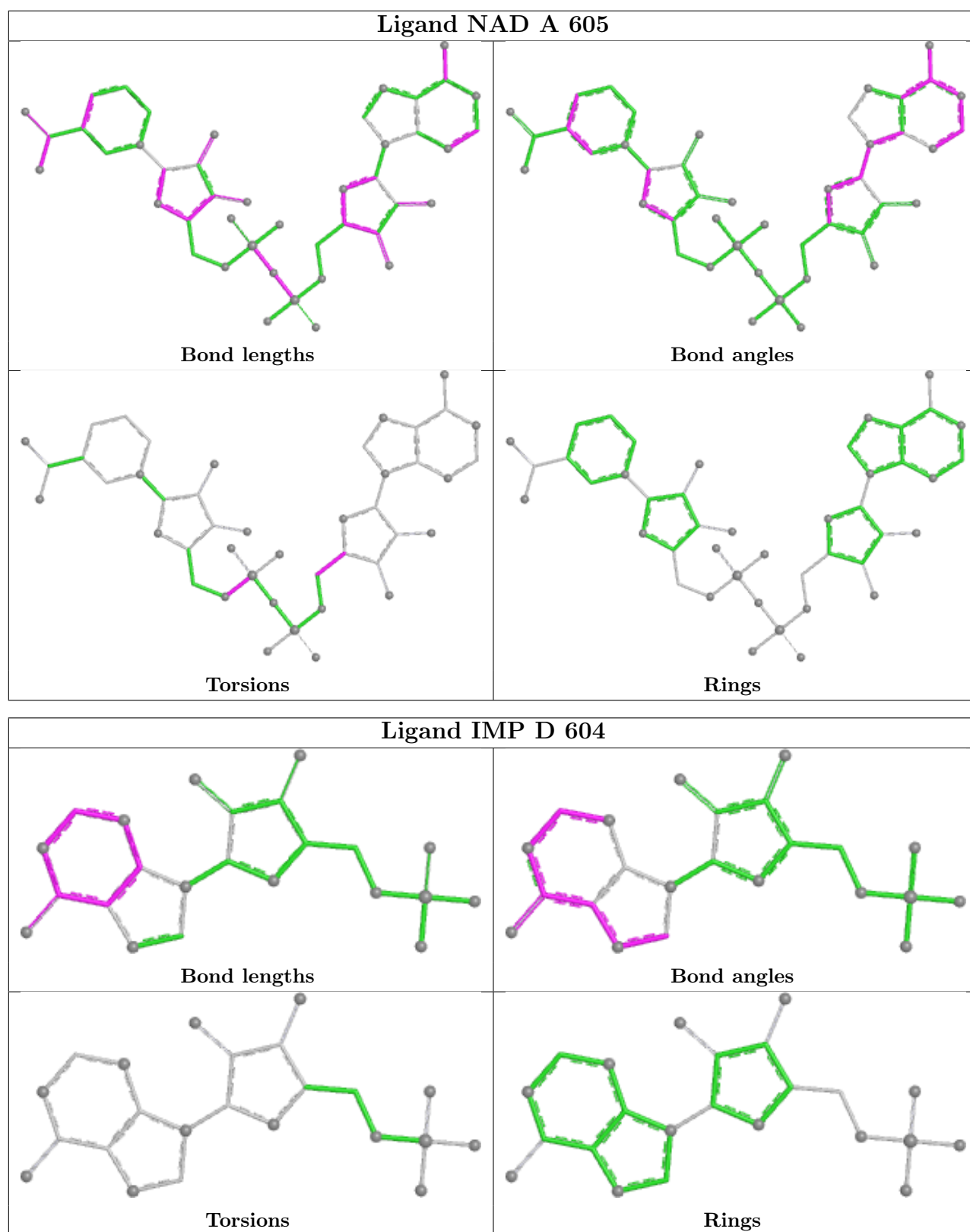


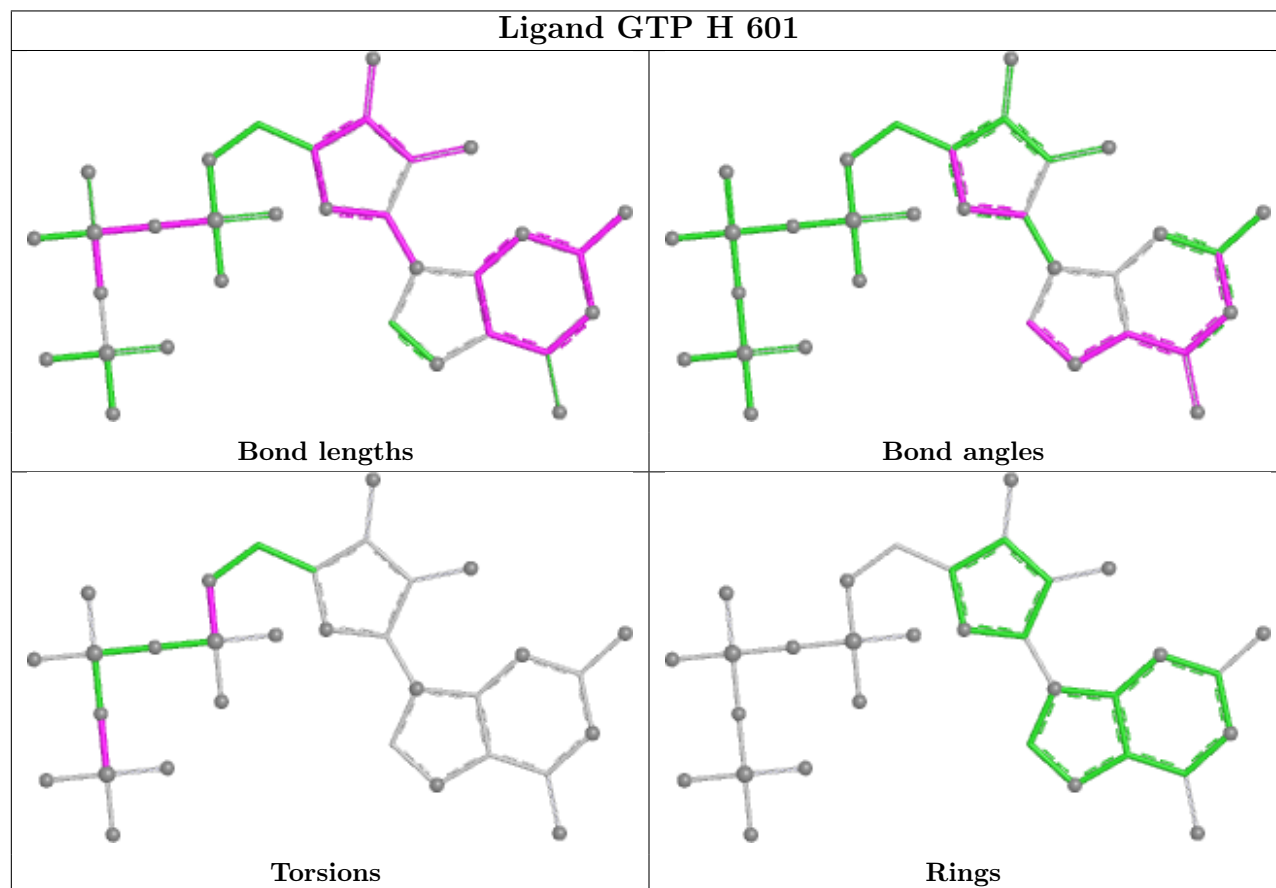
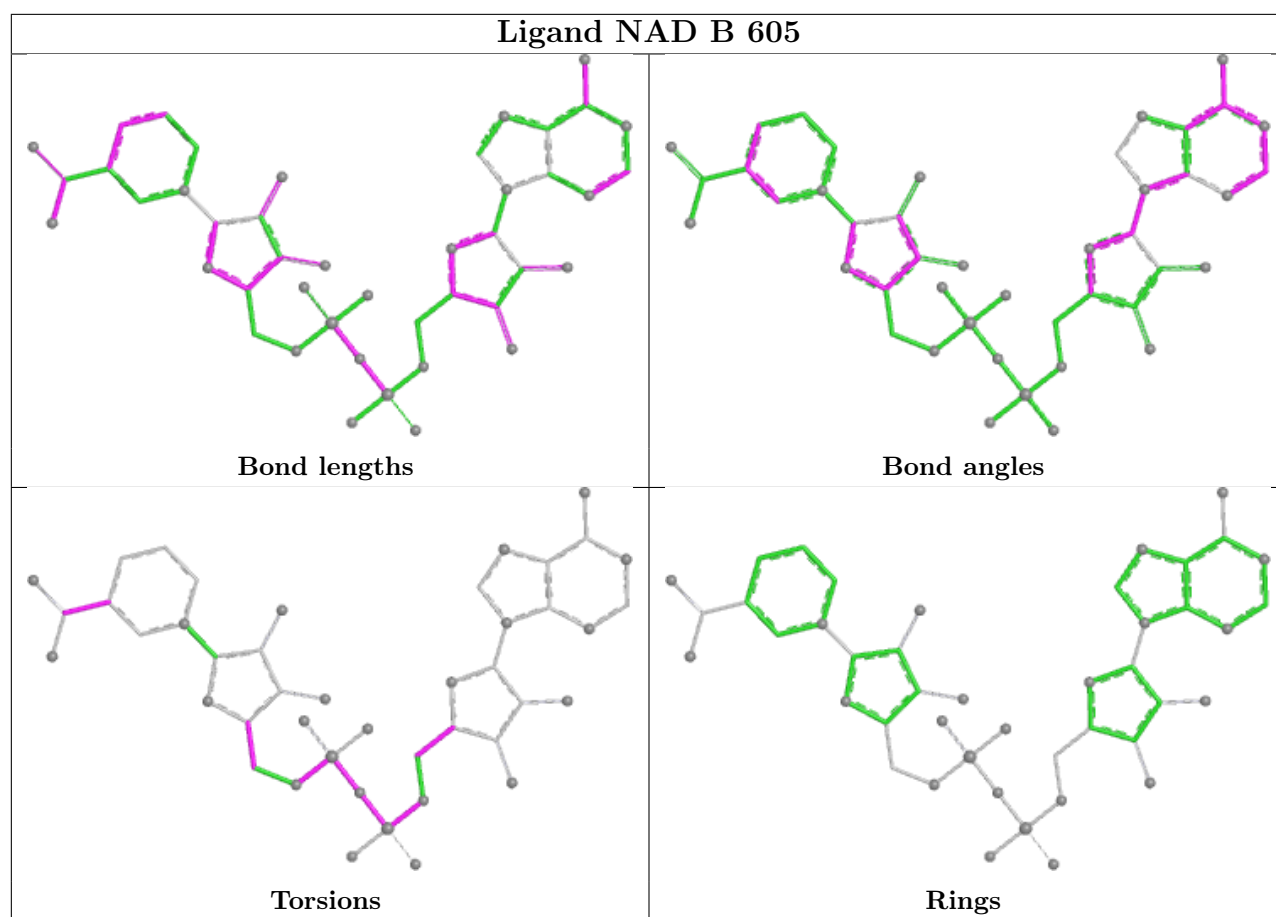
Torsions

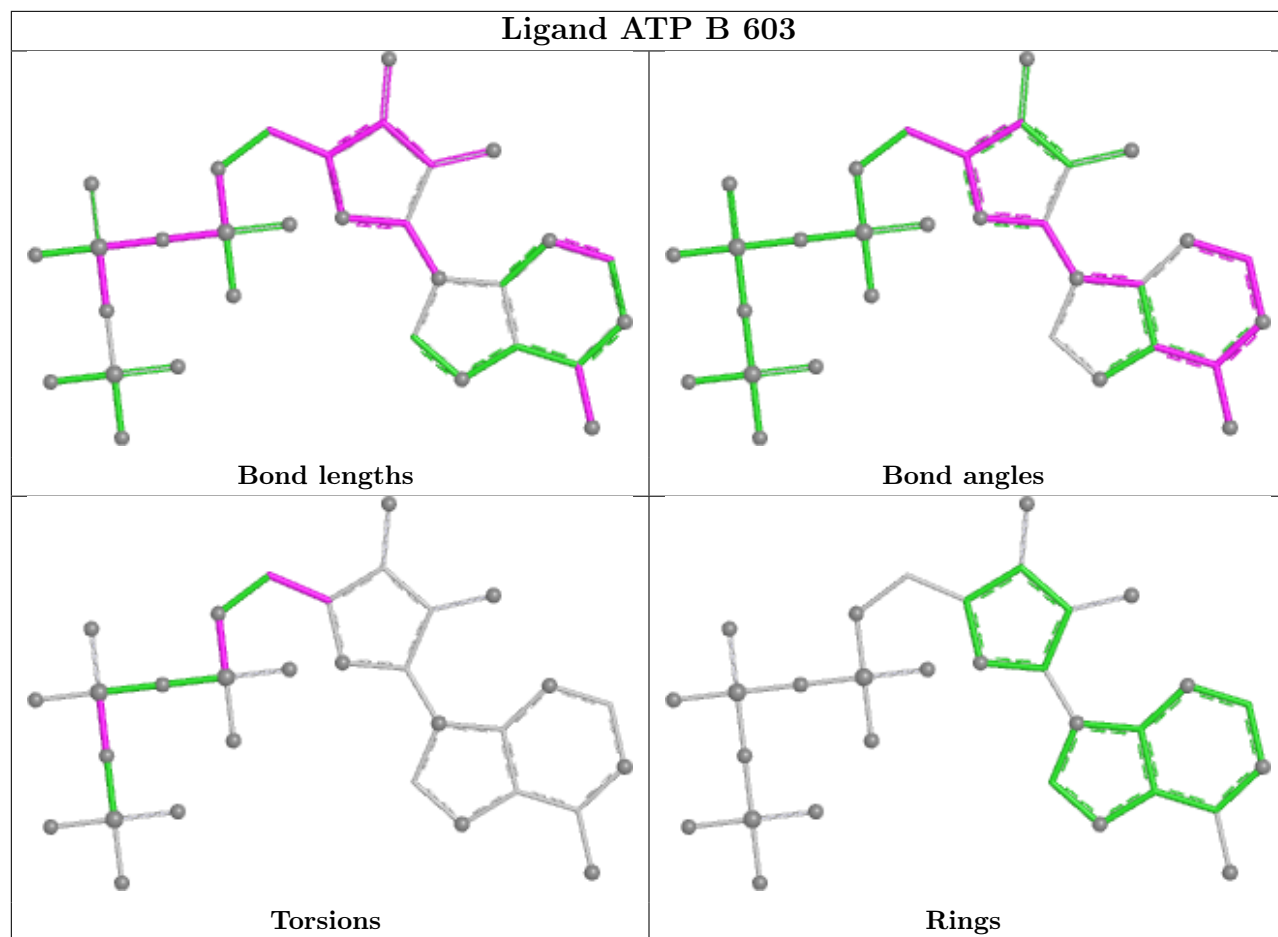


Rings

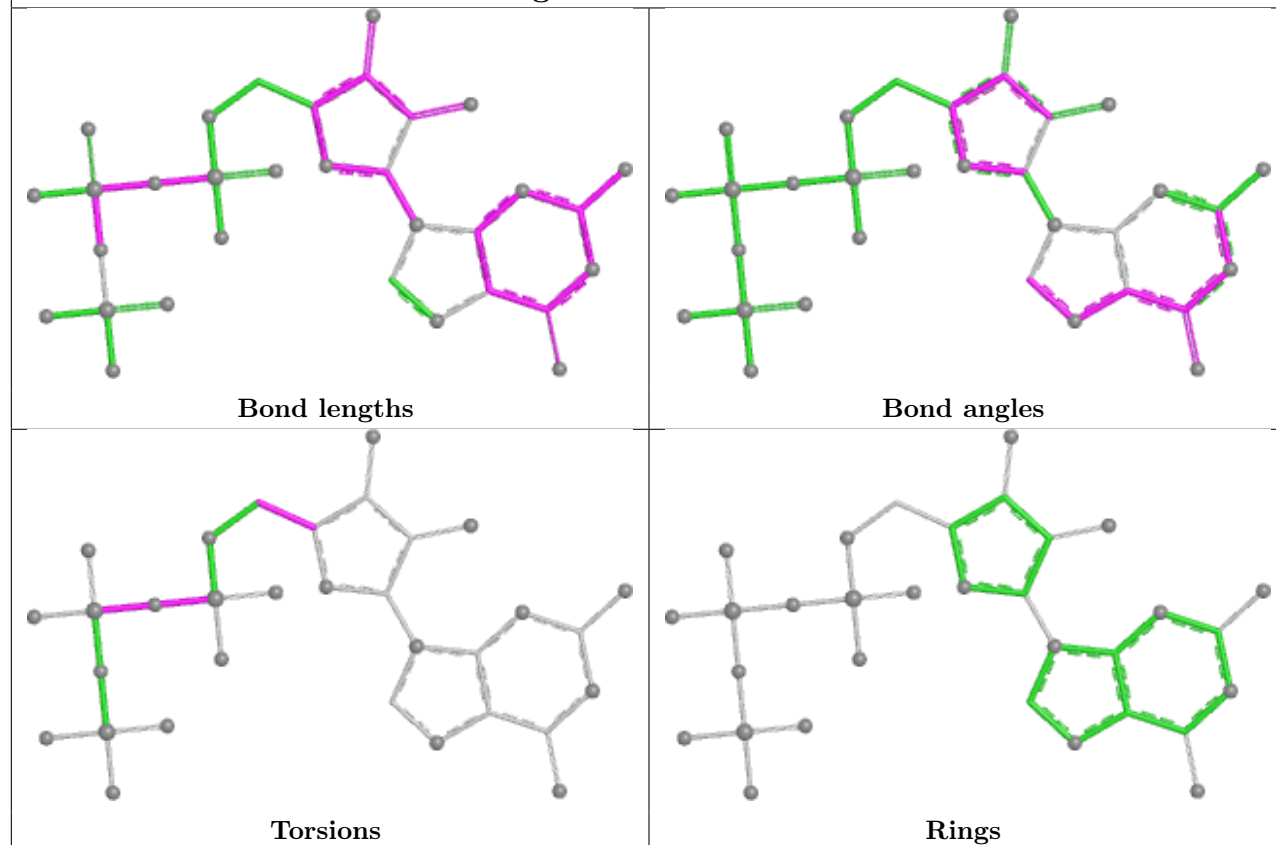




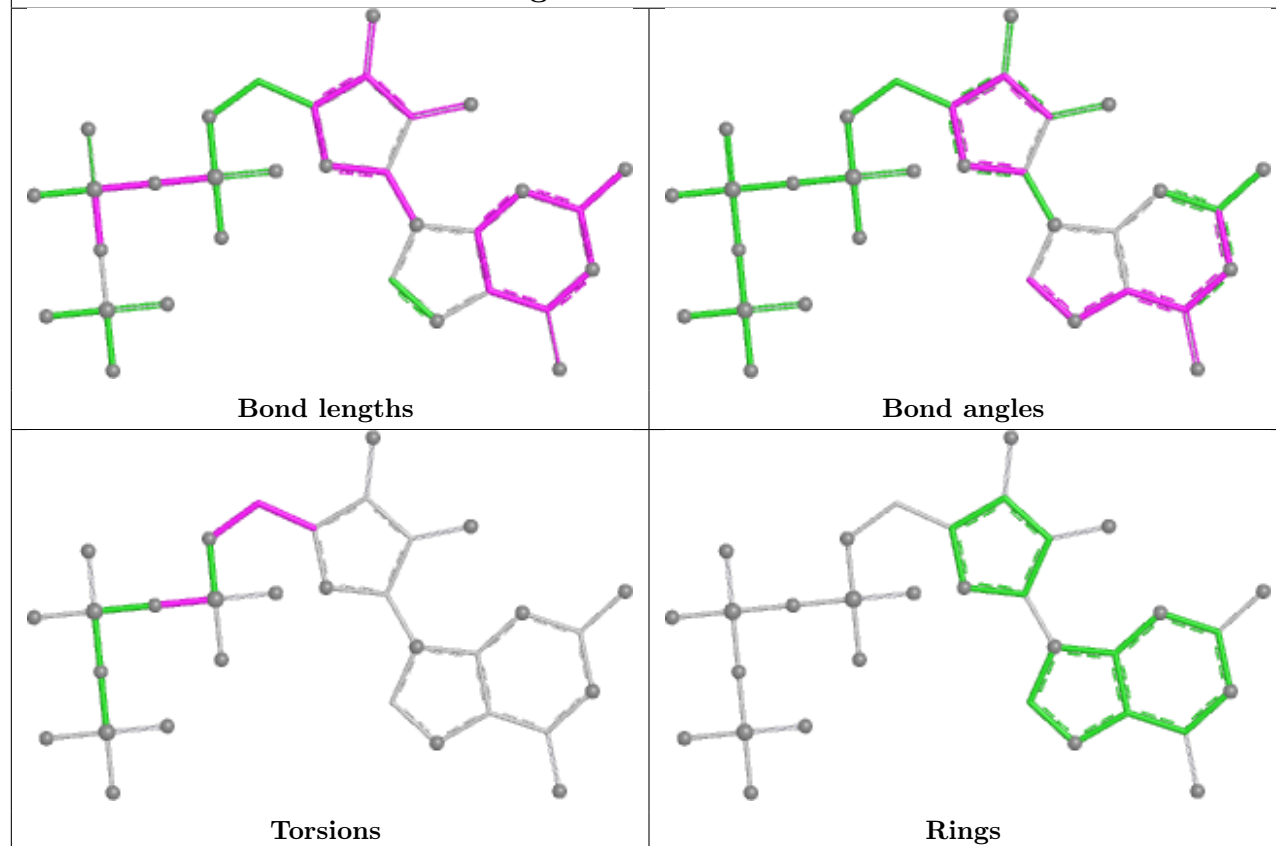


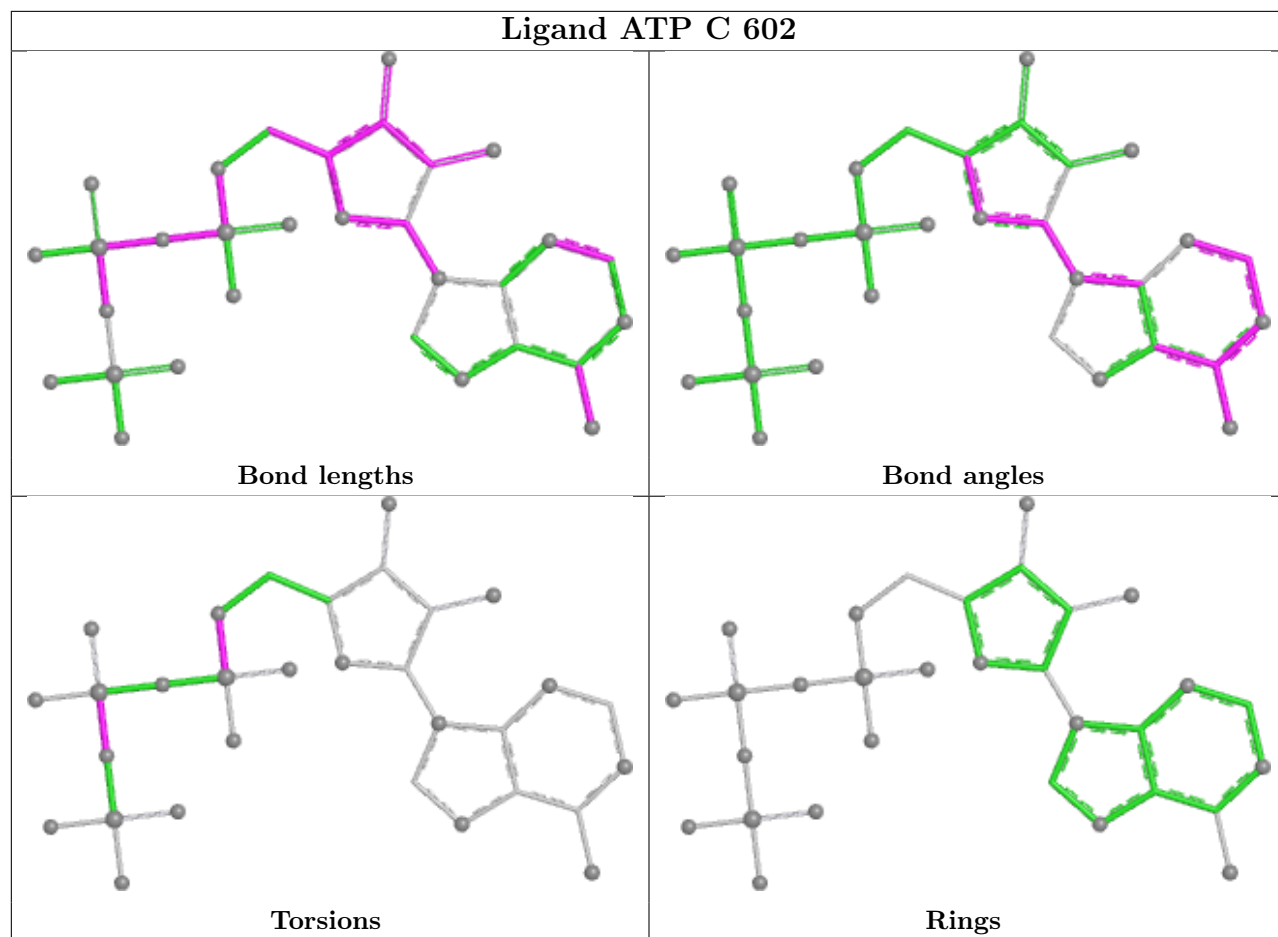


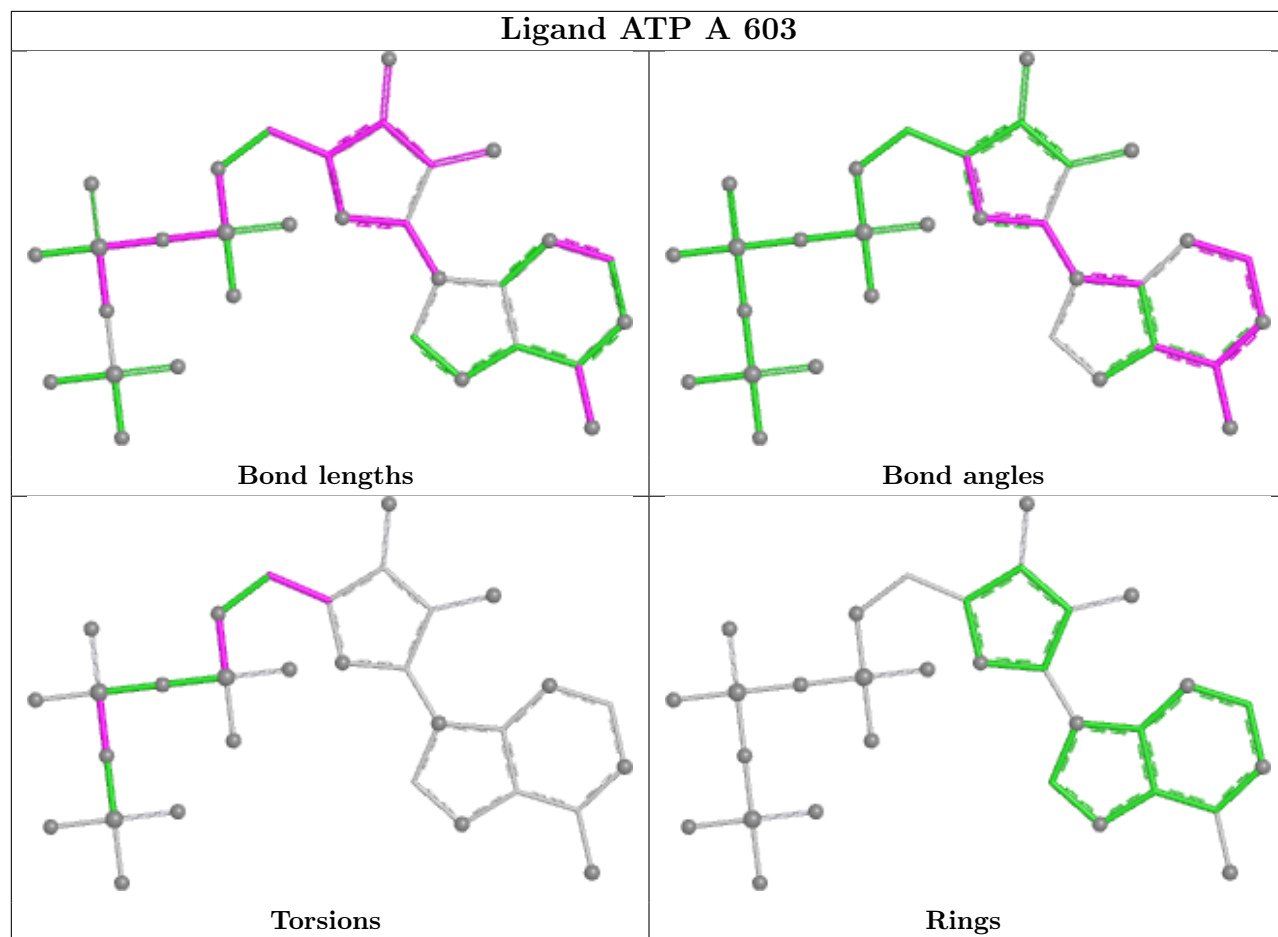
Ligand GTP F 602

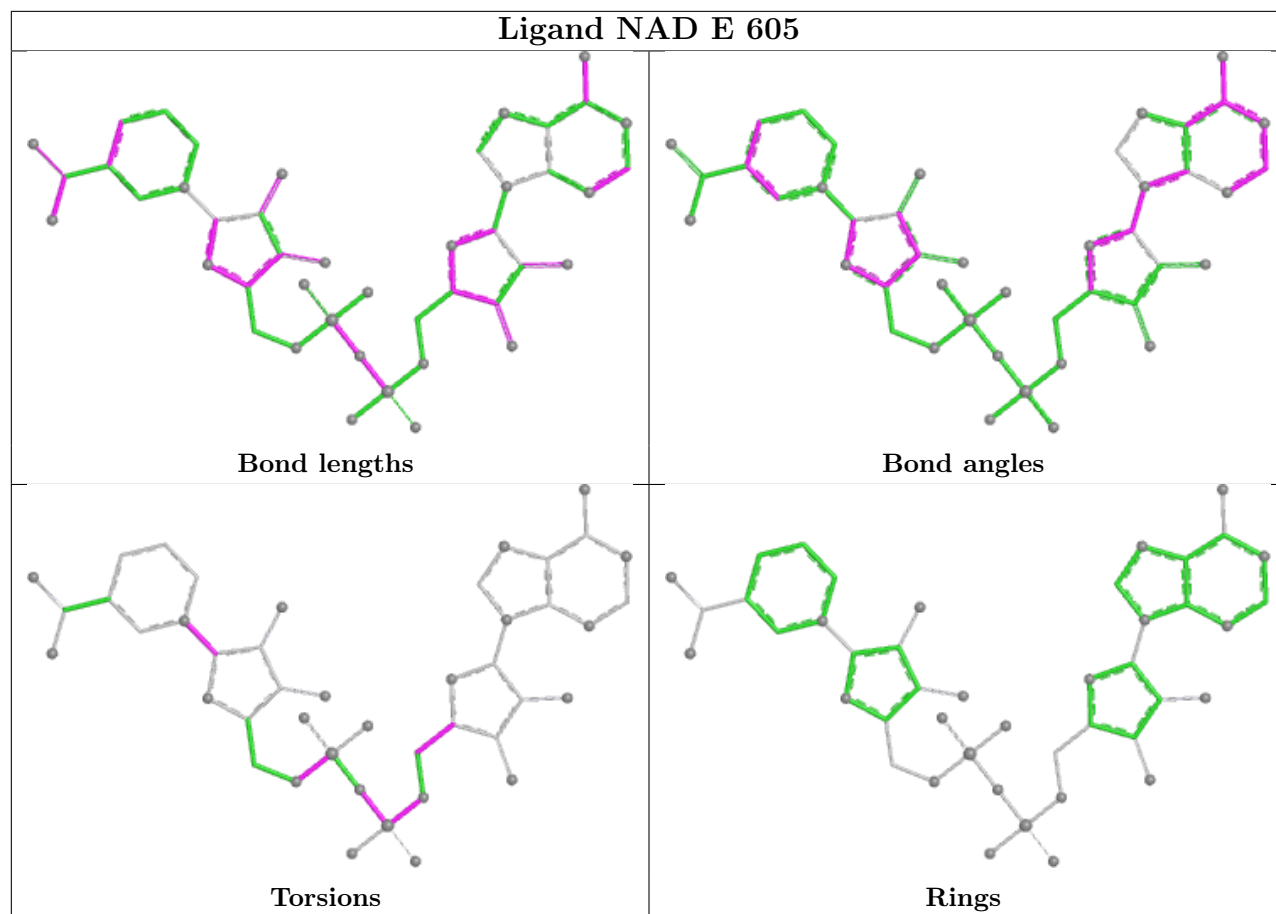


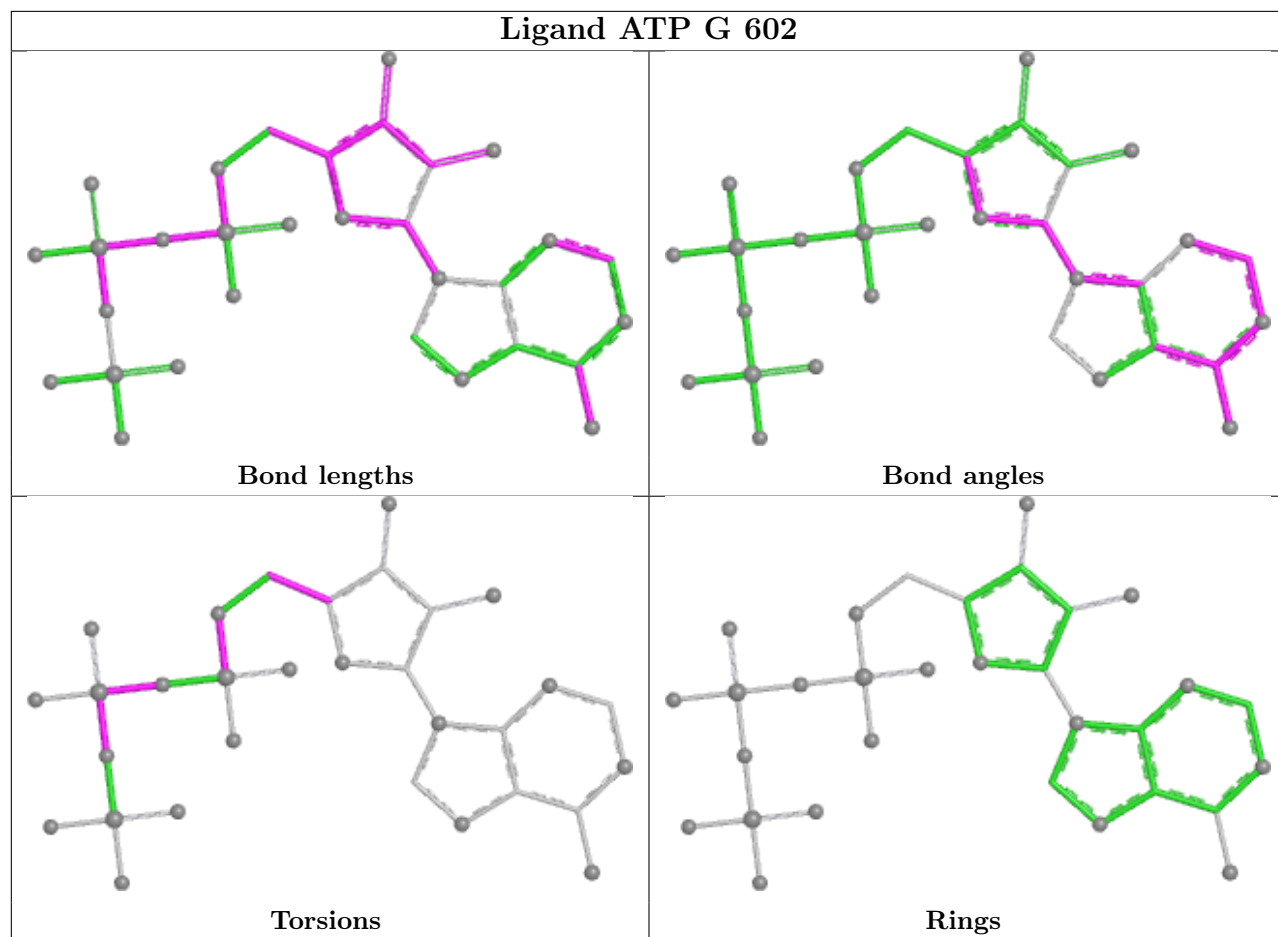
Ligand GTP A 602



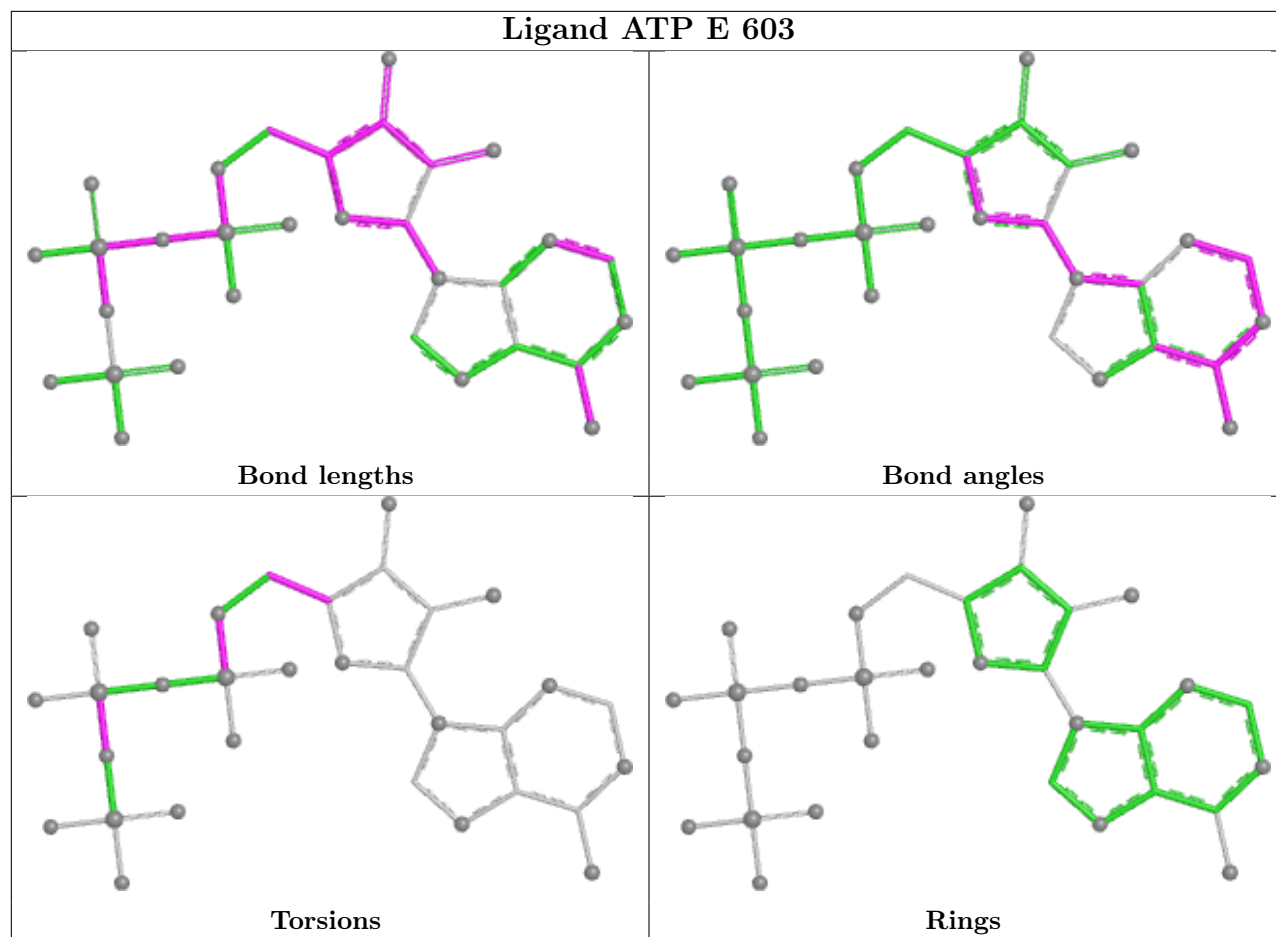




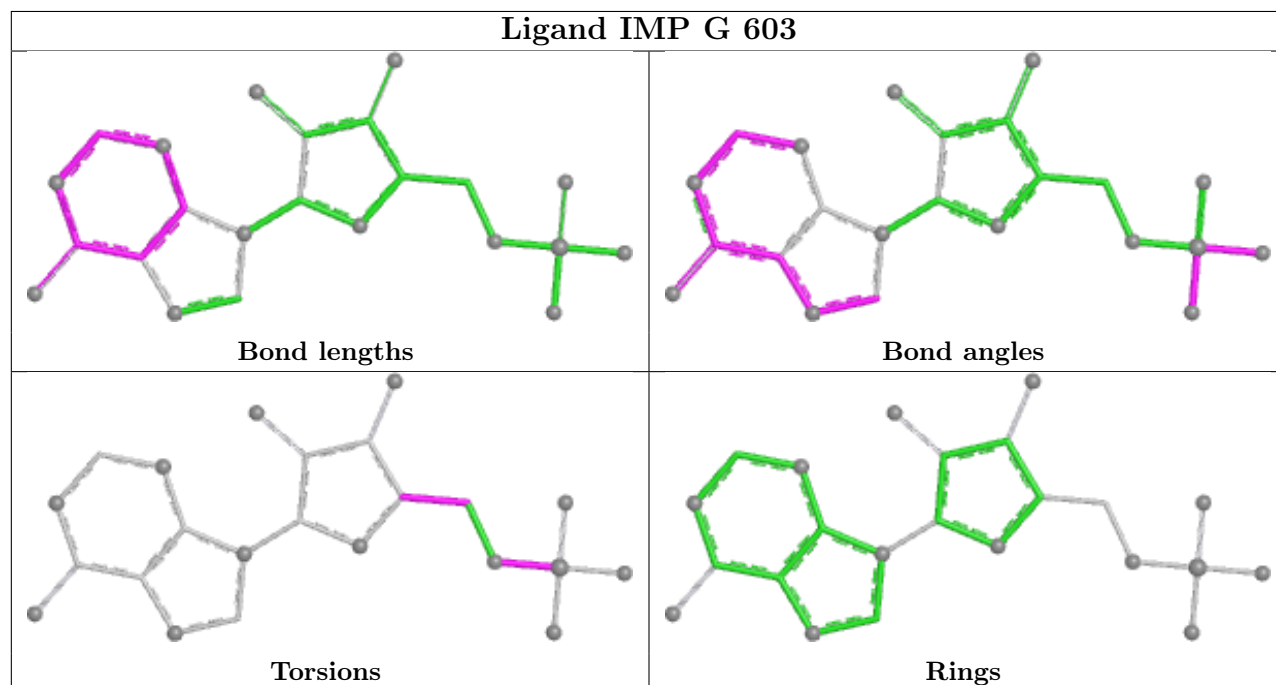


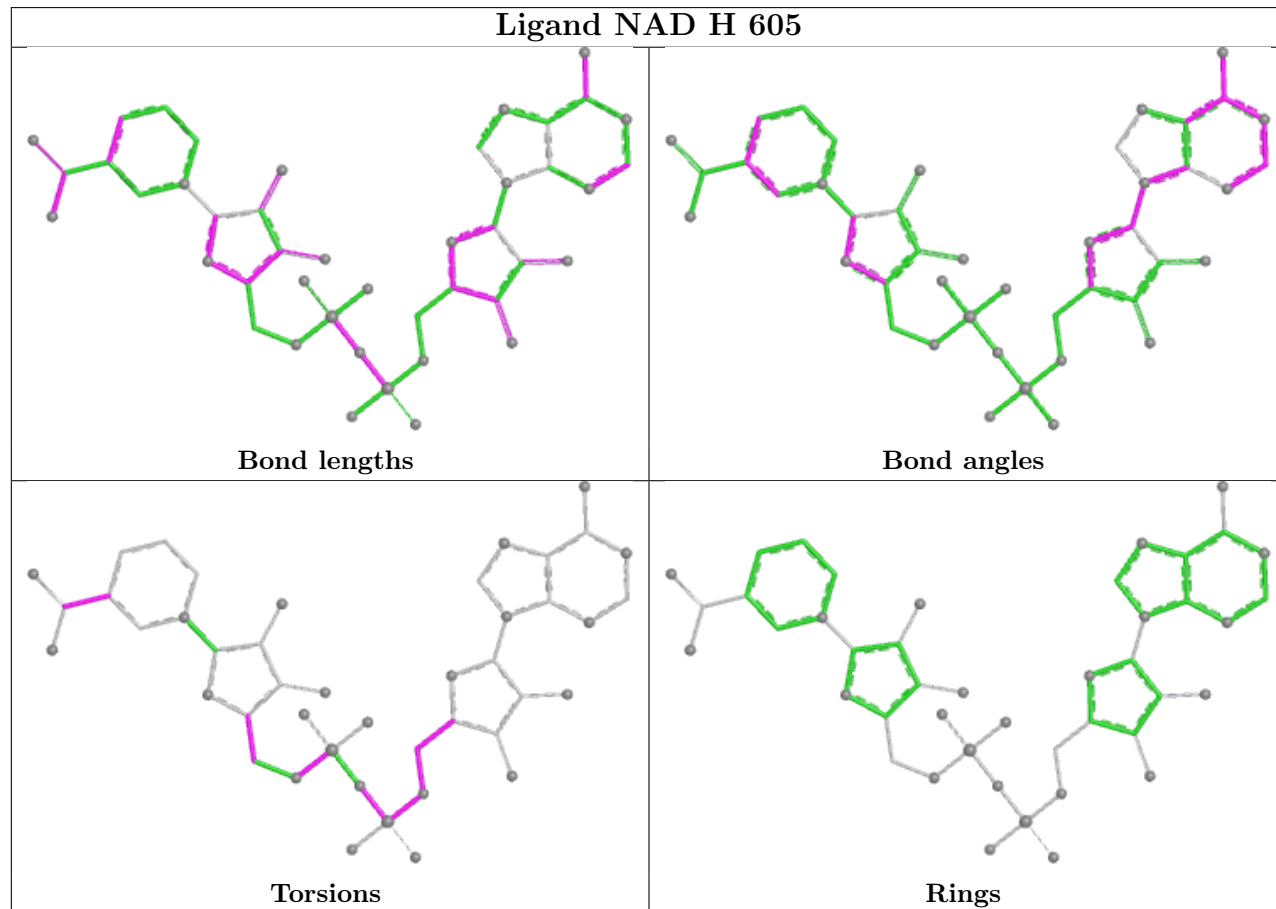
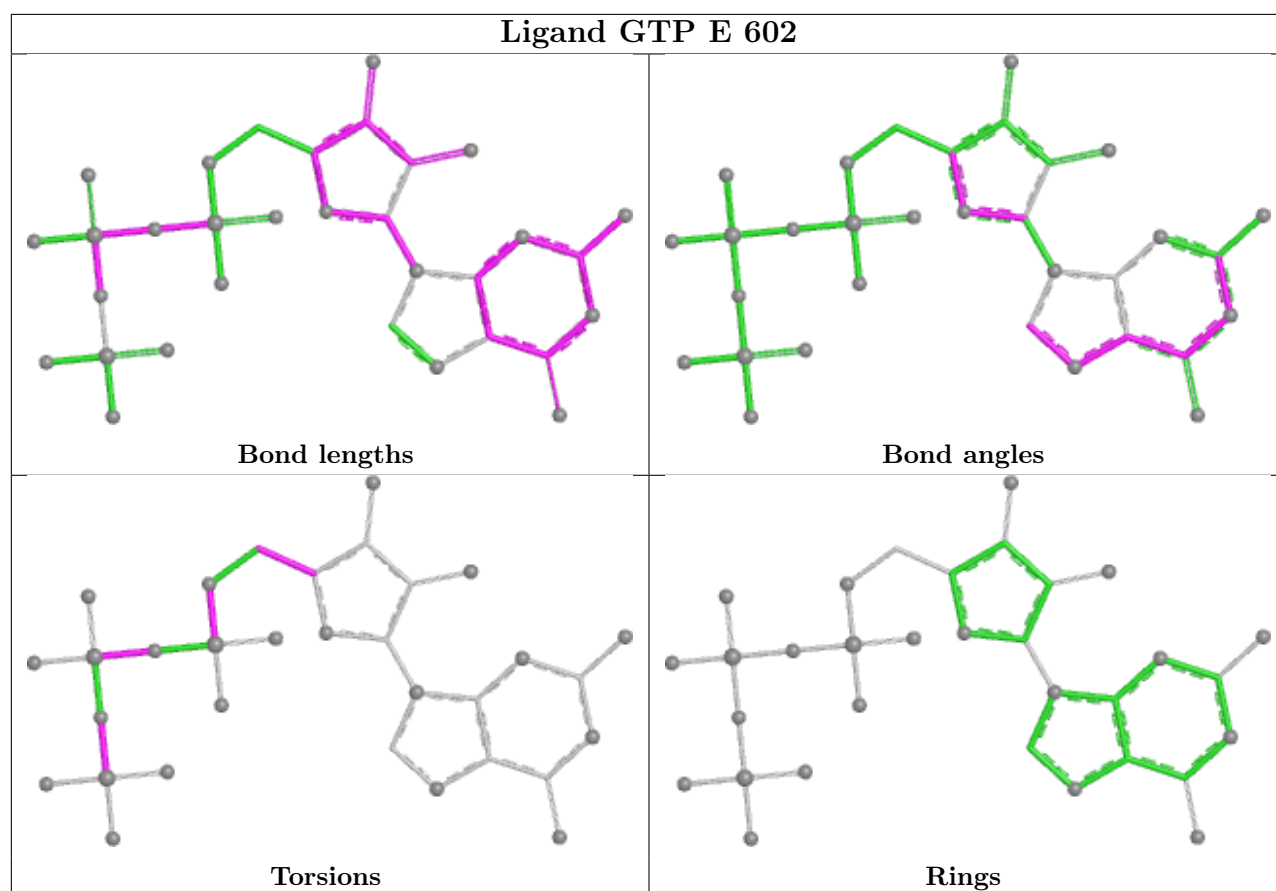


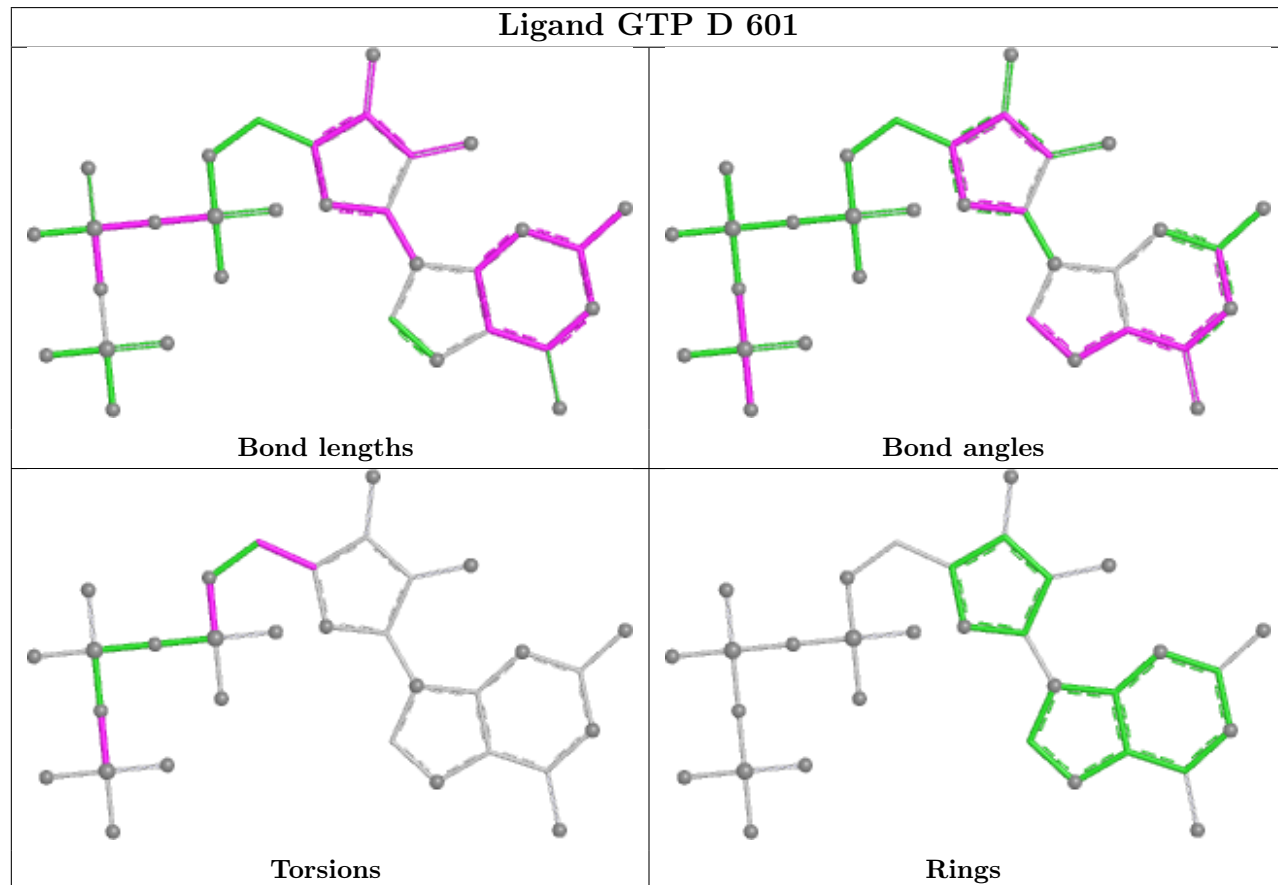
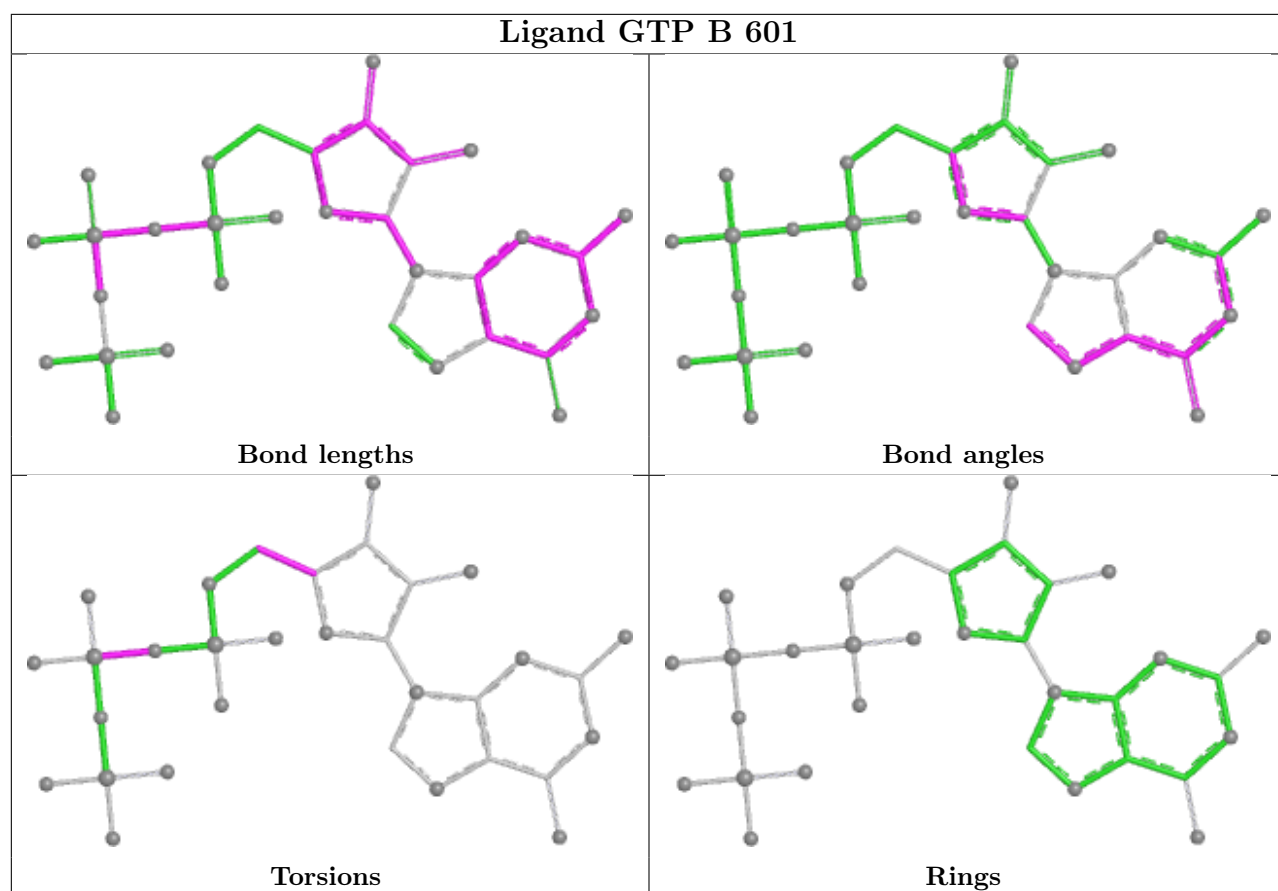
Ligand ATP E 603



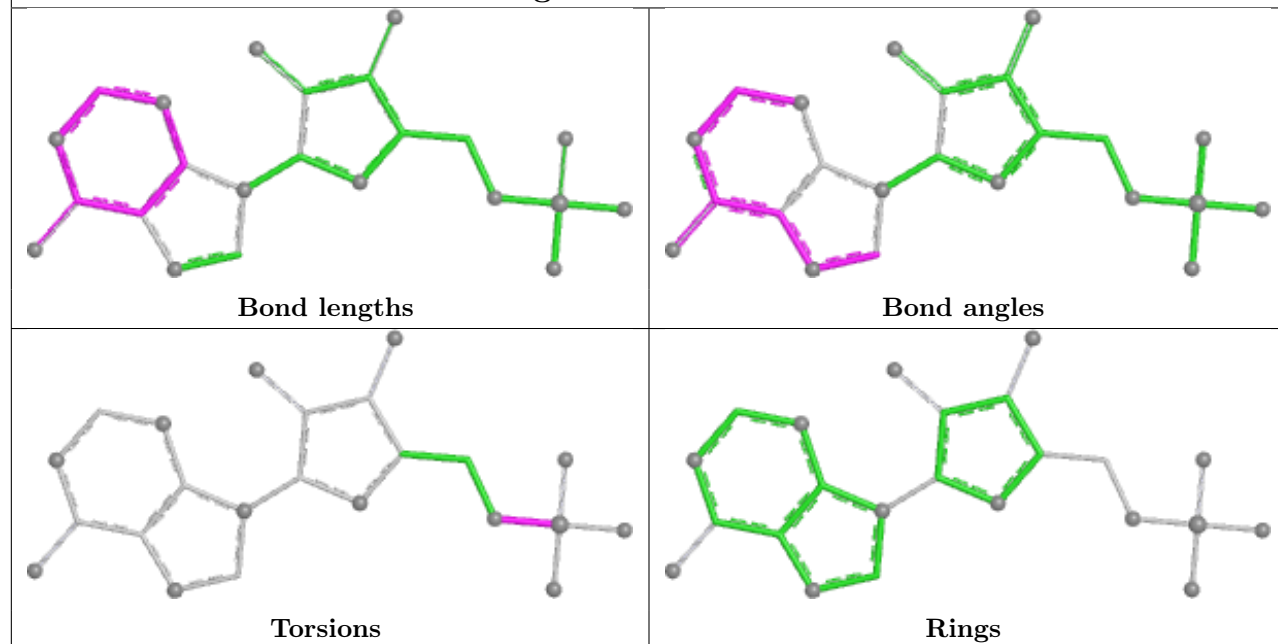
Ligand IMP G 603



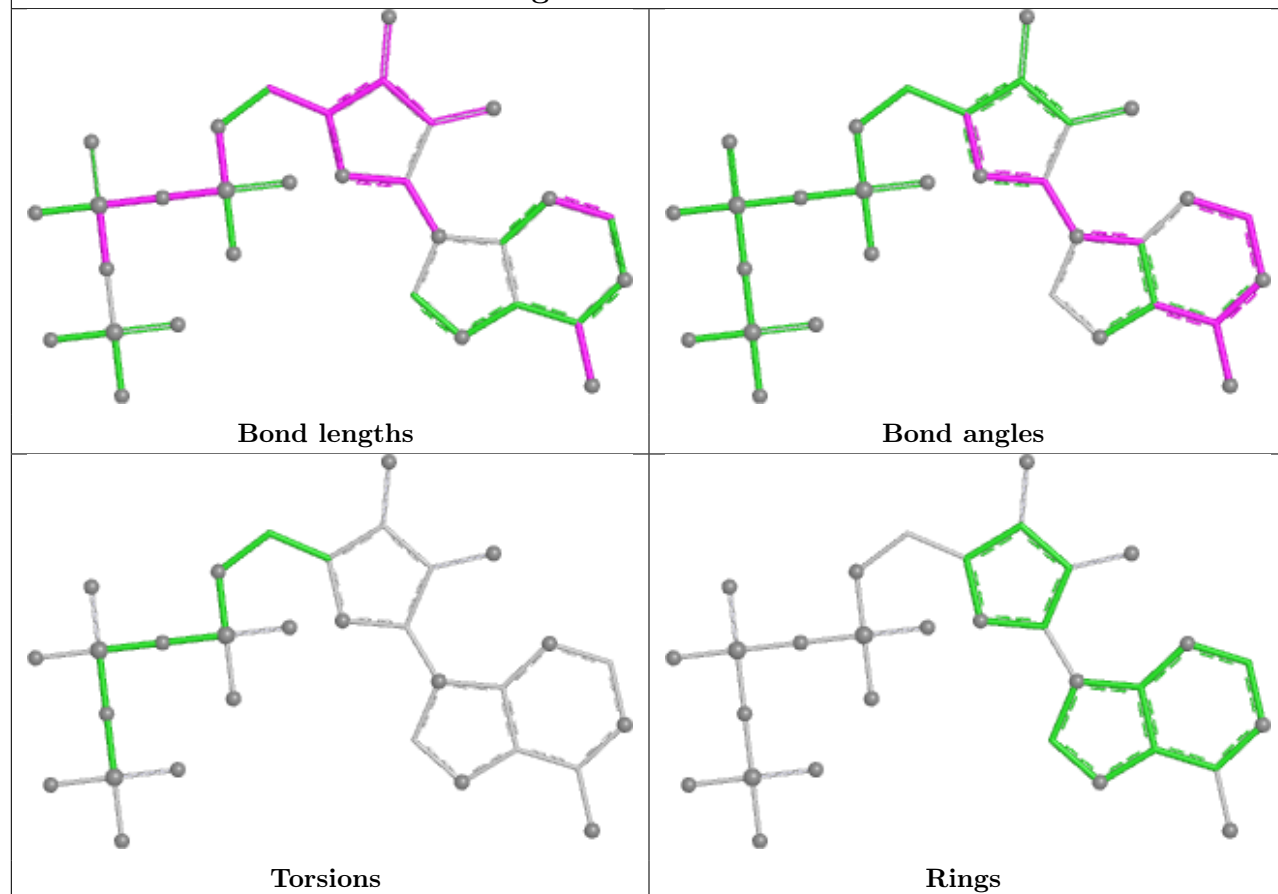


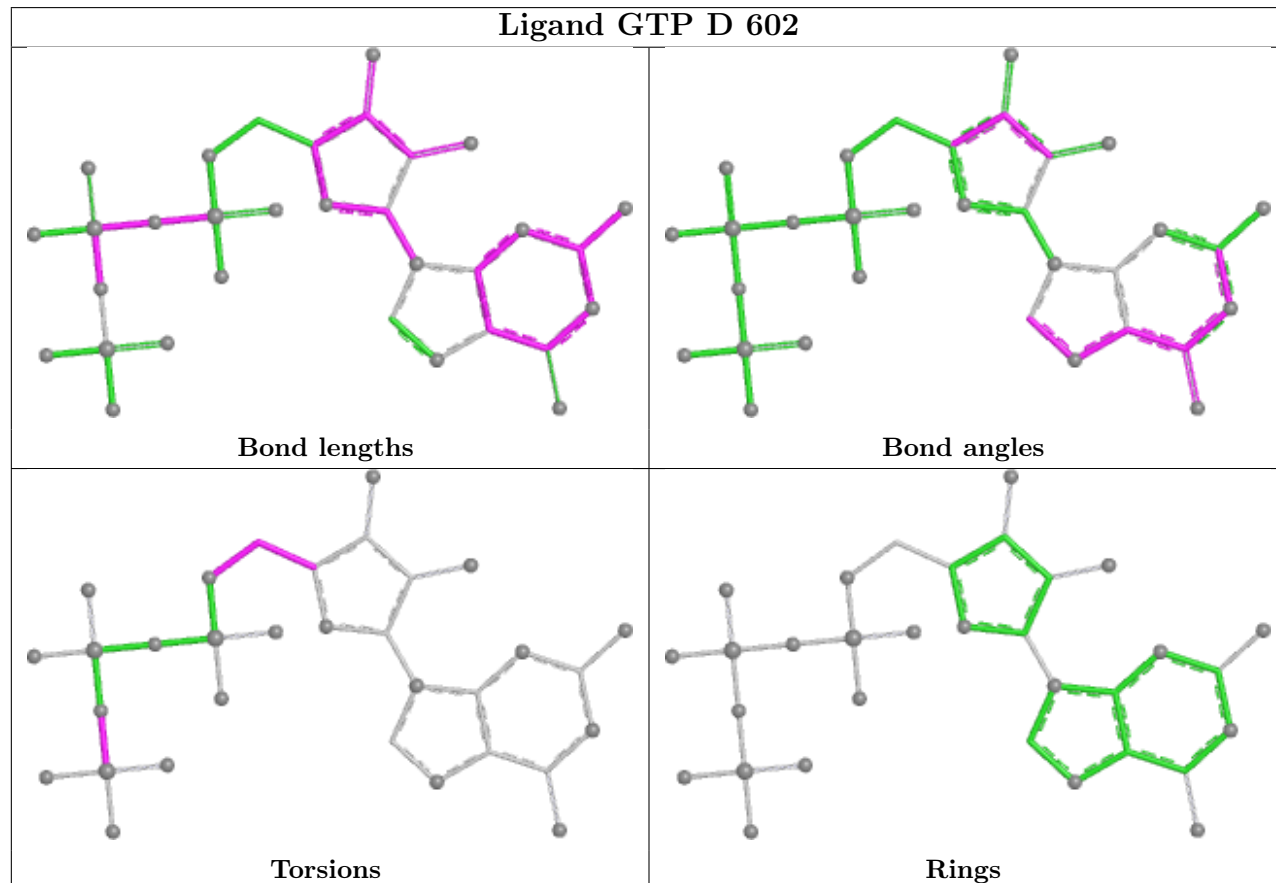
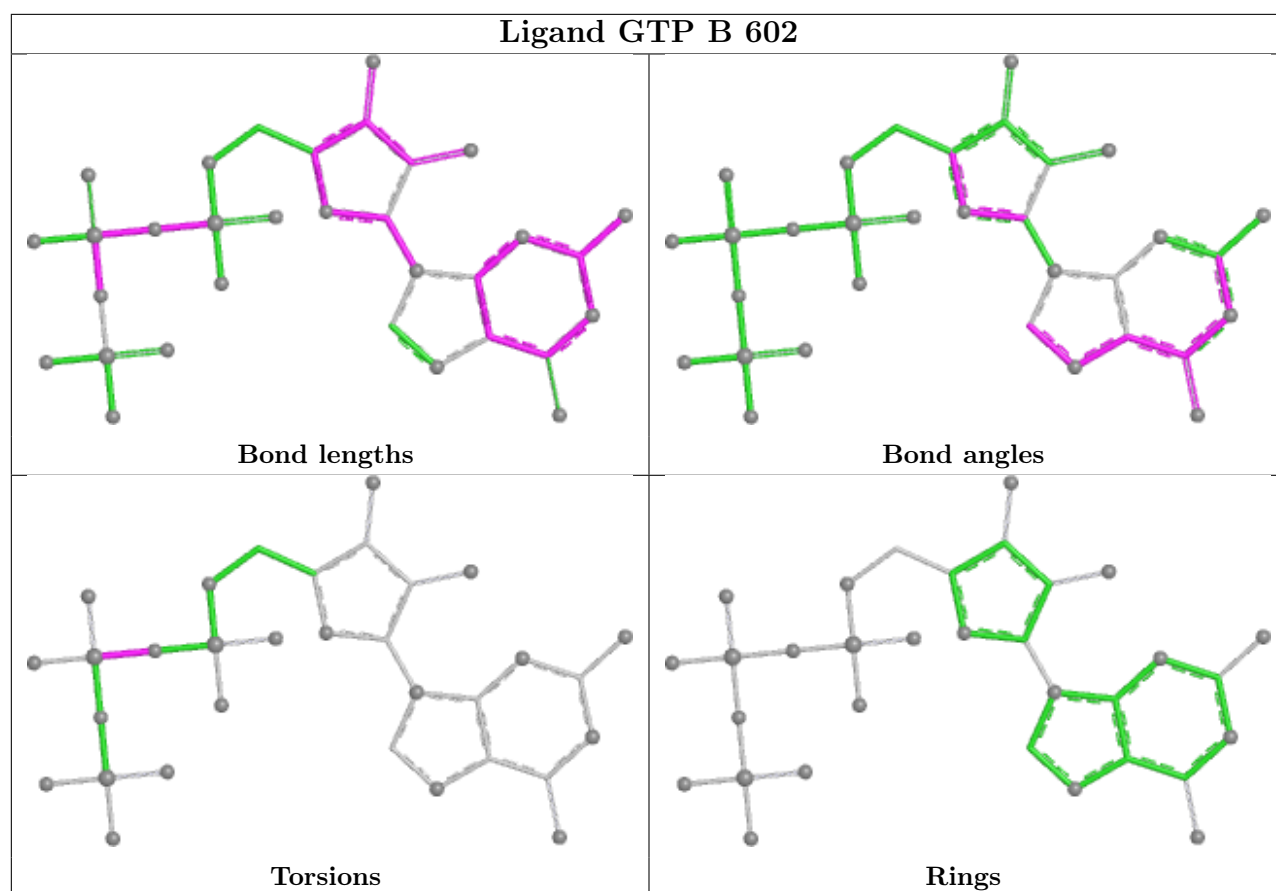


Ligand IMP B 604

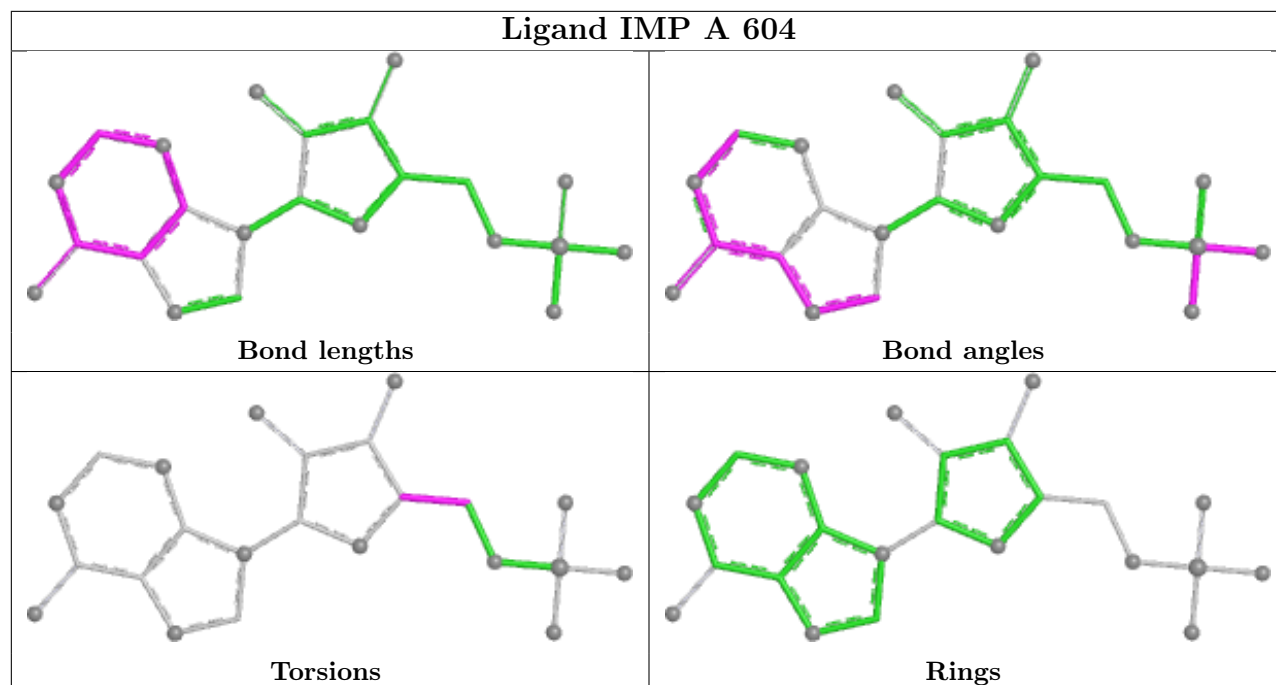


Ligand ATP H 603

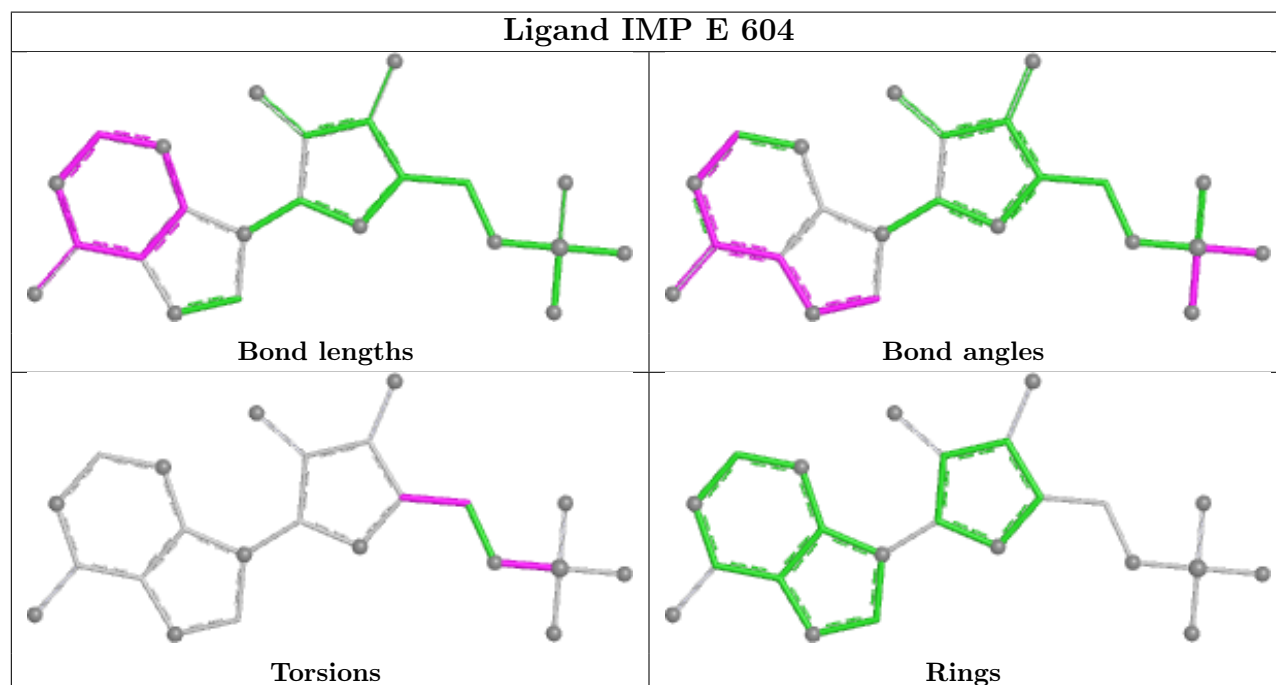


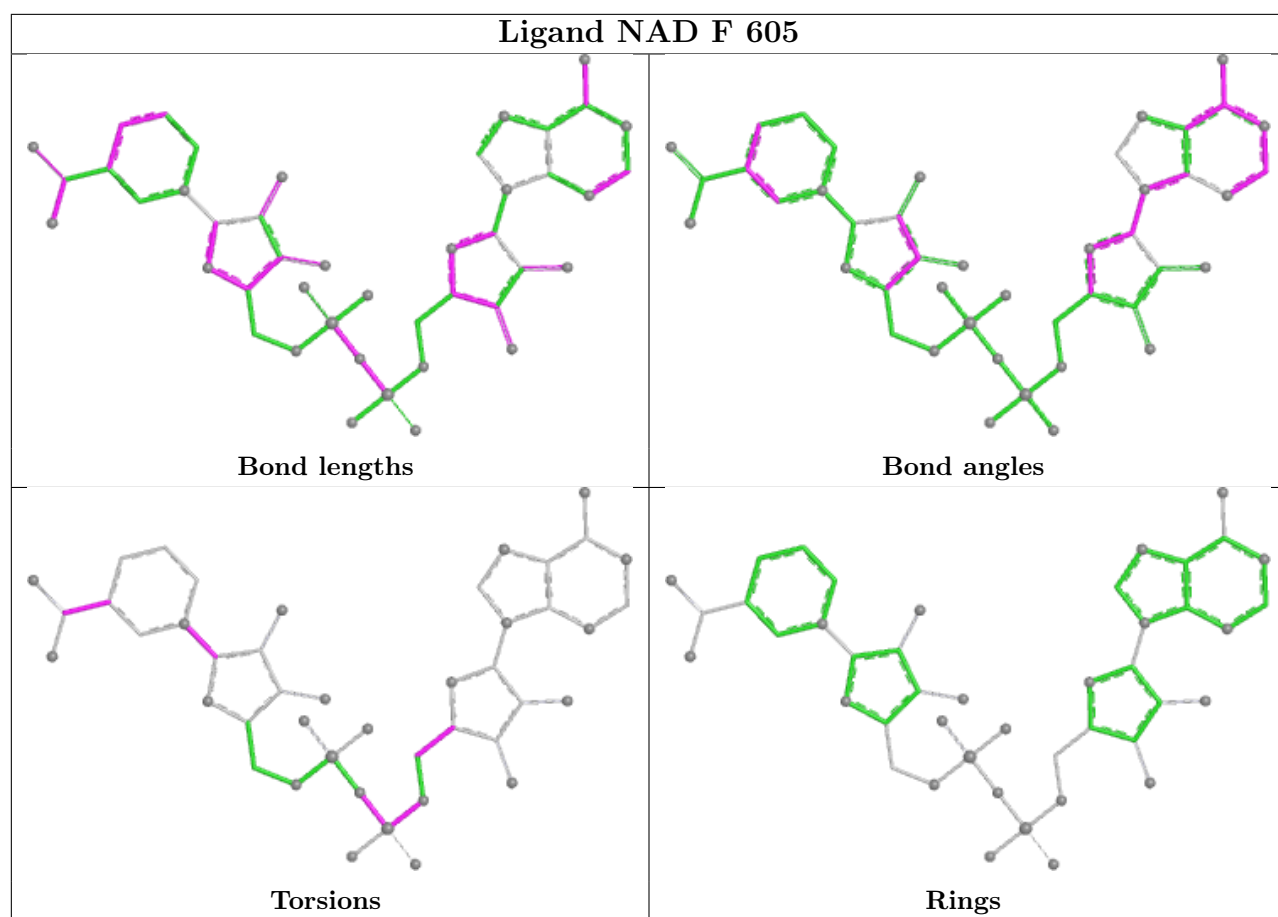


Ligand IMP A 604

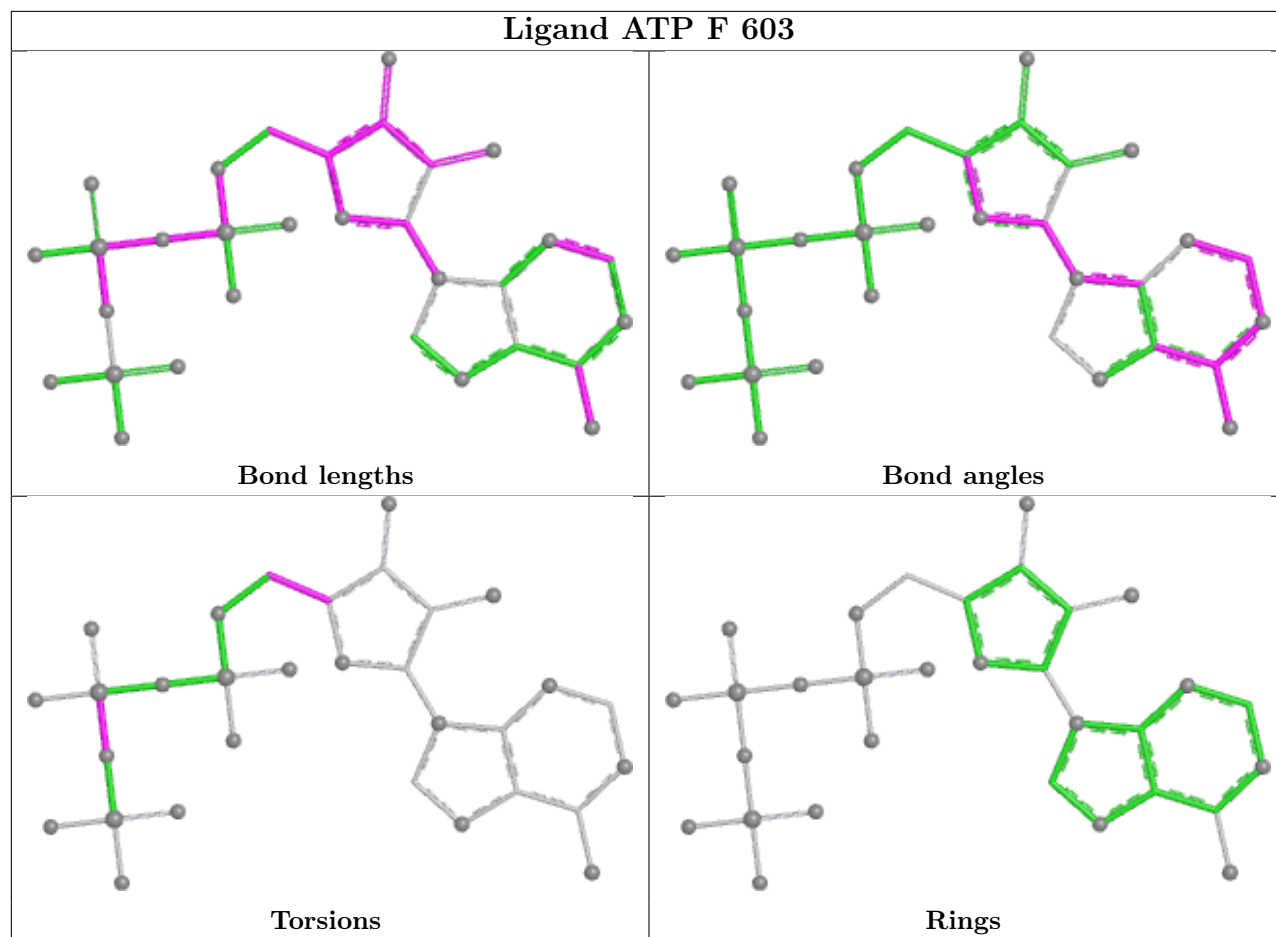


Ligand IMP E 604

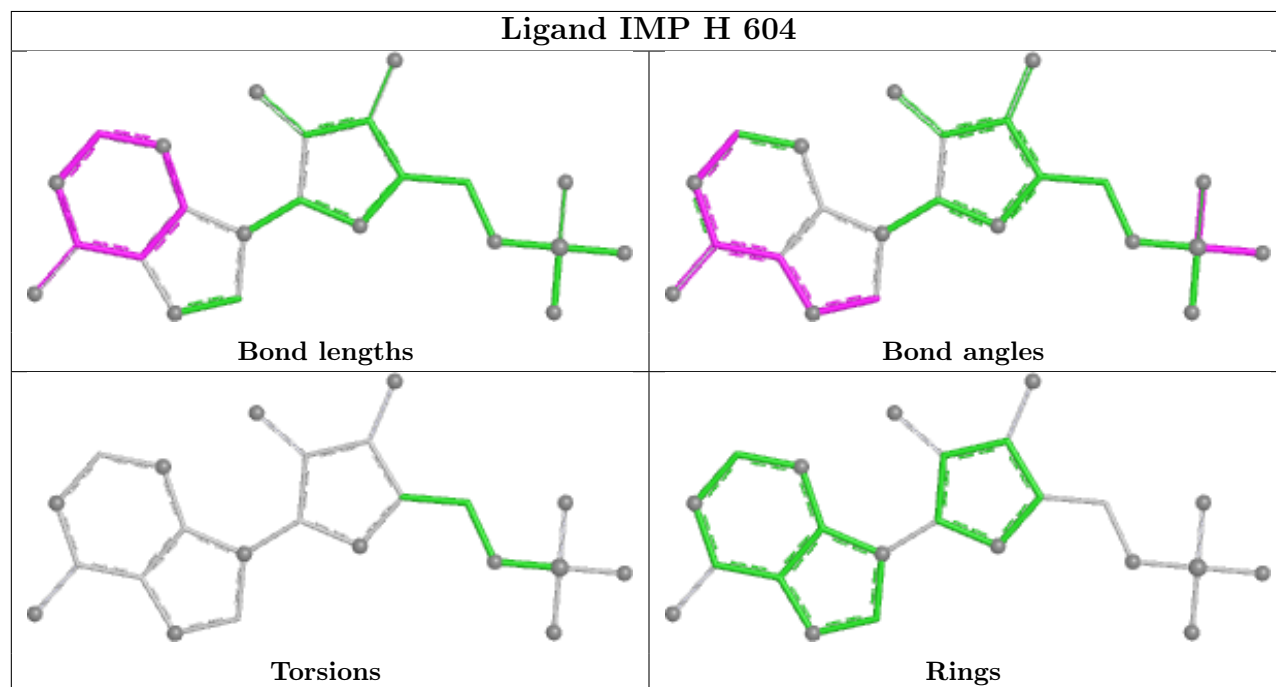




Ligand ATP F 603



Ligand IMP H 604



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.

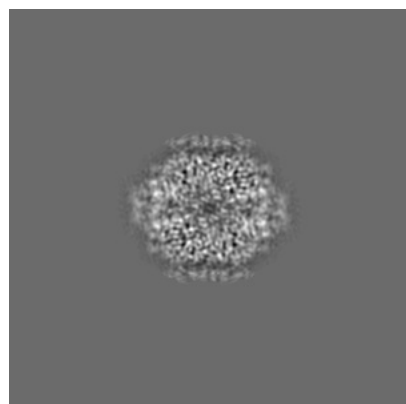
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20705. These allow visual inspection of the internal detail of the map and identification of artifacts.

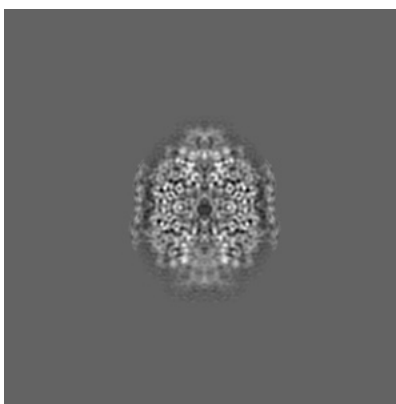
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

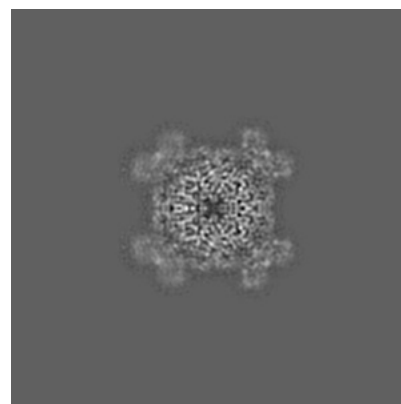
6.1.1 Primary map



X

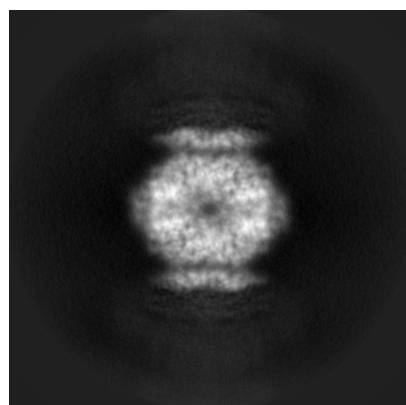


Y

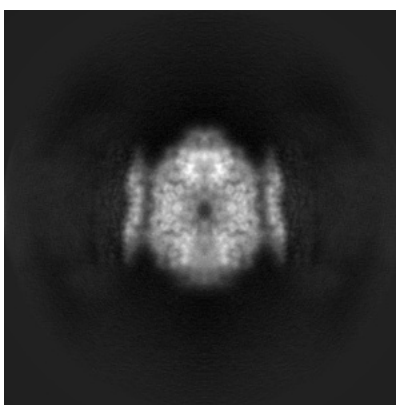


Z

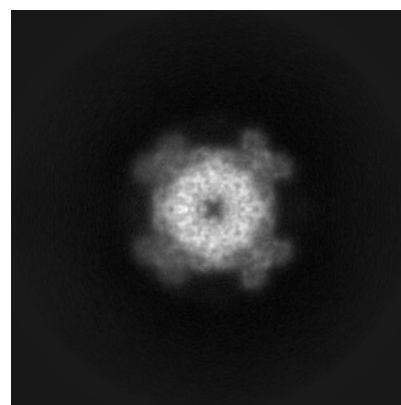
6.1.2 Raw map



X



Y

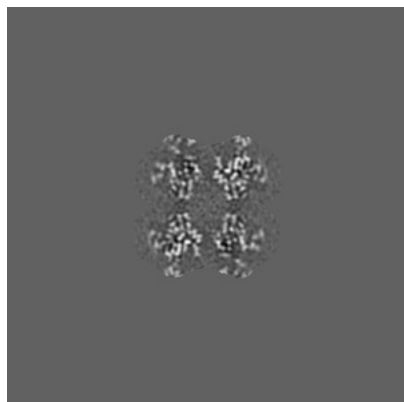


Z

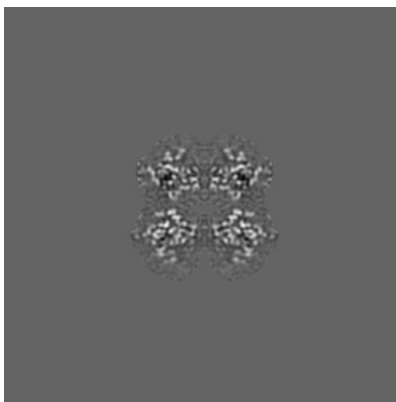
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

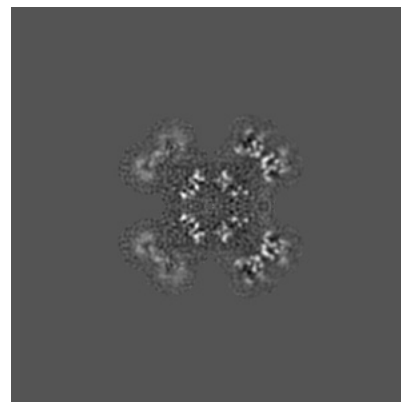
6.2.1 Primary map



X Index: 160

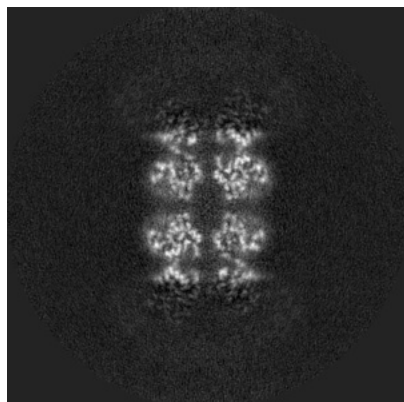


Y Index: 160

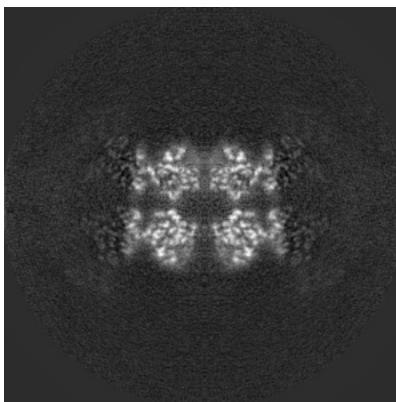


Z Index: 160

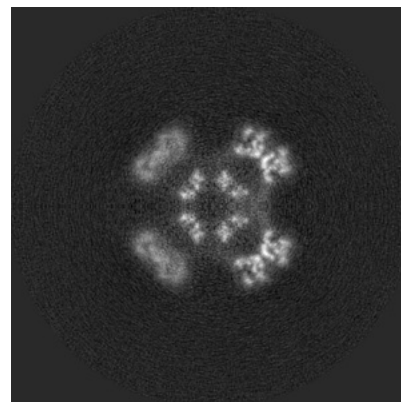
6.2.2 Raw map



X Index: 160



Y Index: 160

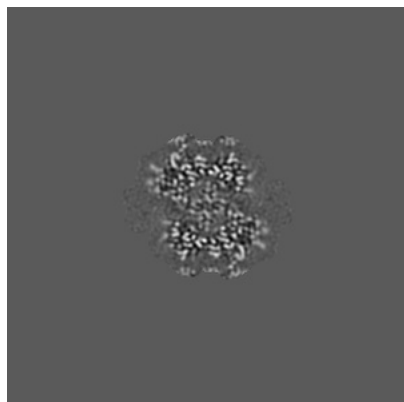


Z Index: 160

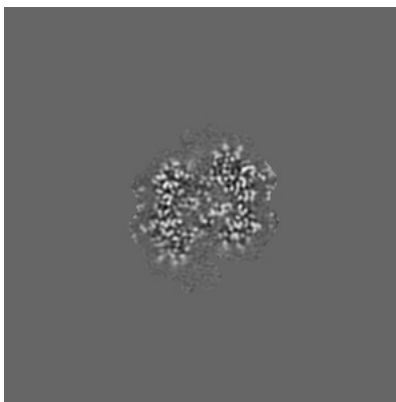
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

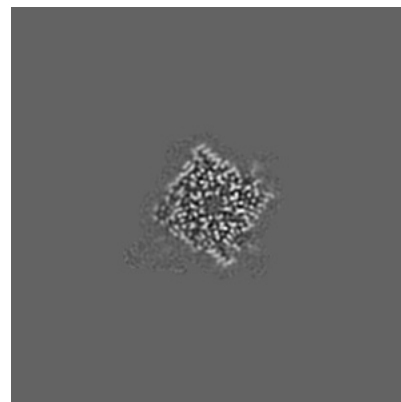
6.3.1 Primary map



X Index: 176

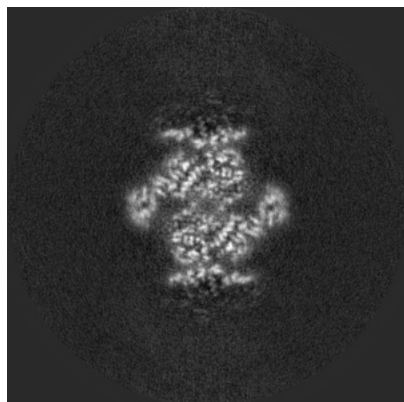


Y Index: 175

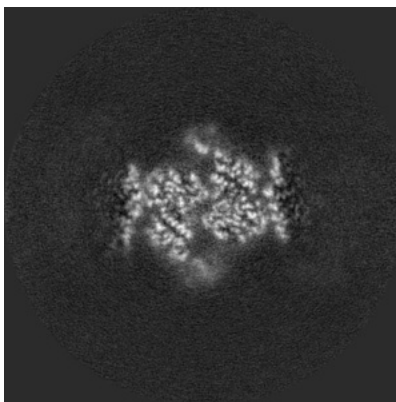


Z Index: 191

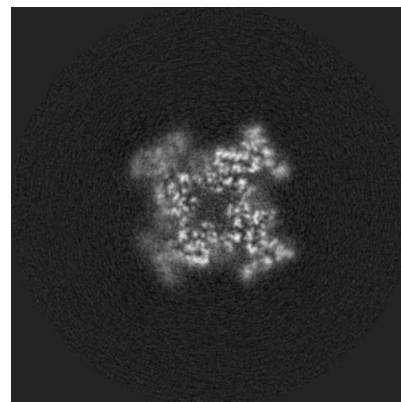
6.3.2 Raw map



X Index: 186



Y Index: 183

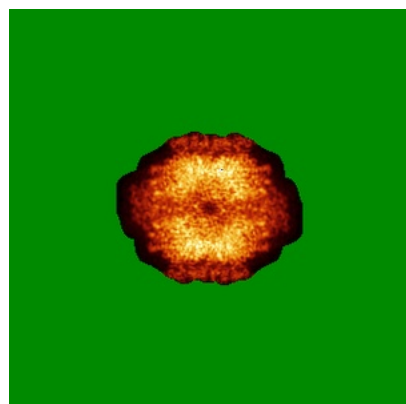


Z Index: 147

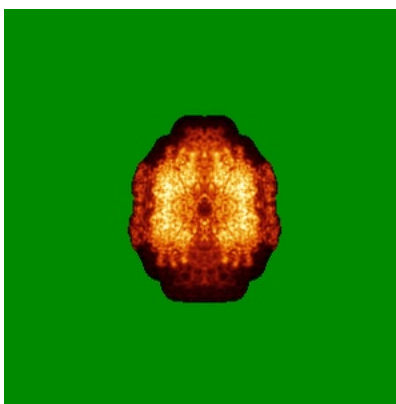
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

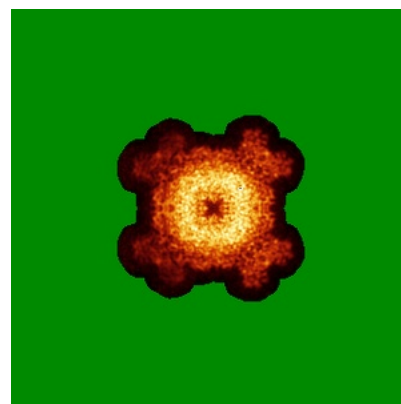
6.4.1 Primary map



X

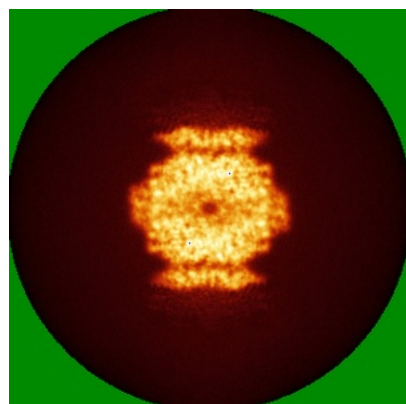


Y

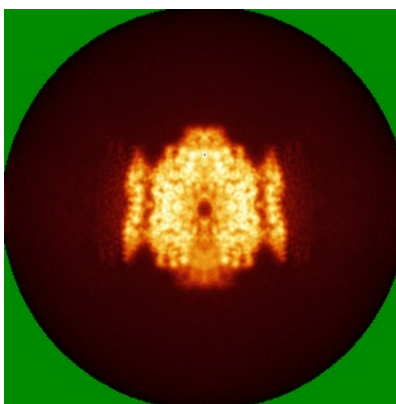


Z

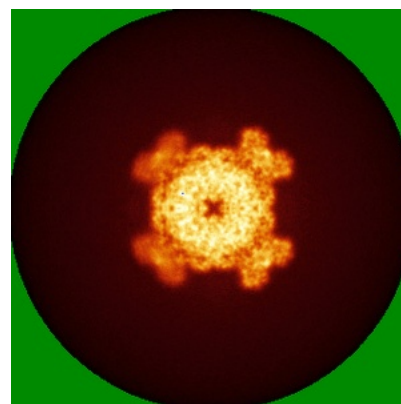
6.4.2 Raw map



X



Y

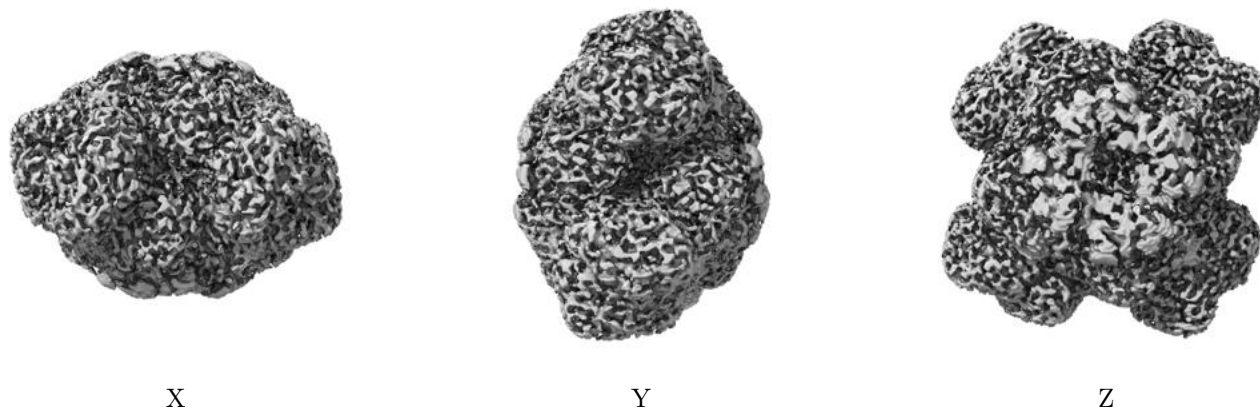


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

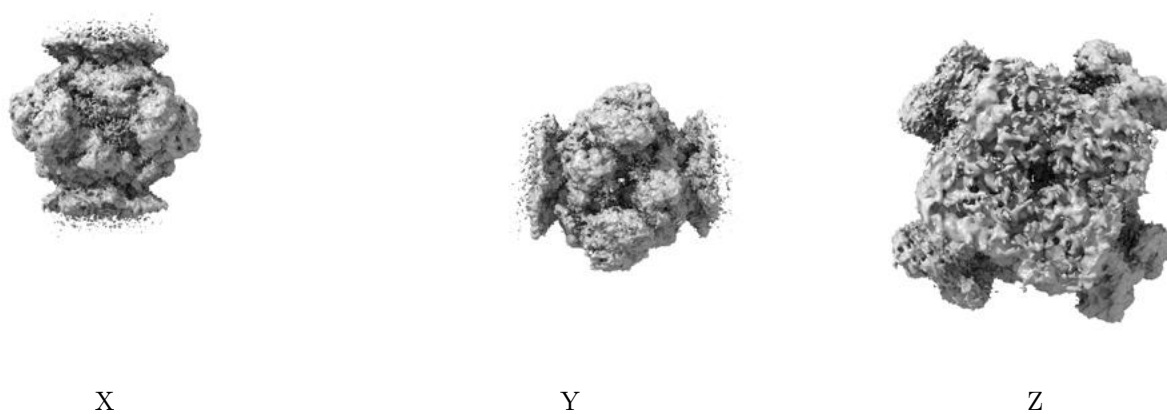
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

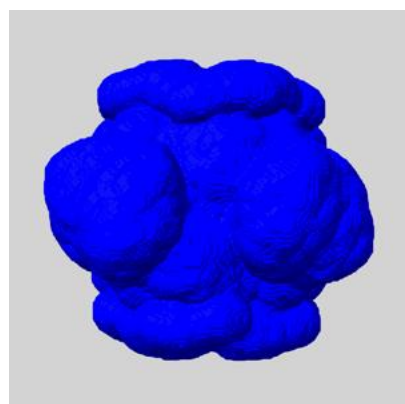
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

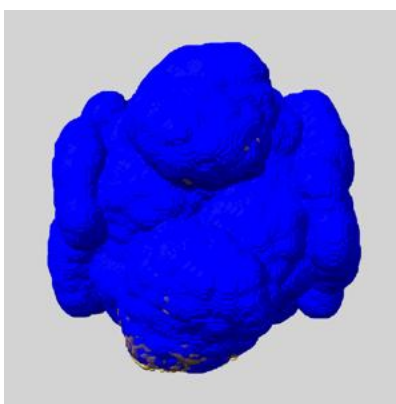
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

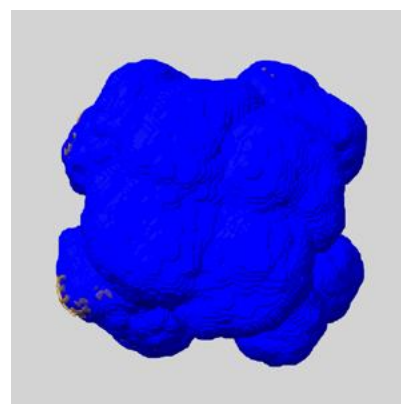
6.6.1 emd_20705_msk_1.map [i](#)



X



Y

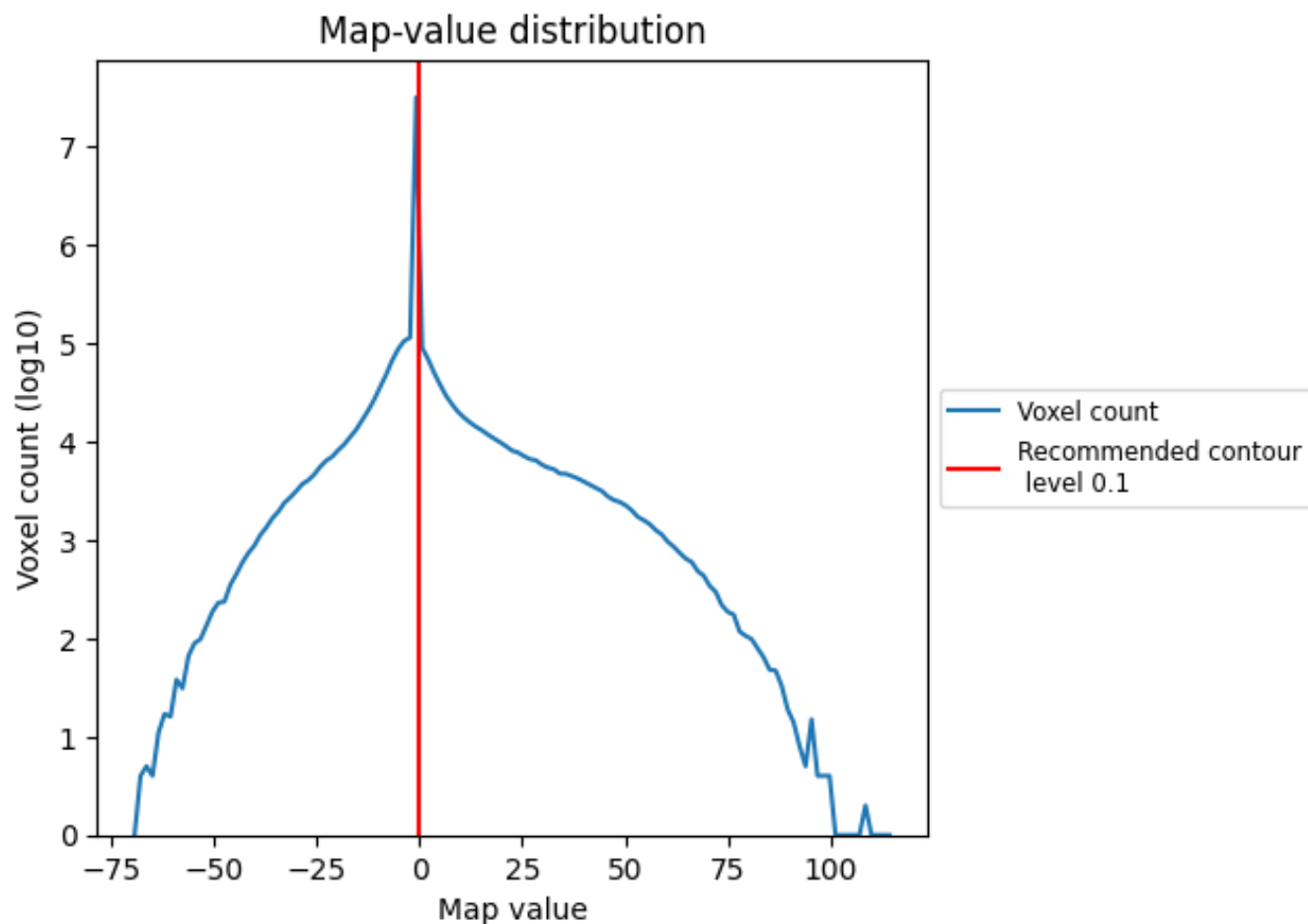


Z

7 Map analysis [i](#)

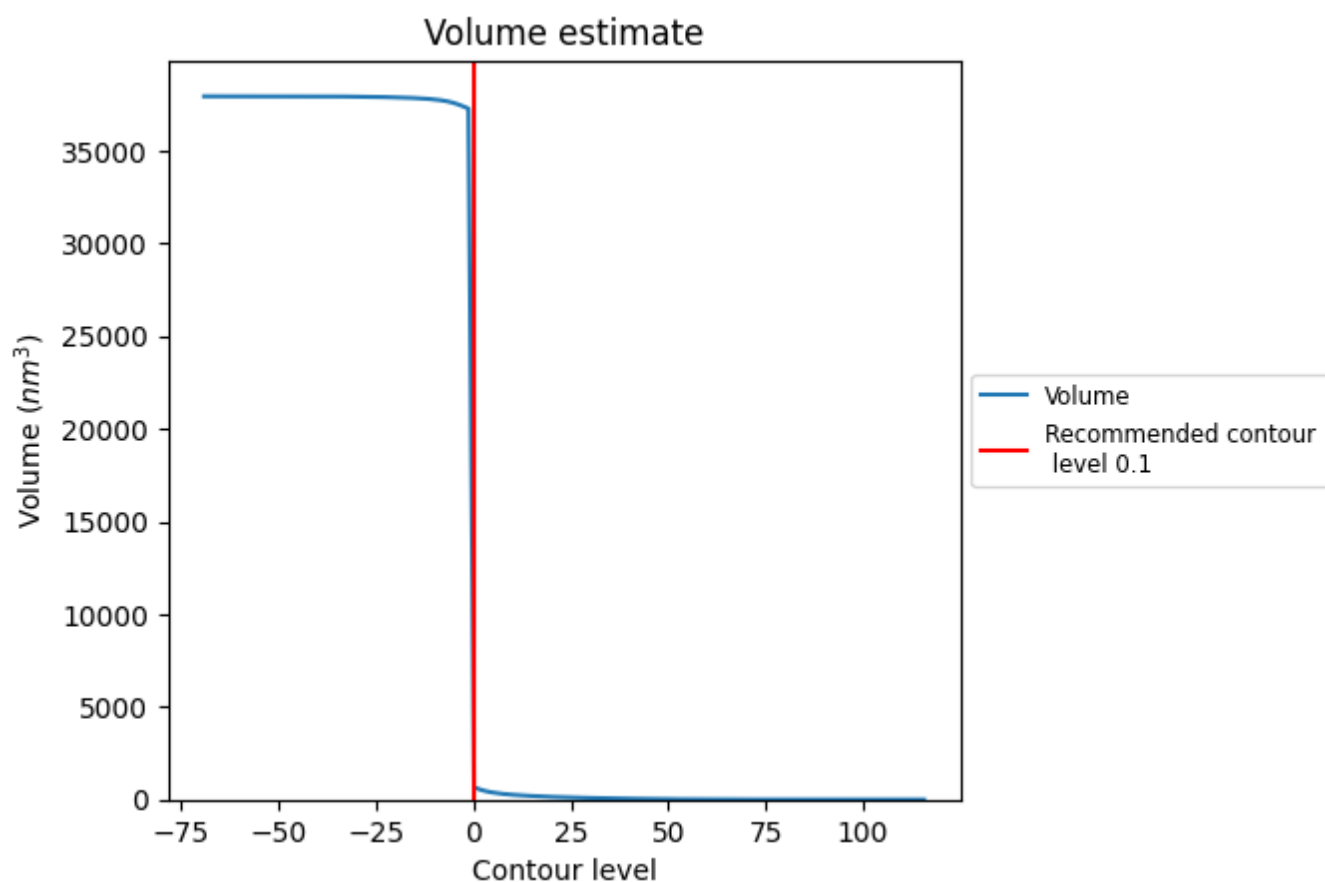
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

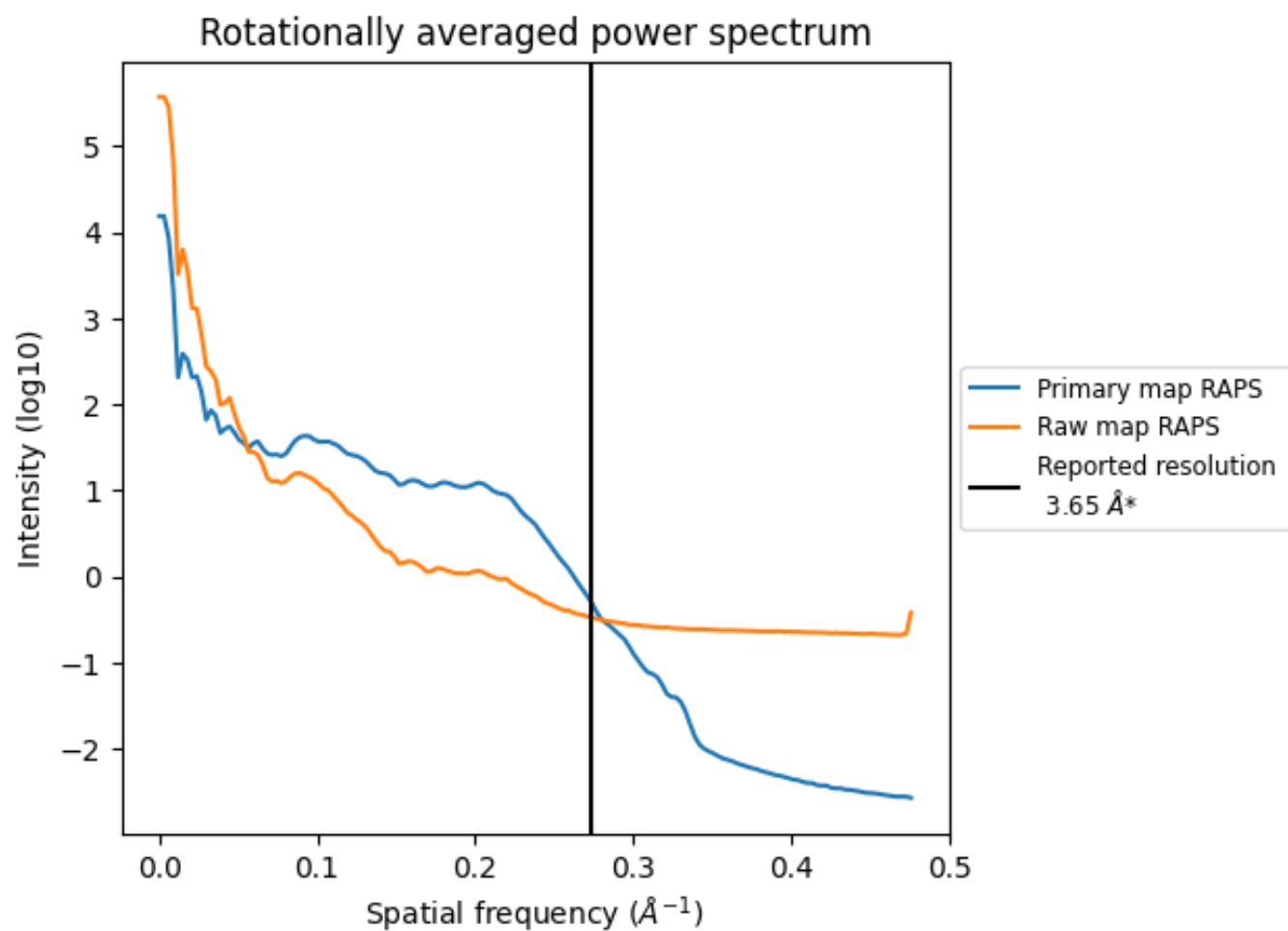
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1358 nm^3 ; this corresponds to an approximate mass of 1227 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

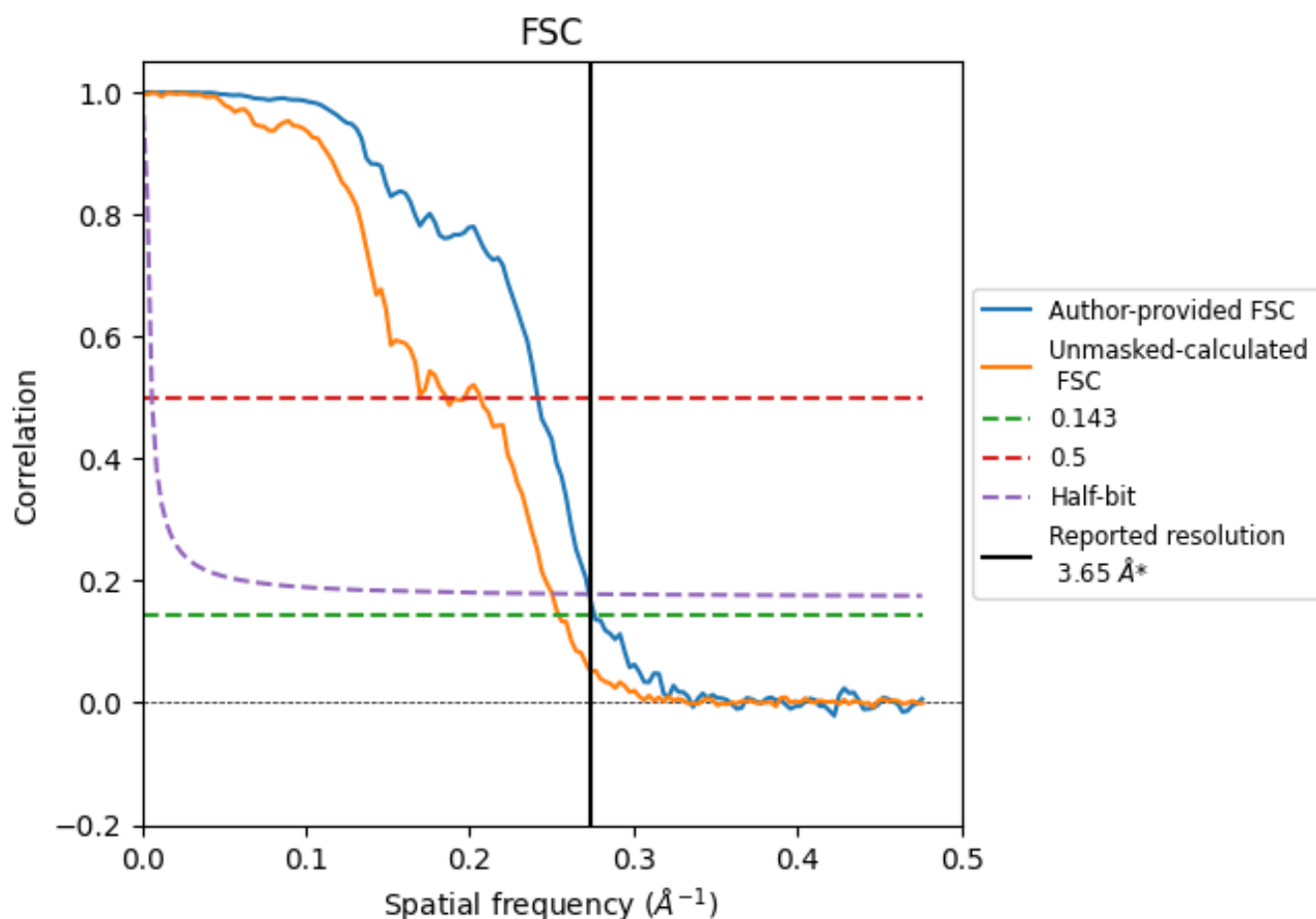


*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.274 \AA^{-1}

8.2 Resolution estimates [i](#)

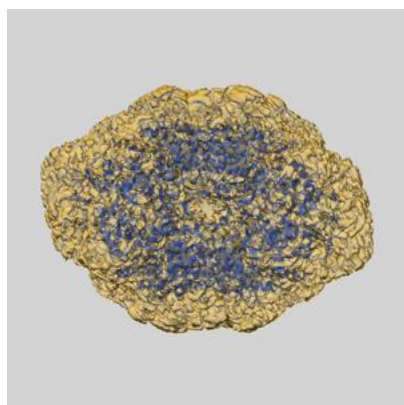
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.62	4.14	3.66
Unmasked-calculated*	3.93	5.39	4.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

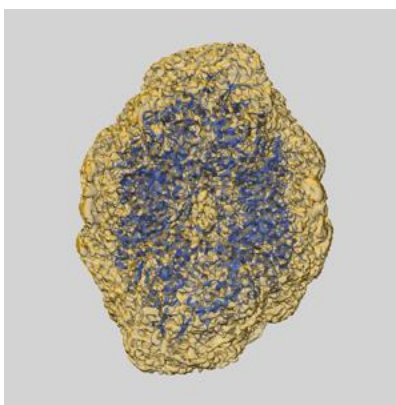
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20705 and PDB model 6UA4. Per-residue inclusion information can be found in section [3](#) on page [11](#).

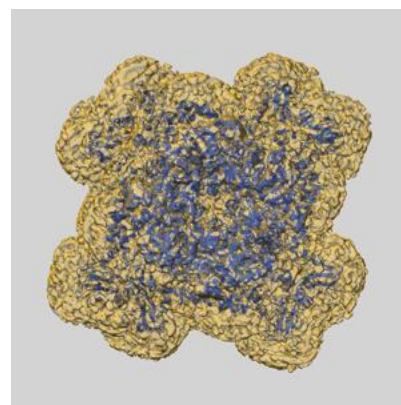
9.1 Map-model overlay [i](#)



X



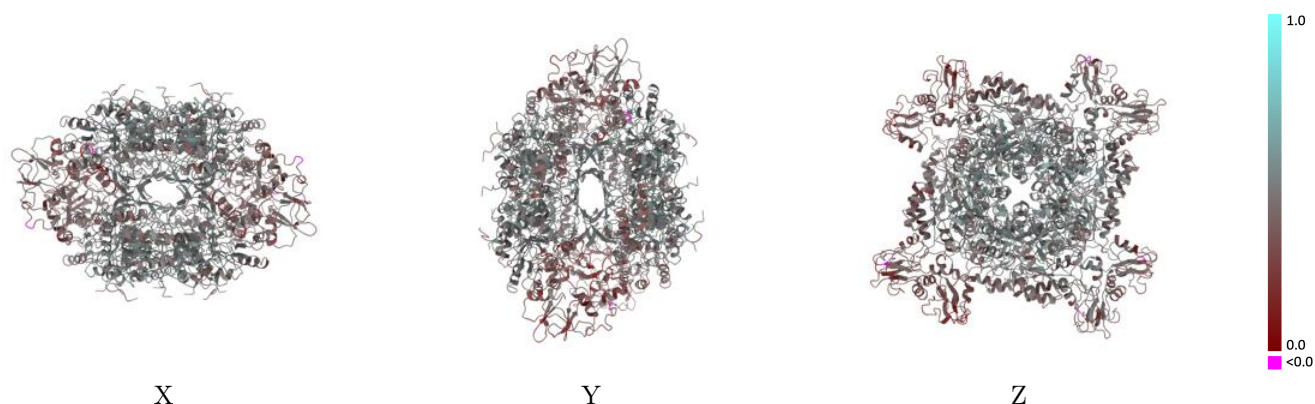
Y



Z

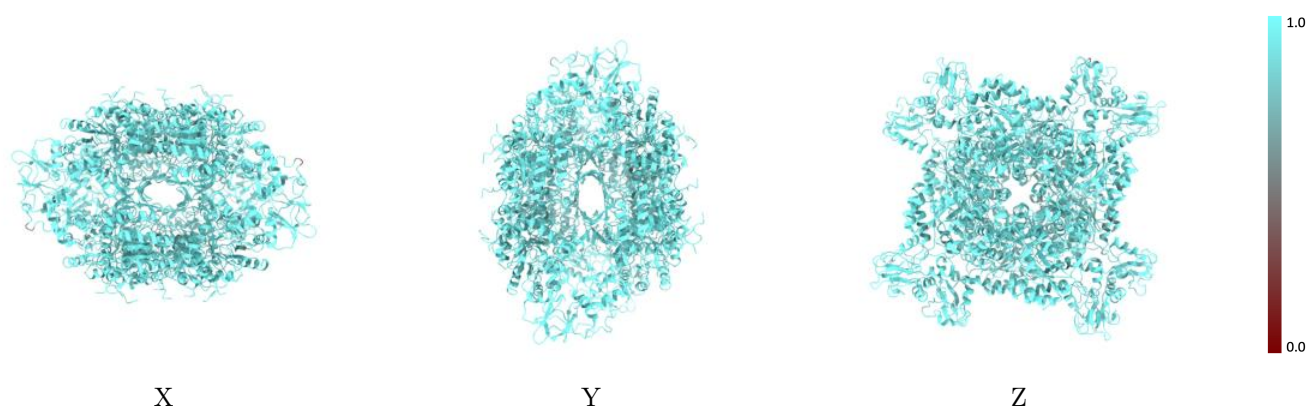
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



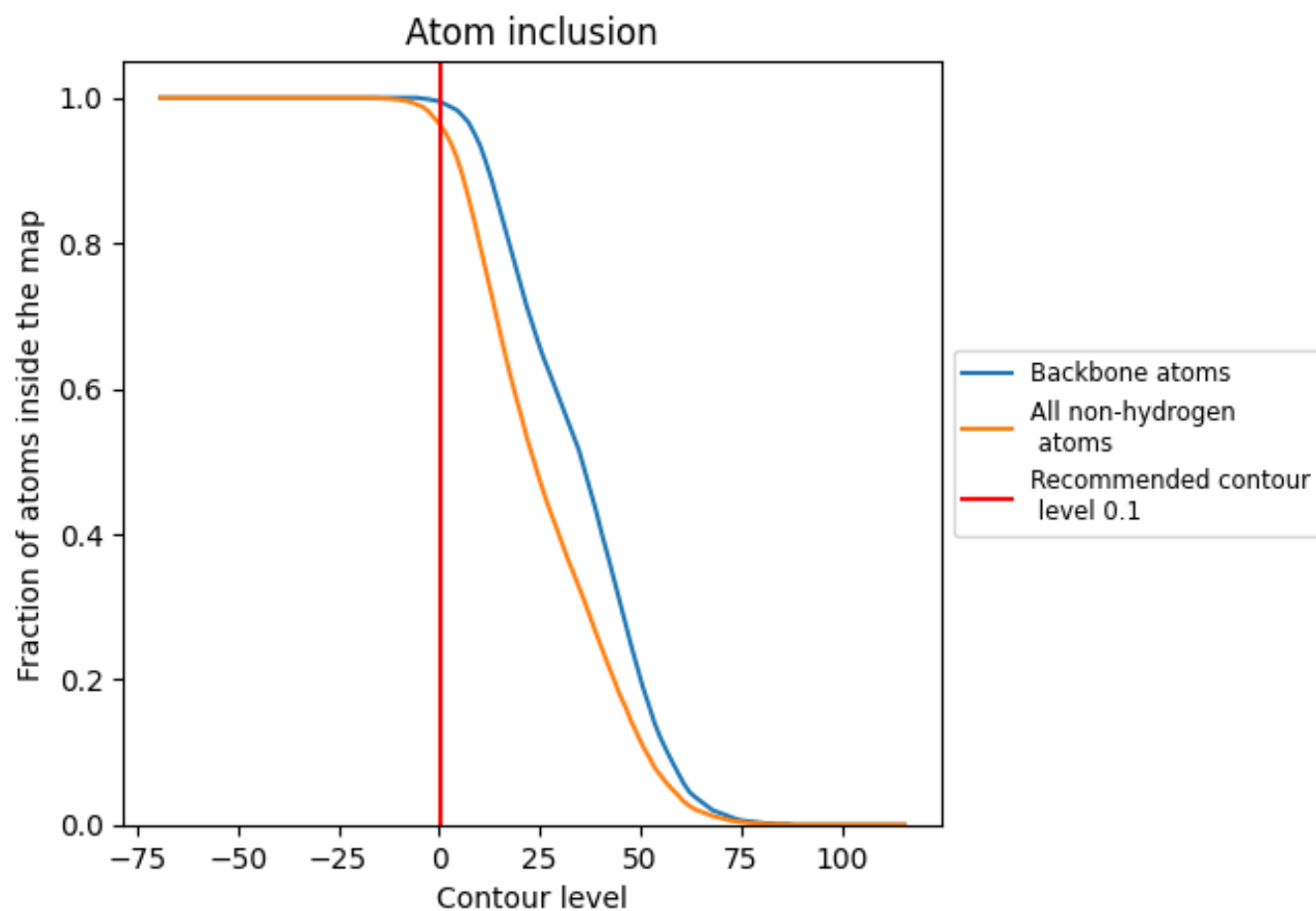
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.4380
A	 0.9640	 0.4480
B	 0.9630	 0.4570
C	 0.9660	 0.4190
D	 0.9680	 0.4320
E	 0.9640	 0.4500
F	 0.9630	 0.4560
G	 0.9660	 0.4180
H	 0.9660	 0.4290
I	 0.9300	 0.4350
J	 0.9600	 0.4310
K	 0.9600	 0.4270
L	 0.9400	 0.4180
M	 0.9400	 0.4410
N	 0.9600	 0.4300
O	 0.9500	 0.4260
P	 0.9300	 0.4270

