



## wwPDB EM Validation Summary Report ⓘ

May 18, 2025 – 06:04 PM EDT

PDB ID : 6UDO / pdb\_00006udo  
EMDB ID : EMD-20741  
Title : Human IMPDH2 treated with ATP, IMP, and 20 mM GTP. Fully compressed filament segment reconstruction.  
Authors : Johnson, M.C.; Kollman, J.M.  
Deposited on : 2019-09-19  
Resolution : 3.21 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](mailto: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>.

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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

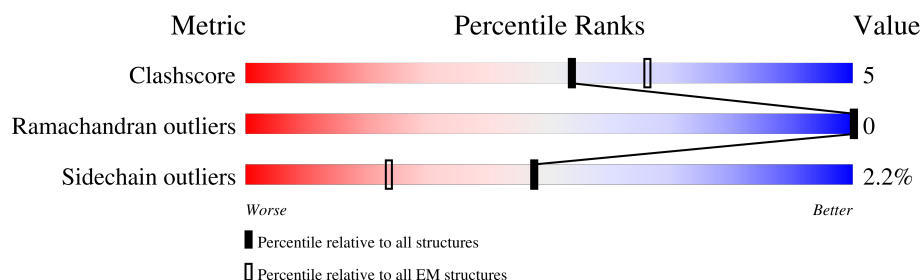
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.21 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.



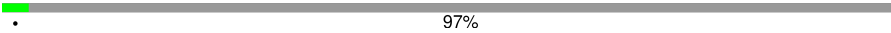
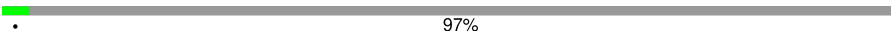
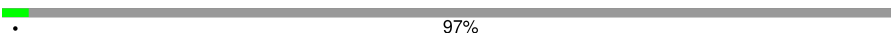
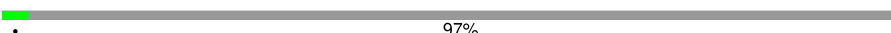
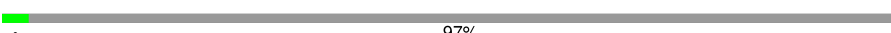
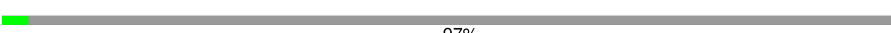


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	80% 13% • 6%
1	B	519	80% 13% • 6%
1	C	519	81% 13% • 6%
1	D	519	80% 14% • 6%
1	E	519	80% 13% • 6%
1	F	519	79% 14% • 6%
1	G	519	81% 13% • 6%
1	H	519	80% 14% • 6%

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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 4 unique types of molecules in this entry. The entry contains 31392 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	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
1	B	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
1	C	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
1	D	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
1	E	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
1	F	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
1	G	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
1	H	487	Total	C	N	O	S	0	0
			3704	2337	639	707	21		
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		
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		

There are 80 discrepancies between the modelled and reference sequences:

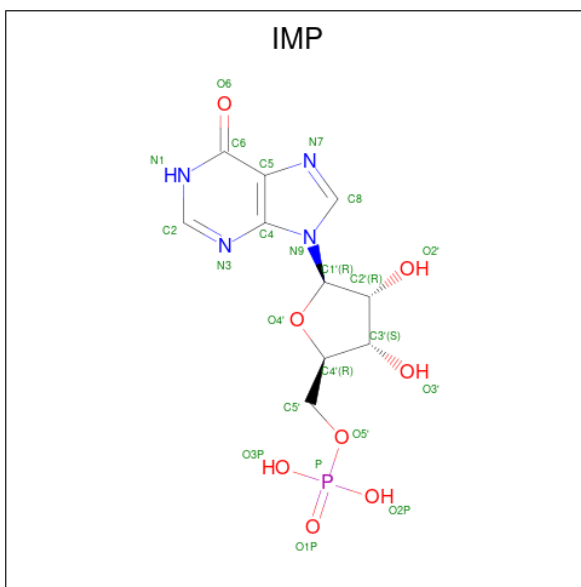
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP P12268
A	-3	GLU	-	expression tag	UNP P12268
A	-2	PHE	-	expression tag	UNP P12268
A	-1	GLU	-	expression tag	UNP P12268
A	0	LEU	-	expression tag	UNP P12268
B	-4	SER	-	expression tag	UNP P12268
B	-3	GLU	-	expression tag	UNP P12268
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
I	-4	SER	-	expression tag	UNP P12268
I	-3	GLU	-	expression tag	UNP P12268
I	-2	PHE	-	expression tag	UNP P12268

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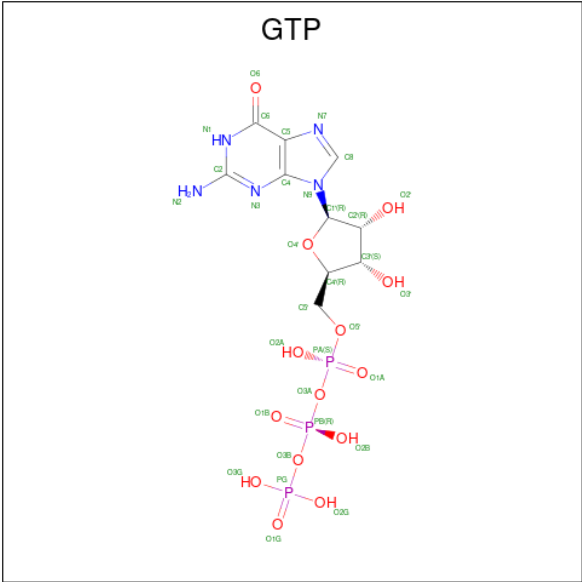
Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLU	-	expression tag	UNP P12268
I	0	LEU	-	expression tag	UNP P12268
J	-4	SER	-	expression tag	UNP P12268
J	-3	GLU	-	expression tag	UNP P12268
J	-2	PHE	-	expression tag	UNP P12268
J	-1	GLU	-	expression tag	UNP P12268
J	0	LEU	-	expression tag	UNP P12268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

- Molecule 2 is INOSINIC ACID (CCD ID: IMP) (formula:  $C_{10}H_{13}N_4O_8P$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 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	C	N	O	P	0
			32	10	5	14	3	
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	

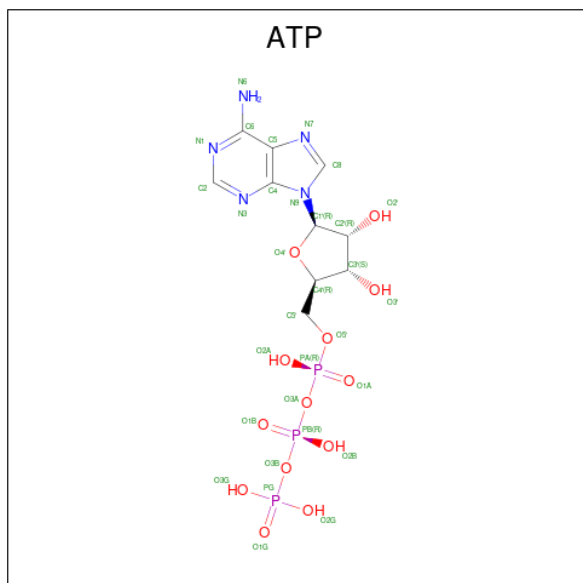
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Mol	Chain	Residues	Atoms					AltConf
3	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	H	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

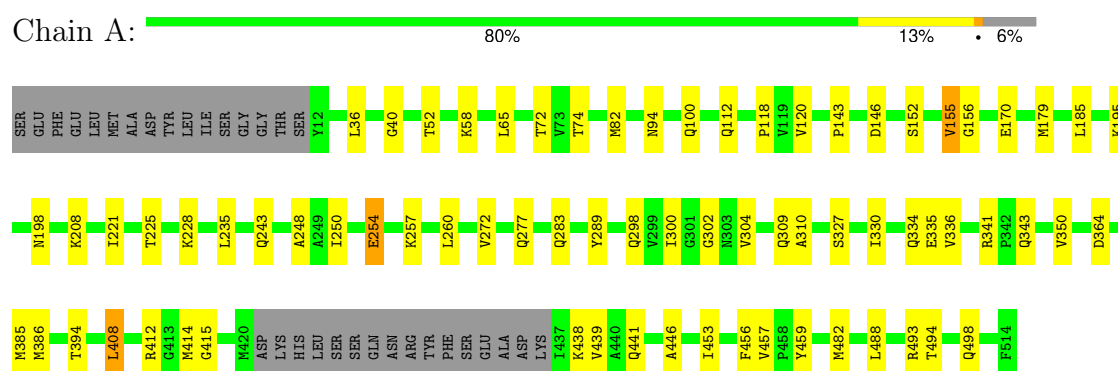


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	G	1	Total	C	N	O	P	0
			31	10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

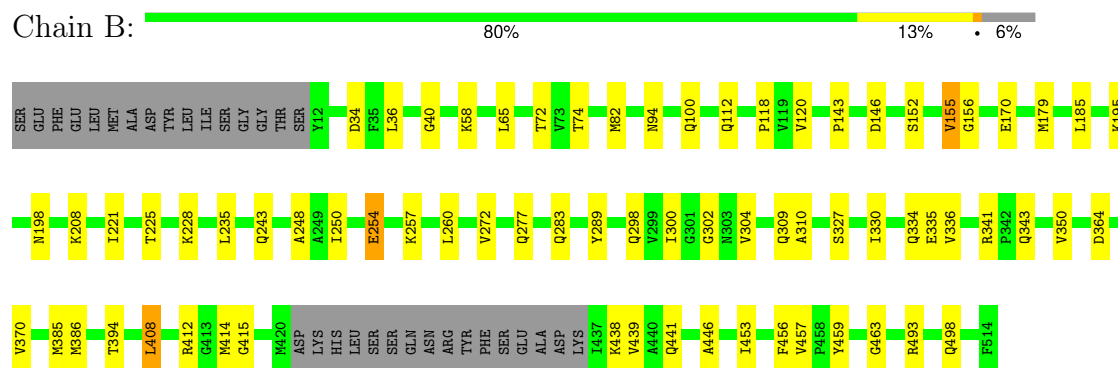
### 3 Residue-property plots

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.

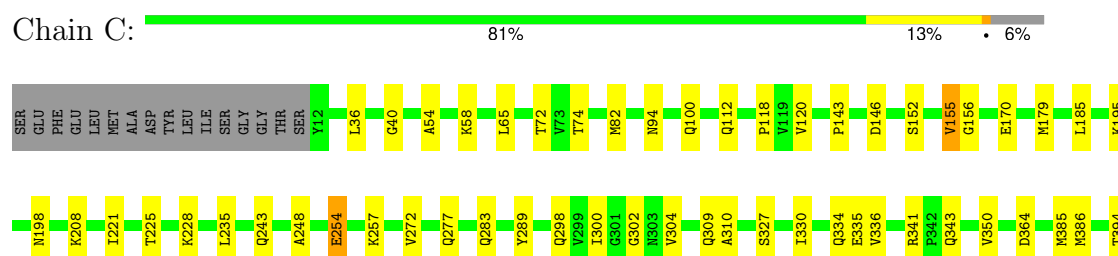
- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

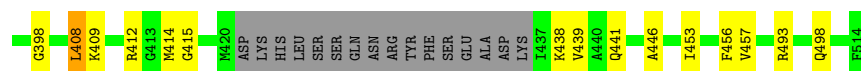


- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



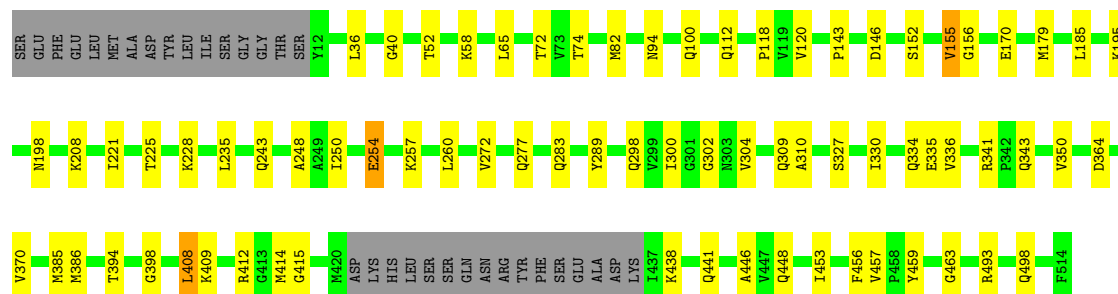
- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2





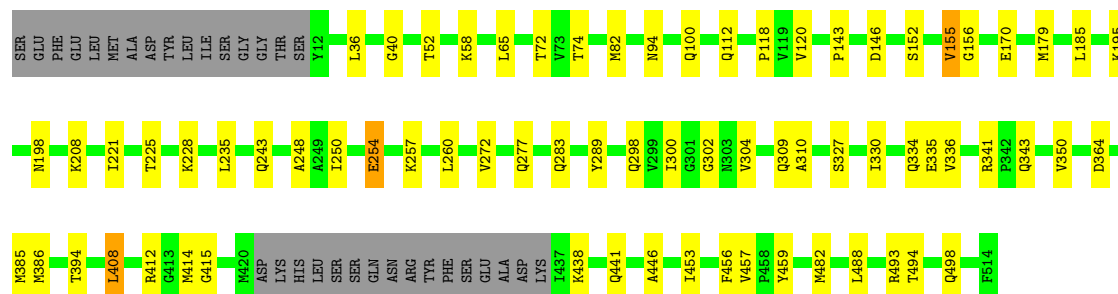
- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain D: 80% 14% 6%



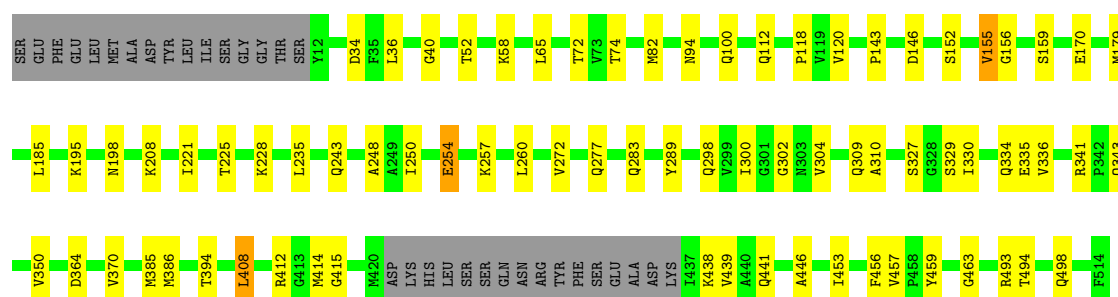
- Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain E: 80% 13% 6%



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

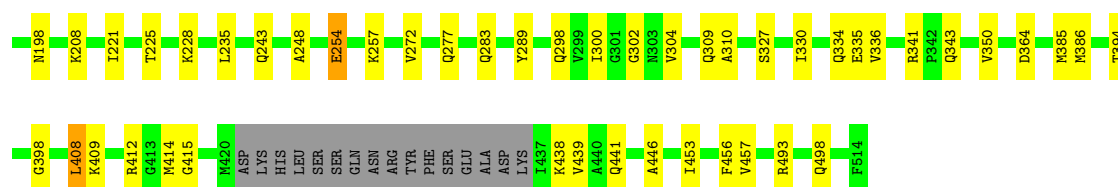
Chain F: 79% 14% 6%



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

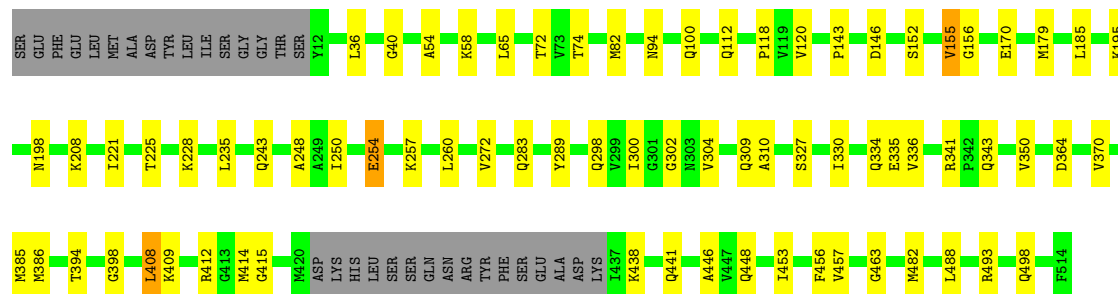
Chain G: 81% 13% 6%





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

Chain H: 80% 14% 6%



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

Chain I: 97% 1% 2%



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

Chain J: 97% 1% 2%

[illegible]

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

Chain K: 

97%

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

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

97%

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

97%



SER	GLY	GLU	GLU	LEU	PHE	PHE	GLU	LYS	ARG	THR	SER	SER	ALA	GLN	VAL	GLY	GLY	GLN	VAL	HIS	SER	SER	PHE
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● Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain N: . 97%

SER	GLU	PHE	GLU	LEU	M1	L5	P14	ASP	ASP	GLY	LEU	THR	THR	ASN	CYS	GLY	GLY	ASP	GLY	LEU	THR	TYR	ASN	ASP	PHE	LEU	ILE	LEU	PRO	GLY	TYR	ASP	PHE	THR	ASP	GLN	VAL	GLY	THR	LYS	LEU	ILE	THR	LYS	PRO	
LEU	VAL	SER	SER	PRO	MET	THR	VAL	THR	GLU	ALA	GLY	MET	ALA	ILE	CYS	GLY	GLY	ILE	ARG	GLY	PHE	ILE	HIS	HIS	ASN	CYS	THR	PRO	GLU	ILE	SER	PHE	VAL	LYS	GLY	VAL	GLY	LYS	THR	THR	GLU	THR	LEU	LYS	PRO	
ASP	ARG	VAL	ARG	ARG	VAL	PHE	LYS	LYS	ALA	ALA	ARG	GLY	HIS	GLY	PHE	CYS	GLY	ILE	PRO	ILE	THR	THR	ASP	THR	GLY	LEU	ILE	ILE	ILE	GLY	SER	ARG	LEU	GLY	PHE	ARG	LEU	GLY	GLU	GLY	GLU	GLY	GLY	GLY	ASP	
LEU	VAL	VAL	ALA	PRO	GLY	ILE	THR	LEU	LYS	GLY	ASP	LYS	ASN	GLY	GLY	ILE	GLY	GLN	SER	LEU	ILE	VAL	ASN	ASN	GLY	ASP	GLY	LEU	VAL	VAL	ASN	GLY	THR	THR	LEU	ASP	THR	ASN	GLY	GLY	GLY	GLY	GLY	GLY	LEU	
LEU	CYS	GLY	ALA	ALA	ILE	THR	HIS	GLY	ASP	ASP	GLY	LYS	TYR	ARG	GLY	LEU	ASP	LEU	LEU	ALA	GLY	VAL	LYS	GLN	GLY	VAL	GLY	GLY	ASN	GLY	ASN	GLY	ILE	ASN	THR	ASN	GLY	ASP	TYR	PRO	LEU	LEU	GLY	ASN	VAL	
VAL	THR	ALA	ALA	GLN	ALA	LYS	ASN	LEU	ILE	ASP	ALA	GLY	VAL	ASP	ALA	GLY	ALA	VAL	GLY	GLY	MET	GLY	SER	GLY	GLY	VAL	VAL	LEU	ALA	ALA	GLY	CYS	ILE	THR	THR	GLY	GLY	GLY	VAL	LYS	VAL	THR	GLY	GLY	ASP	
GLY	GLY	ILE	GLN	ASN	VAL	GLY	ILE	ASP	LYS	ALA	ALA	GLY	VAL	THR	VAL	GLY	VAL	THR	THR	VAL	MET	GLY	MET	GLY	GLY	VAL	VAL	LEU	ALA	VAL	GLY	GLY	GLY	GLY	THR	THR	ILE	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
SER	SER	GLN	ASN	ARG	TYR	PHE	THR	LYS	ASP	LYS	ILE	VAL	VAL	SER	GLY	LEU	GLN	ASP	LEU	VAL	GLY	ALA	ALA	THR	THR	GLY	GLY	PRO	GLY	GLY	TYR	GLY	GLY	GLY	ILE	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
SER	GLU	LEU	GLY	GLY	SER	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ALA	THR	ARG	THR	ARG	THR	ARG	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
SER	SER	SER	SER	LYS	ALA	GLN	GLN	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
THR	ARG	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
SER	SER	SER	SER	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ALA	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					

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

Chain O: . 97%

SER	GLU	PHE	GLU	LEU	M1	L5	P14	ASP	ASP	GLY	LEU	THR	THR	ASN	CYS	GLY	GLY	ASP	GLY	LEU	THR	TYR	ASN	ASP	PHE	LEU	ILE	PRO	GLU	PRO	GLY	TYR	ASP	ASP	GLY	THR	ASP	GLU	VAL	GLN	VAL	SER	SER	LEU				
LEU	VAL	SER	SER	PRO	MET	ASP	THR	VAL	GLU	ALA	GLY	MET	ALA	THR	ALA	ILE	ALA	GLN	MET	ALA	LEU	THR	ASN	CYS	GLY	GLY	ILE	PRO	GLU	PRO	PHE	GLN	GLY	ASP	THR	THR	GLU	VAL	GLN	VAL	SER	SER	LEU					
ASP	VAL	ARG	ARG	VAL	PHE	GLY	GLU	ALA	LYS	ALA	HIS	GLY	PHE	CYS	GLY	GLY	THR	THR	ASP	MET	GLY	SER	ARG	LEU	VAL	ILE	ILE	PRO	GLU	ILE	SER	ARG	LEU	VAL	ASP	THR	GLU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
LEU	VAL	ALA	PRO	ALA	GLY	ILE	THR	LEU	LYS	LYS	ALA	ASN	GLU	ILE	ILE	GLY	GLN	ARG	SER	PRO	ILE	VAL	LYS	ASP	GLY	GLU	ILE	ILE	VAL	VAL	ASN	ARG	ASP	THR	HIS	HIS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU		
LEU	CYS	GLY	ALA	ALA	ILE	GLY	THR	HIS	ASP	ASP	GLY	LYS	TYR	ARG	GLY	LEU	ASP	LEU	LEU	ALA	GLY	VAL	GLN	LYS	LYS	GLY	ILE	VAL	VAL	ASN	LEU	ASP	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
VAL	THR	ALA	GLN	GLN	ALA	LYS	ASN	LEU	ILE	ASP	ALA	VAL	ASP	LEU	ALA	GLY	ARG	VAL	VAL	GLY	MET	GLY	GLY	GLY	GLY	GLY	ILE	CYS	VAL	ILE	THR	GLN	GLY	ASN	ASN	GLN	ASN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	
GLY	GLY	ILE	GLN	ASN	VAL	GLY	HIS	ILE	LYS	LYS	ALA	LEU	VAL	LEU	GLY	ALA	THR	THR	THR	VAL	GLY	GLY	GLY	GLY	GLY	GLY	ILE	ALA	ALA	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

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

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

Chain P:  97%

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

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

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

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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	31392	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	138.716	Depositor
Minimum map value	-88.945	Depositor
Average map value	0.058	Depositor
Map value standard deviation	3.698	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	330.6, 330.6, 330.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8265, 0.8265, 0.8265	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, IMP, GTP

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	0.32	0/3760	0.63	5/5070 (0.1%)
1	B	0.32	0/3760	0.63	5/5070 (0.1%)
1	C	0.32	0/3760	0.63	5/5070 (0.1%)
1	D	0.32	0/3760	0.63	5/5070 (0.1%)
1	E	0.32	0/3760	0.63	5/5070 (0.1%)
1	F	0.32	0/3760	0.63	5/5070 (0.1%)
1	G	0.32	0/3760	0.63	5/5070 (0.1%)
1	H	0.32	0/3760	0.63	5/5070 (0.1%)
1	I	0.28	0/104	0.75	0/141
1	J	0.28	0/104	0.75	0/141
1	K	0.28	0/104	0.75	0/141
1	L	0.28	0/104	0.75	0/141
1	M	0.28	0/104	0.75	0/141
1	N	0.28	0/104	0.75	0/141
1	O	0.28	0/104	0.75	0/141
1	P	0.28	0/104	0.75	0/141
All	All	0.32	0/30912	0.63	40/41688 (0.1%)

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	GLU	CB-CG-CD	5.92	122.67	112.60
1	G	254	GLU	CB-CG-CD	5.92	122.67	112.60
1	D	254	GLU	CB-CG-CD	5.92	122.66	112.60
1	B	254	GLU	CB-CG-CD	5.92	122.66	112.60
1	E	254	GLU	CB-CG-CD	5.91	122.65	112.60

There are no chirality outliers.

There are no planarity outliers.

## 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	3704	0	3760	43	0
1	B	3704	0	3760	42	0
1	C	3704	0	3760	40	0
1	D	3704	0	3760	43	0
1	E	3704	0	3760	42	0
1	F	3704	0	3760	46	0
1	G	3704	0	3760	40	0
1	H	3704	0	3760	42	0
1	I	102	0	99	1	0
1	J	102	0	99	0	0
1	K	102	0	99	1	0
1	L	102	0	99	1	0
1	M	102	0	99	1	0
1	N	102	0	99	1	0
1	O	102	0	99	2	0
1	P	102	0	99	1	0
2	A	23	0	11	1	0
2	B	23	0	11	1	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
2	E	23	0	11	1	0
2	F	23	0	11	2	0
2	G	23	0	11	1	0
2	H	23	0	11	1	0
3	A	64	0	23	3	0
3	B	64	0	23	4	0
3	C	64	0	23	3	0
3	D	64	0	23	3	0
3	E	64	0	23	3	0
3	F	64	0	23	4	0
3	G	64	0	23	3	0
3	H	64	0	23	3	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
4	C	31	0	12	1	0
4	D	31	0	12	1	0
4	E	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	31	0	12	2	0
4	G	31	0	12	1	0
4	H	31	0	12	1	0
All	All	31392	0	31240	310	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 5.

The worst 5 of 310 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASN:HB2	1:A:414:MET:HE1	1.77	0.66
1:E:94:ASN:HB2	1:E:414:MET:HE1	1.77	0.66
1:B:94:ASN:HB2	1:B:414:MET:HE1	1.77	0.66
1:F:94:ASN:HB2	1:F:414:MET:HE1	1.77	0.66
1:H:94:ASN:HB2	1:H:414:MET:HE1	1.77	0.66

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	483/519 (93%)	459 (95%)	24 (5%)	0	100	100
1	B	483/519 (93%)	459 (95%)	24 (5%)	0	100	100
1	C	483/519 (93%)	459 (95%)	24 (5%)	0	100	100
1	D	483/519 (93%)	459 (95%)	24 (5%)	0	100	100
1	E	483/519 (93%)	459 (95%)	24 (5%)	0	100	100
1	F	483/519 (93%)	459 (95%)	24 (5%)	0	100	100
1	G	483/519 (93%)	459 (95%)	24 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	483/519 (93%)	459 (95%)	24 (5%)	0	100	100
1	I	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	J	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	K	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	L	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	M	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	N	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	O	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	P	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
All	All	3960/8304 (48%)	3728 (94%)	232 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	397/425 (93%)	388 (98%)	9 (2%)	45	70
1	B	397/425 (93%)	388 (98%)	9 (2%)	45	70
1	C	397/425 (93%)	388 (98%)	9 (2%)	45	70
1	D	397/425 (93%)	388 (98%)	9 (2%)	45	70
1	E	397/425 (93%)	388 (98%)	9 (2%)	45	70
1	F	397/425 (93%)	388 (98%)	9 (2%)	45	70
1	G	397/425 (93%)	388 (98%)	9 (2%)	45	70
1	H	397/425 (93%)	388 (98%)	9 (2%)	45	70
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	11 (100%)	0	100	100
All	All	3264/6800 (48%)	3192 (98%)	72 (2%)	47	71

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	228	LYS
1	H	438	LYS
1	G	254	GLU
1	H	225	THR
1	C	330	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	253	HIS
1	H	498	GLN
1	F	253	HIS
1	H	454	HIS
1	H	253	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	A	603	-	29,34,34	4.30	17 (58%)	35,54,54	1.39	6 (17%)
4	ATP	B	604	-	28,33,33	0.92	0	34,52,52	1.19	2 (5%)
4	ATP	E	604	-	28,33,33	0.92	0	34,52,52	1.19	2 (5%)
3	GTP	B	602	-	29,34,34	4.29	17 (58%)	35,54,54	1.52	6 (17%)
3	GTP	H	602	-	29,34,34	4.30	17 (58%)	35,54,54	1.53	6 (17%)
3	GTP	C	602	-	29,34,34	4.29	17 (58%)	35,54,54	1.53	6 (17%)
4	ATP	D	604	-	28,33,33	0.93	0	34,52,52	1.20	2 (5%)
3	GTP	F	602	-	29,34,34	4.29	17 (58%)	35,54,54	1.52	6 (17%)
2	IMP	C	601	-	21,25,25	2.88	7 (33%)	22,38,38	1.58	6 (27%)
4	ATP	A	604	-	28,33,33	0.91	0	34,52,52	1.20	2 (5%)
3	GTP	H	603	-	29,34,34	4.30	17 (58%)	35,54,54	1.38	5 (14%)
4	ATP	F	604	-	28,33,33	0.92	0	34,52,52	1.19	2 (5%)
3	GTP	E	603	-	29,34,34	4.29	17 (58%)	35,54,54	1.39	5 (14%)
2	IMP	D	601	-	21,25,25	2.88	7 (33%)	22,38,38	1.59	6 (27%)
2	IMP	E	601	-	21,25,25	2.87	7 (33%)	22,38,38	1.53	5 (22%)
2	IMP	H	601	-	21,25,25	2.87	7 (33%)	22,38,38	1.52	5 (22%)
3	GTP	A	602	-	29,34,34	4.30	17 (58%)	35,54,54	1.53	6 (17%)
3	GTP	D	603	-	29,34,34	4.30	17 (58%)	35,54,54	1.39	5 (14%)
4	ATP	C	604	-	28,33,33	0.92	0	34,52,52	1.19	2 (5%)
2	IMP	G	601	-	21,25,25	2.87	7 (33%)	22,38,38	1.54	5 (22%)
3	GTP	F	603	-	29,34,34	4.30	17 (58%)	35,54,54	1.39	5 (14%)
4	ATP	H	604	-	28,33,33	0.92	0	34,52,52	1.20	2 (5%)
3	GTP	B	603	-	29,34,34	4.30	17 (58%)	35,54,54	1.39	5 (14%)
4	ATP	G	604	-	28,33,33	0.92	0	34,52,52	1.20	2 (5%)
2	IMP	B	601	-	21,25,25	2.86	7 (33%)	22,38,38	1.60	6 (27%)
2	IMP	F	601	-	21,25,25	2.87	7 (33%)	22,38,38	1.52	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	G	603	-	29,34,34	4.30	17 (58%)	35,54,54	1.38	5 (14%)
3	GTP	D	602	-	29,34,34	4.29	17 (58%)	35,54,54	1.53	6 (17%)
3	GTP	E	602	-	29,34,34	4.29	17 (58%)	35,54,54	1.53	6 (17%)
2	IMP	A	601	-	21,25,25	2.86	7 (33%)	22,38,38	1.60	6 (27%)
3	GTP	C	603	-	29,34,34	4.30	17 (58%)	35,54,54	1.39	5 (14%)
3	GTP	G	602	-	29,34,34	4.30	17 (58%)	35,54,54	1.53	6 (17%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	G	604	-	-	7/18/38/38	0/3/3/3
2	IMP	B	601	-	-	5/6/26/26	0/3/3/3
2	IMP	F	601	-	-	5/6/26/26	0/3/3/3
3	GTP	G	603	-	-	4/18/38/38	0/3/3/3
3	GTP	D	602	-	-	8/18/38/38	0/3/3/3
3	GTP	E	602	-	-	8/18/38/38	0/3/3/3
2	IMP	A	601	-	-	5/6/26/26	0/3/3/3
3	GTP	C	603	-	-	4/18/38/38	0/3/3/3
3	GTP	G	602	-	-	8/18/38/38	0/3/3/3

The worst 5 of 328 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	GTP	C2'-C3'	-11.01	1.23	1.53
3	G	603	GTP	C2'-C3'	-11.01	1.23	1.53
3	C	603	GTP	C2'-C3'	-11.01	1.23	1.53
3	A	603	GTP	C2'-C3'	-11.00	1.23	1.53
3	D	603	GTP	C2'-C3'	-11.00	1.23	1.53

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	602	GTP	C4'-O4'-C1'	-4.39	105.90	109.92
3	E	602	GTP	C4'-O4'-C1'	-4.35	105.94	109.92
3	D	602	GTP	C4'-O4'-C1'	-4.34	105.95	109.92
3	H	602	GTP	C4'-O4'-C1'	-4.34	105.95	109.92
3	A	602	GTP	C4'-O4'-C1'	-4.34	105.95	109.92

There are no chirality outliers.

5 of 192 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	IMP	C5'-O5'-P-O1P
2	A	601	IMP	C5'-O5'-P-O2P
2	A	601	IMP	C5'-O5'-P-O3P
2	B	601	IMP	C5'-O5'-P-O1P
2	B	601	IMP	C5'-O5'-P-O2P

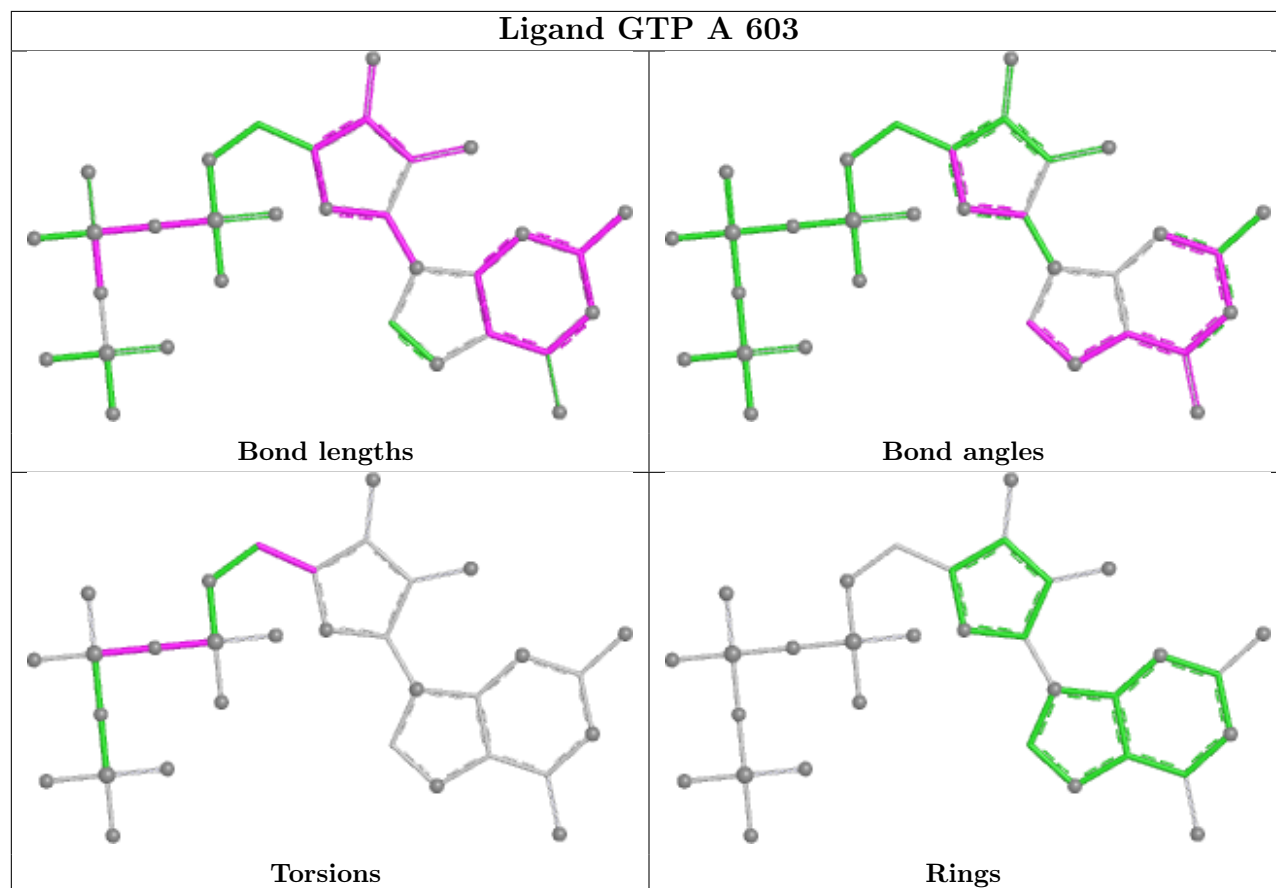
There are no ring outliers.

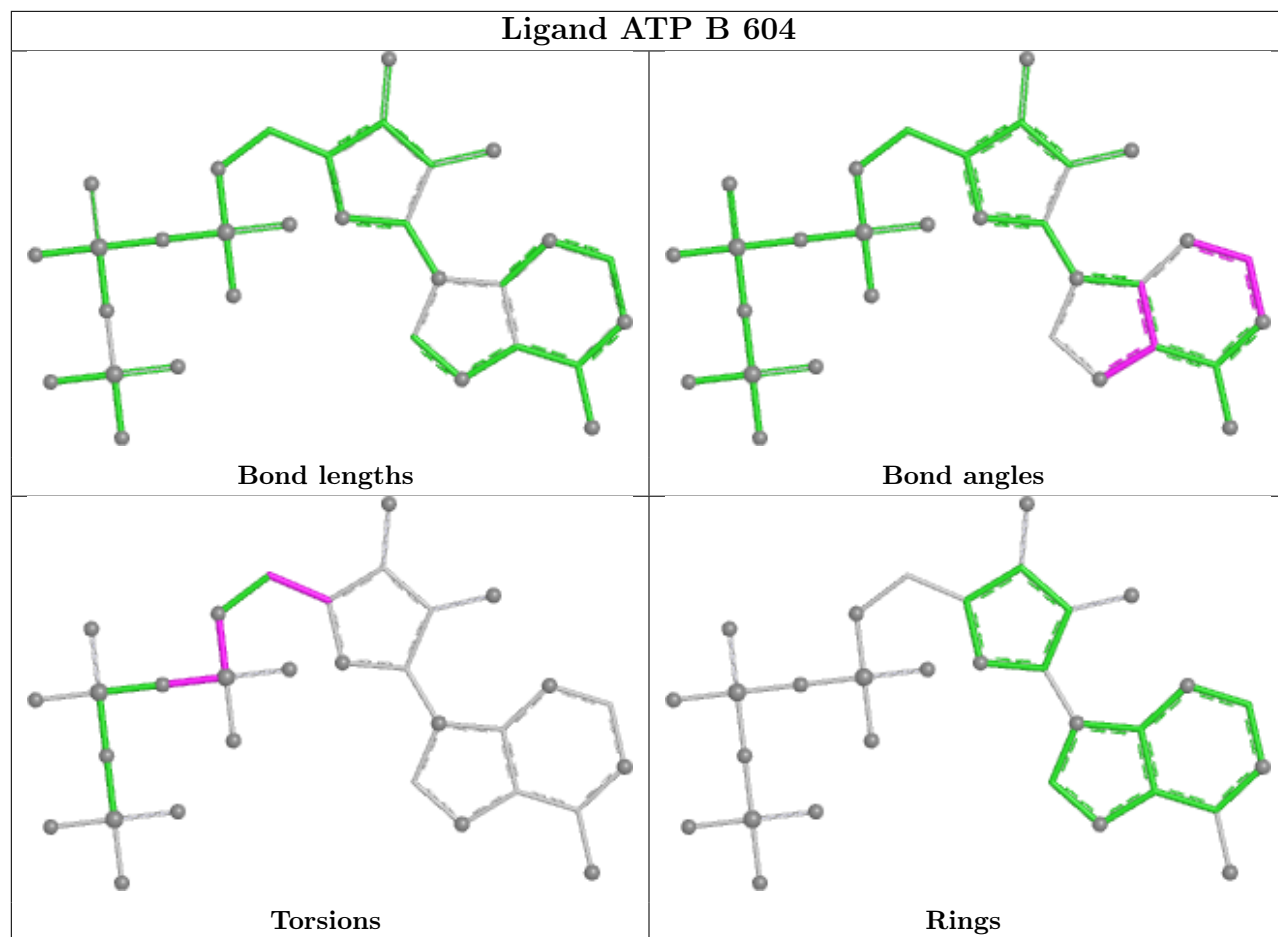
32 monomers are involved in 44 short contacts:

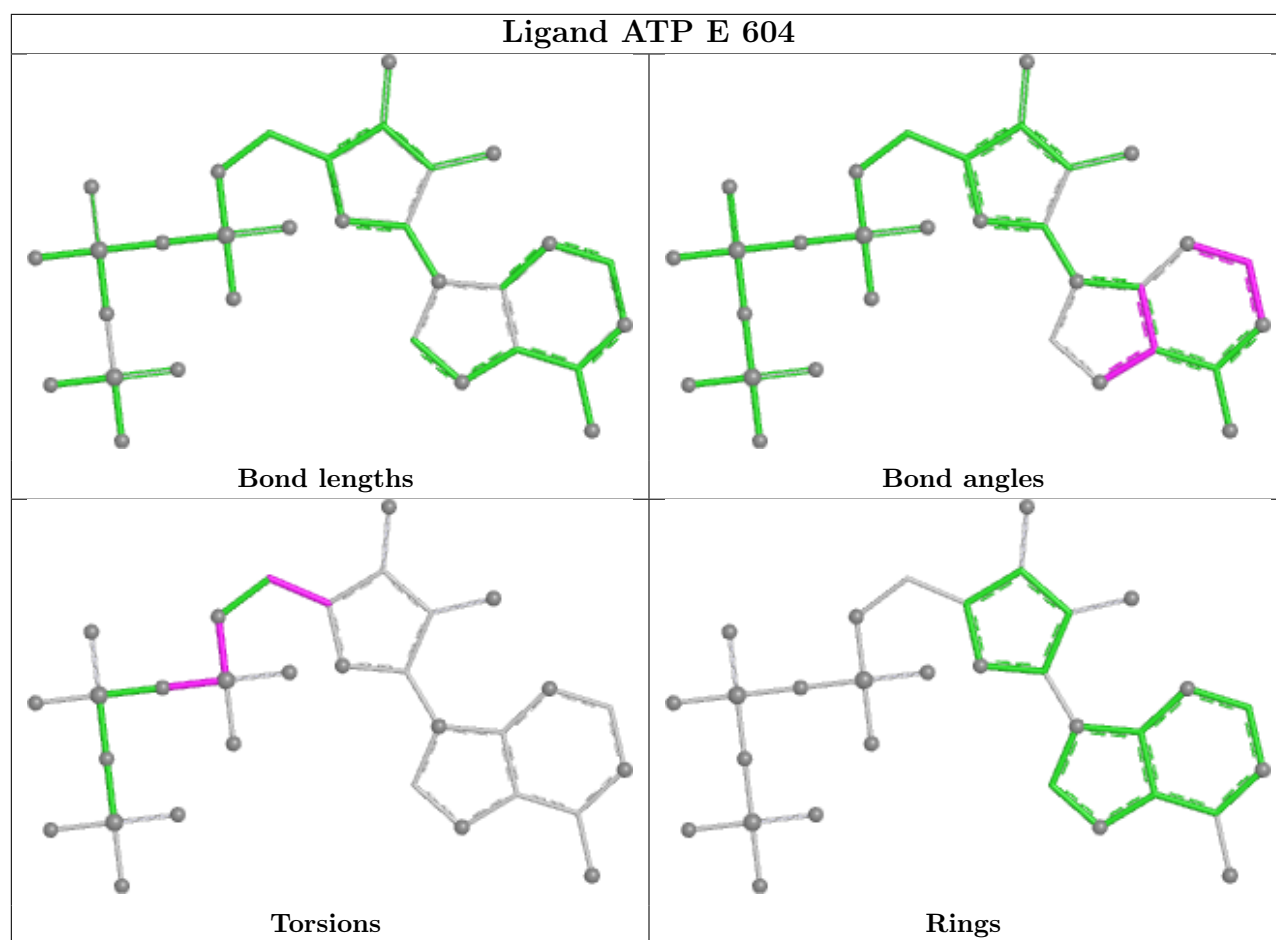
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	GTP	2	0
4	B	604	ATP	1	0
4	E	604	ATP	1	0
3	B	602	GTP	1	0
3	H	602	GTP	1	0
3	C	602	GTP	1	0
4	D	604	ATP	1	0
3	F	602	GTP	1	0
2	C	601	IMP	1	0
4	A	604	ATP	1	0
3	H	603	GTP	2	0
4	F	604	ATP	2	0
3	E	603	GTP	2	0
2	D	601	IMP	1	0
2	E	601	IMP	1	0
2	H	601	IMP	1	0
3	A	602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

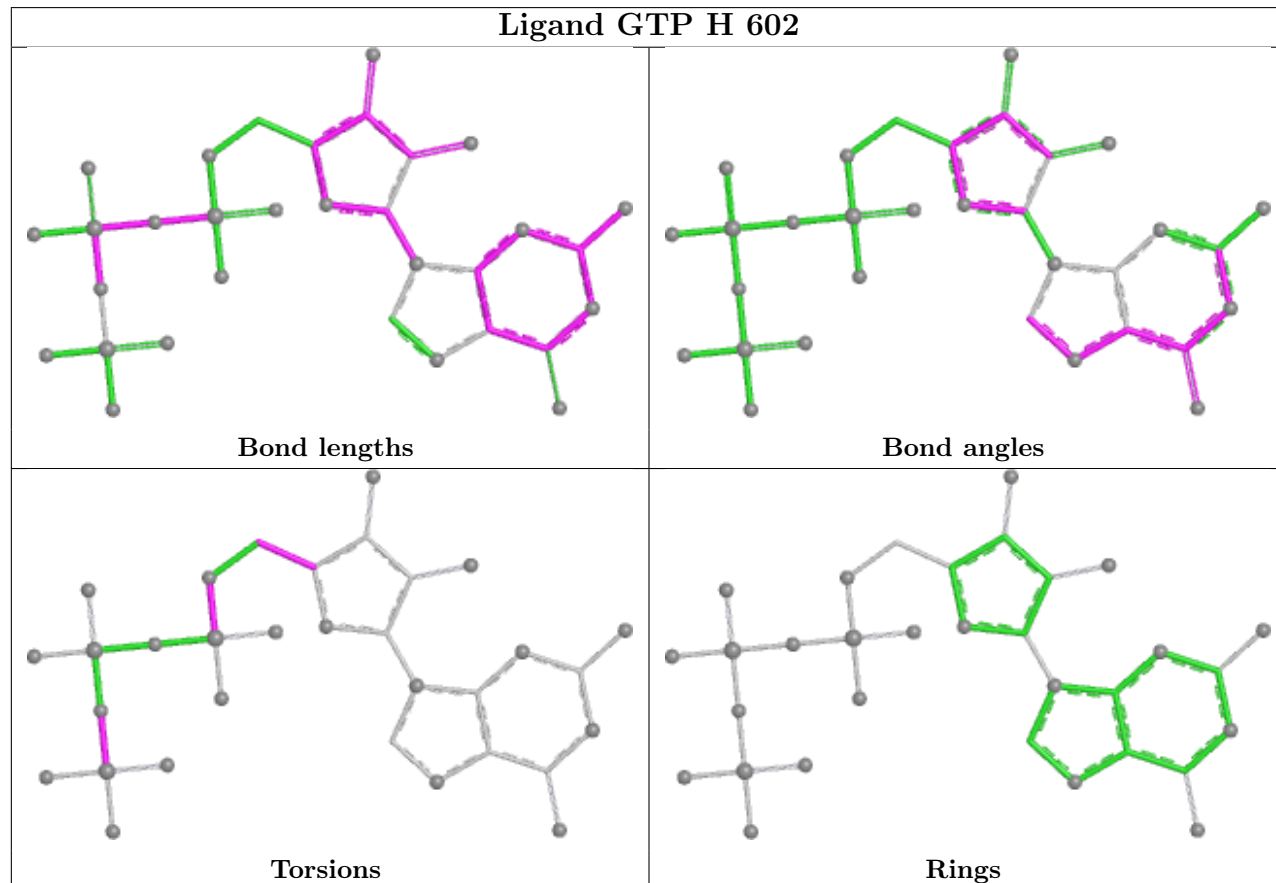
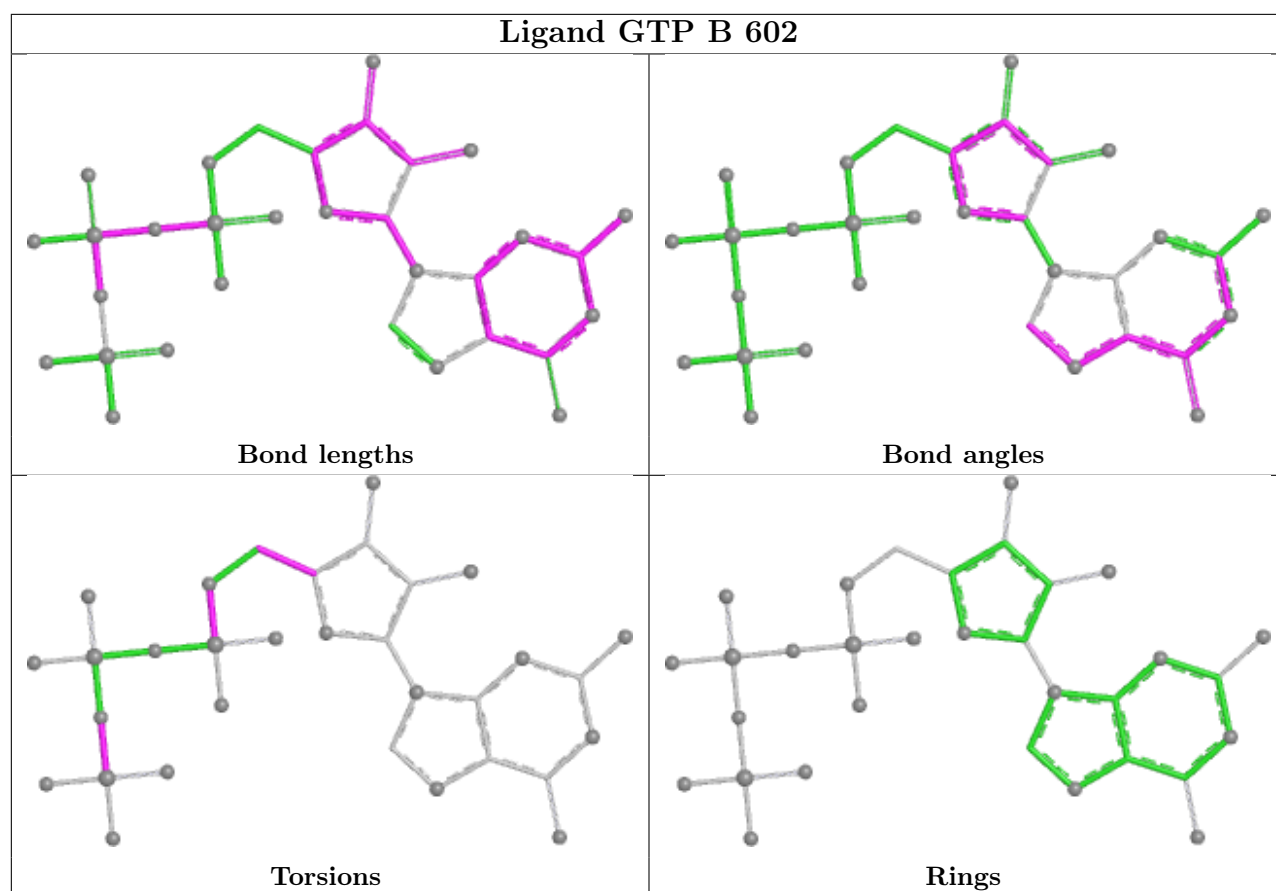
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

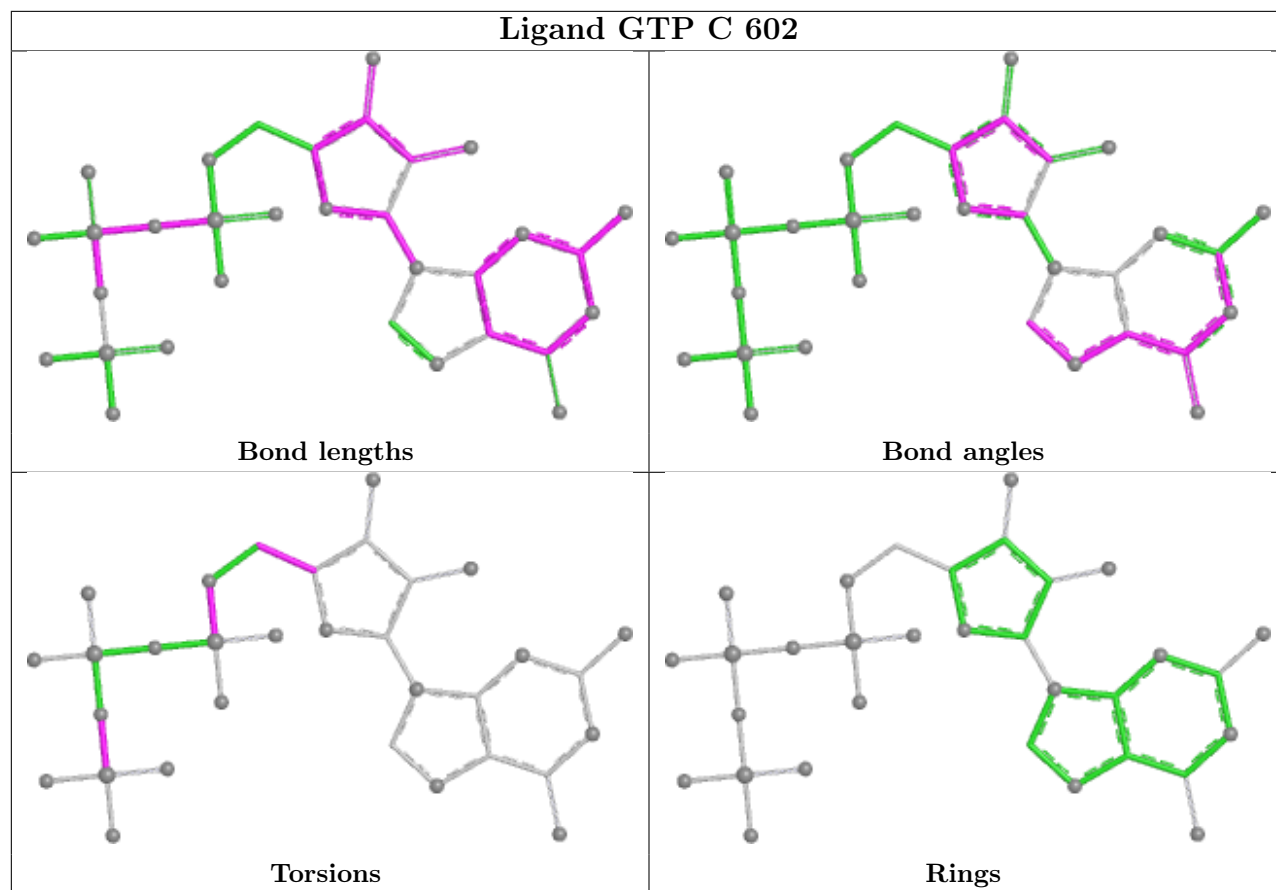
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

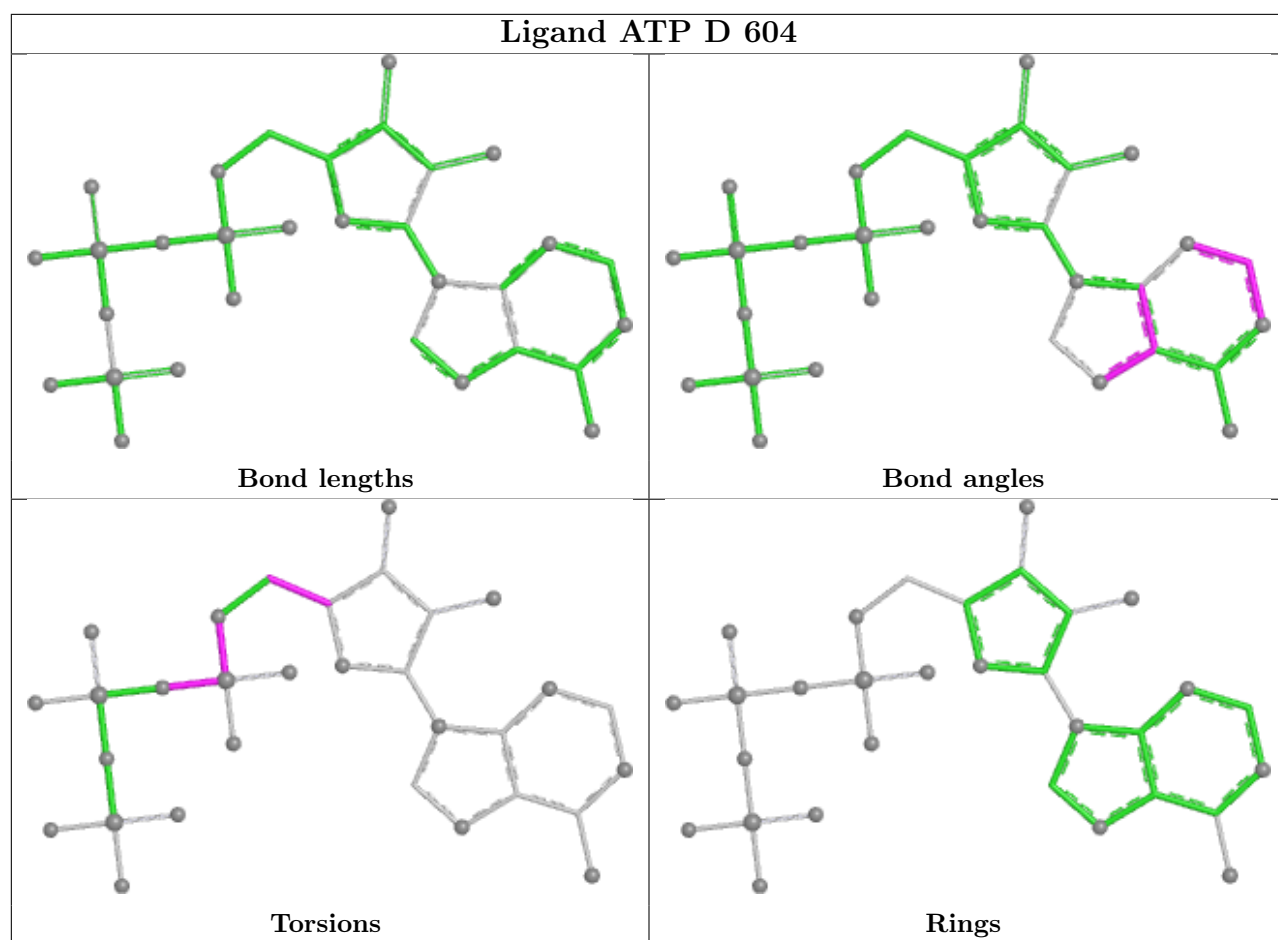






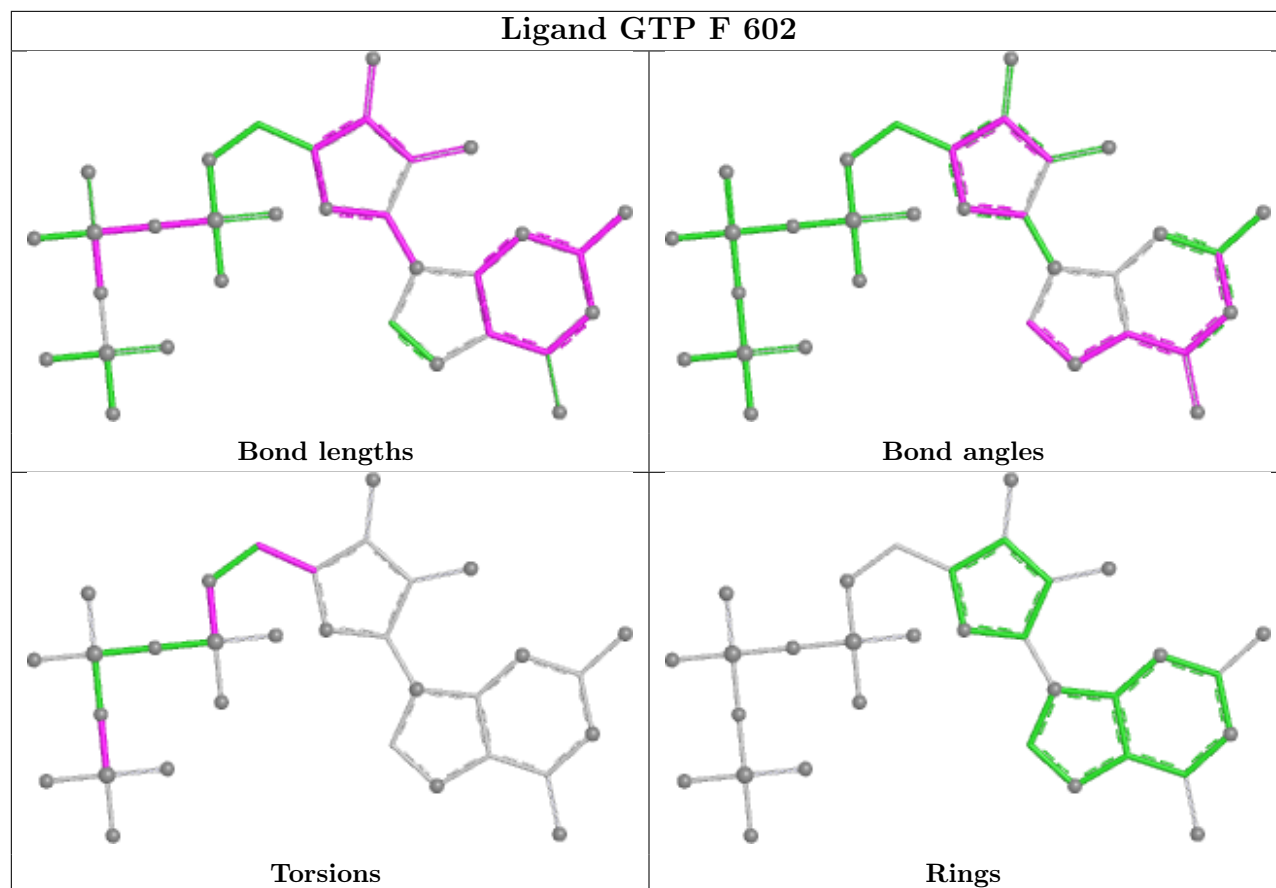




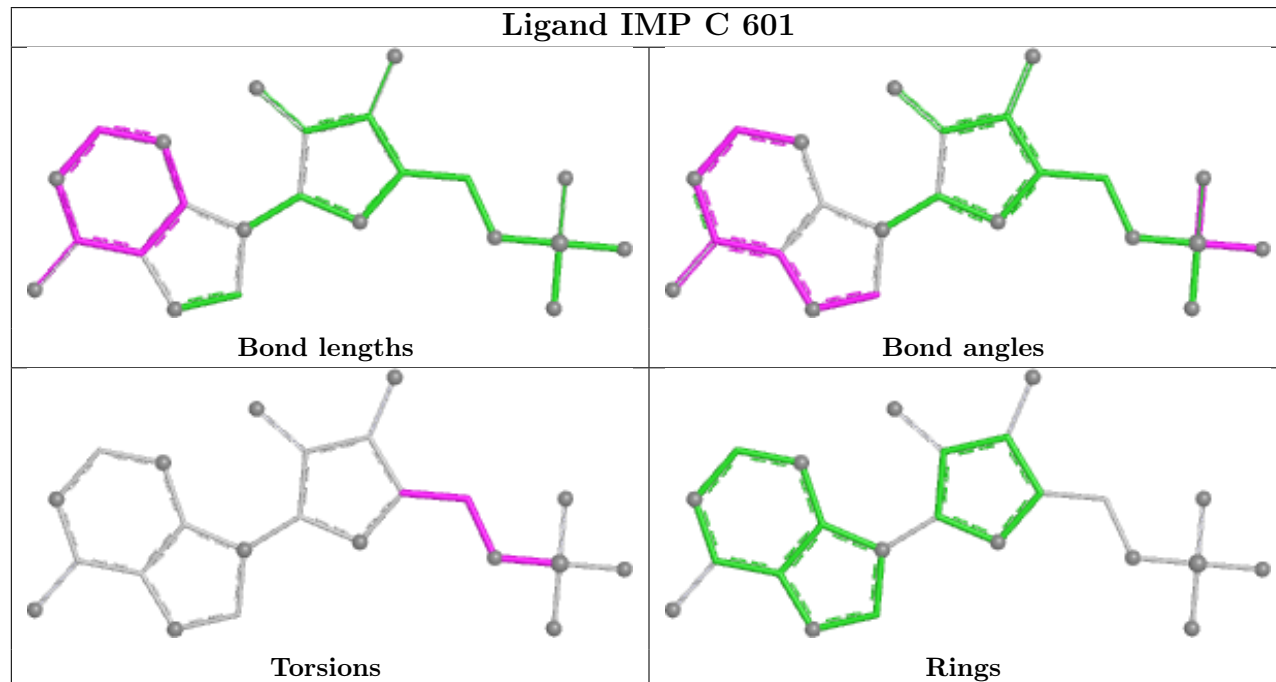


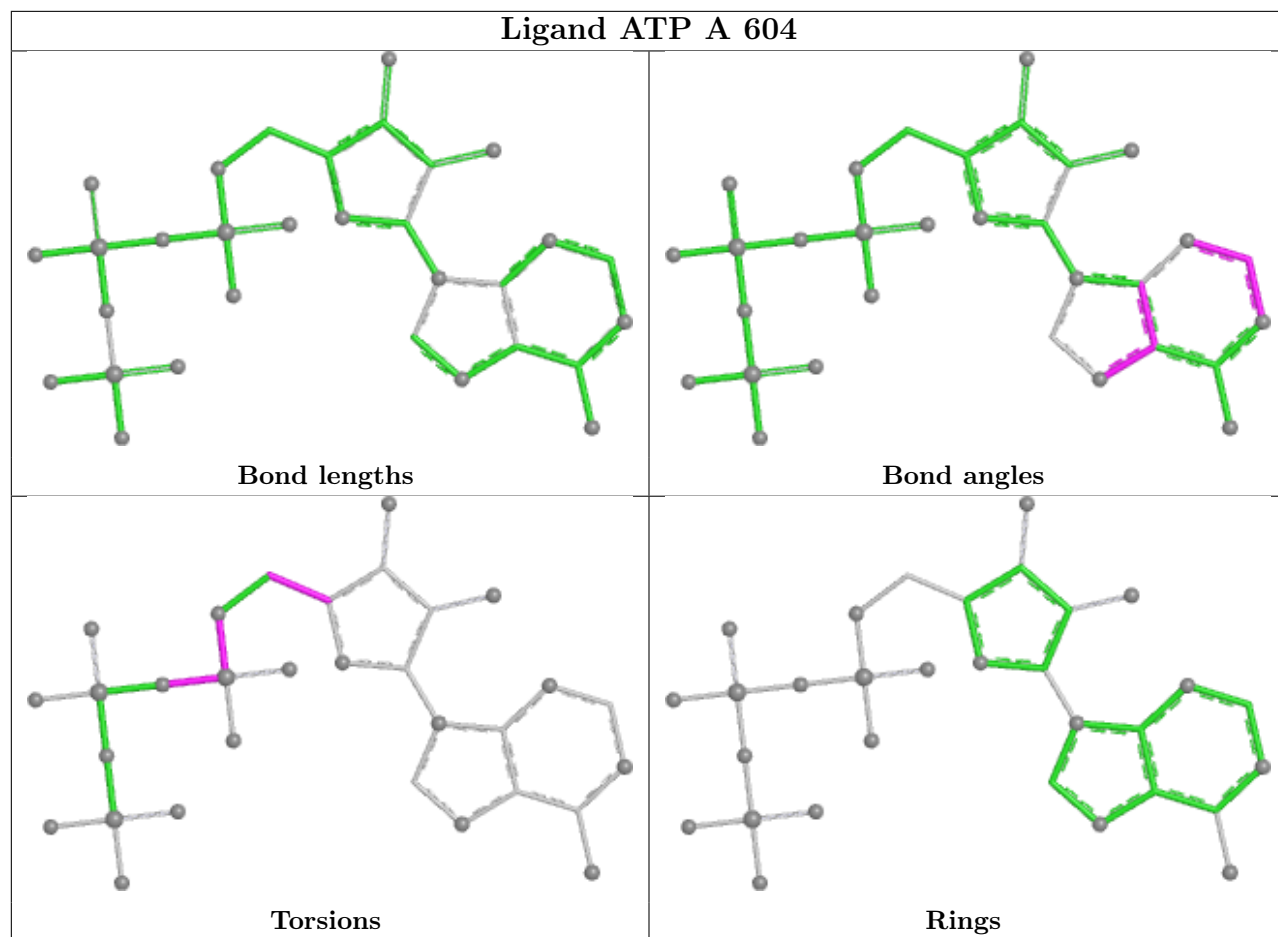


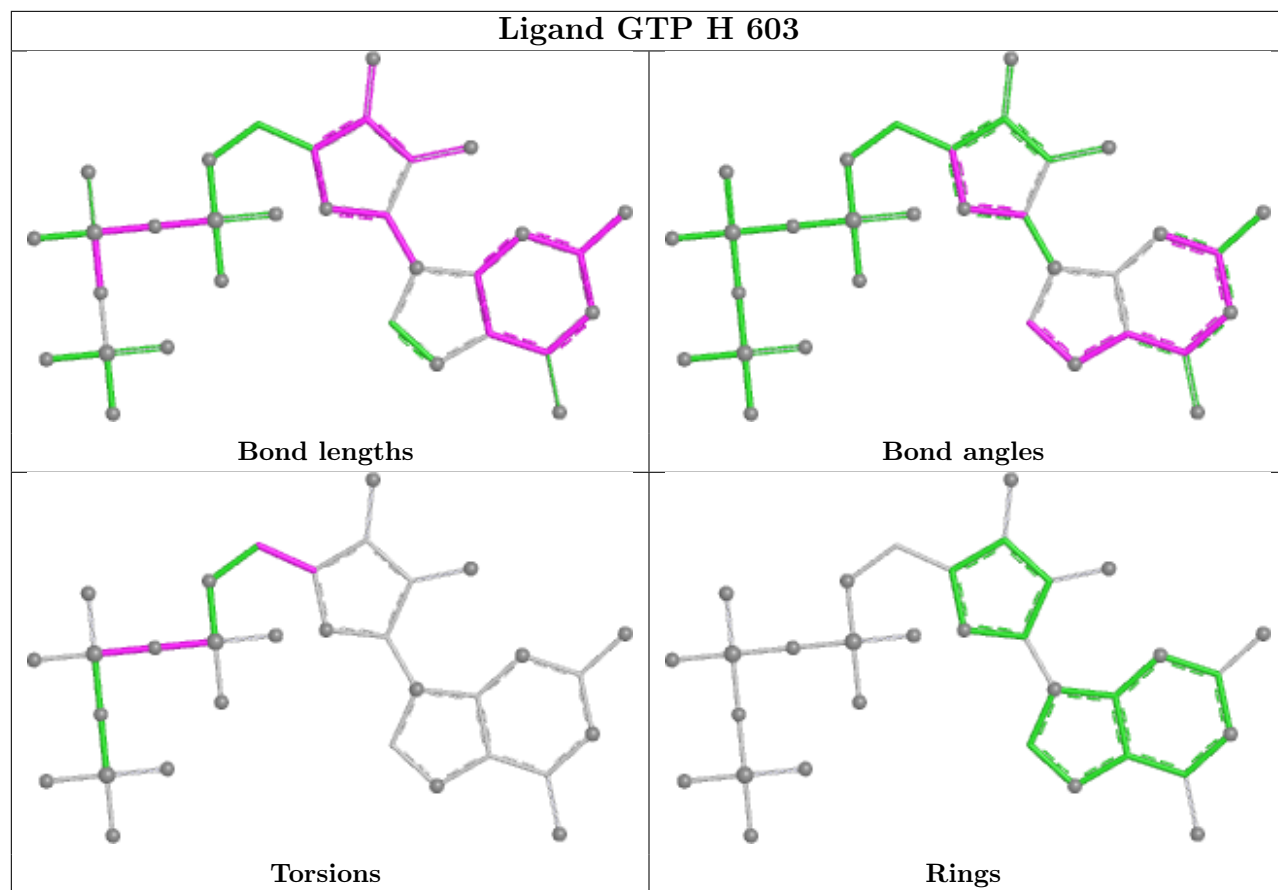
## Ligand GTP F 602

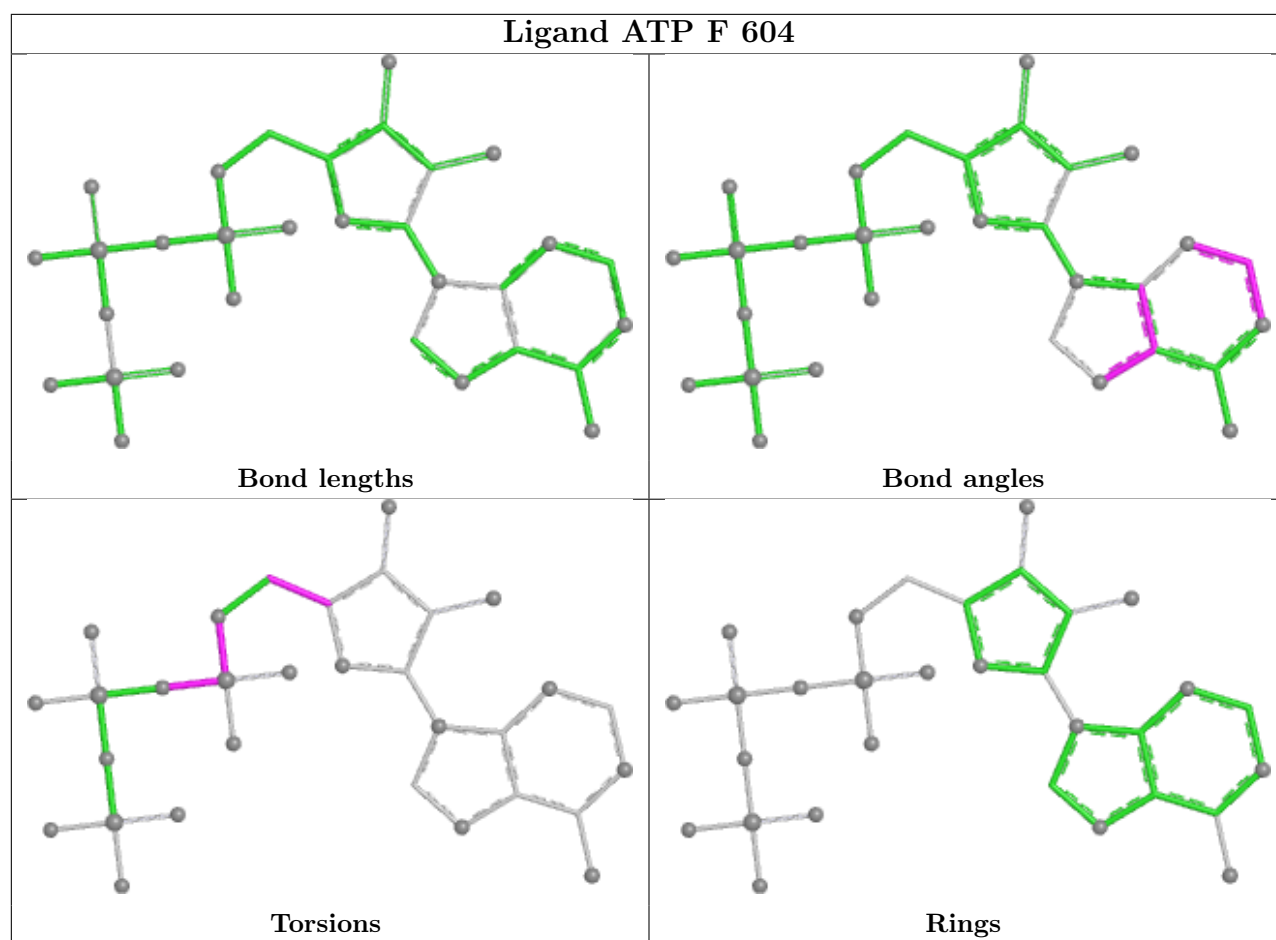


## Ligand IMP C 601

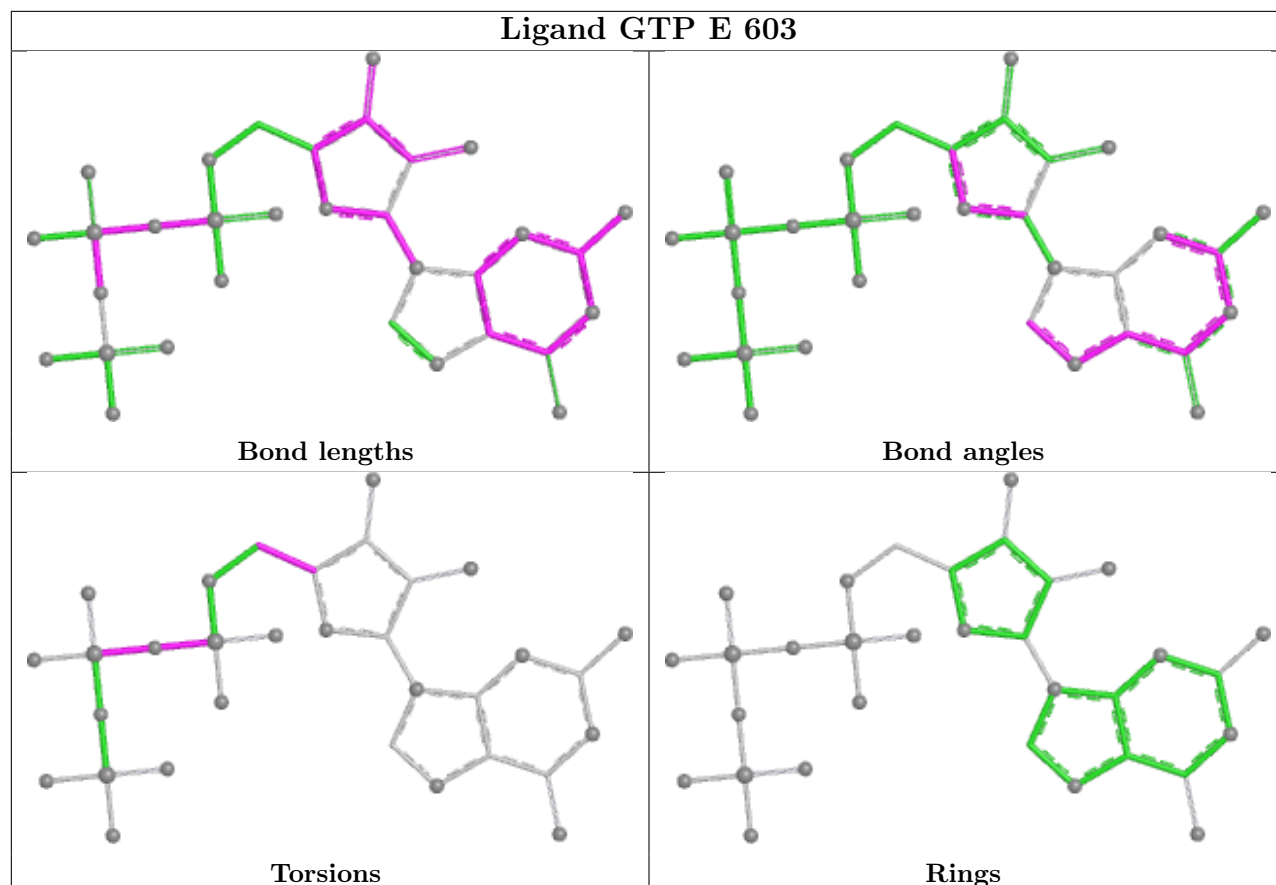




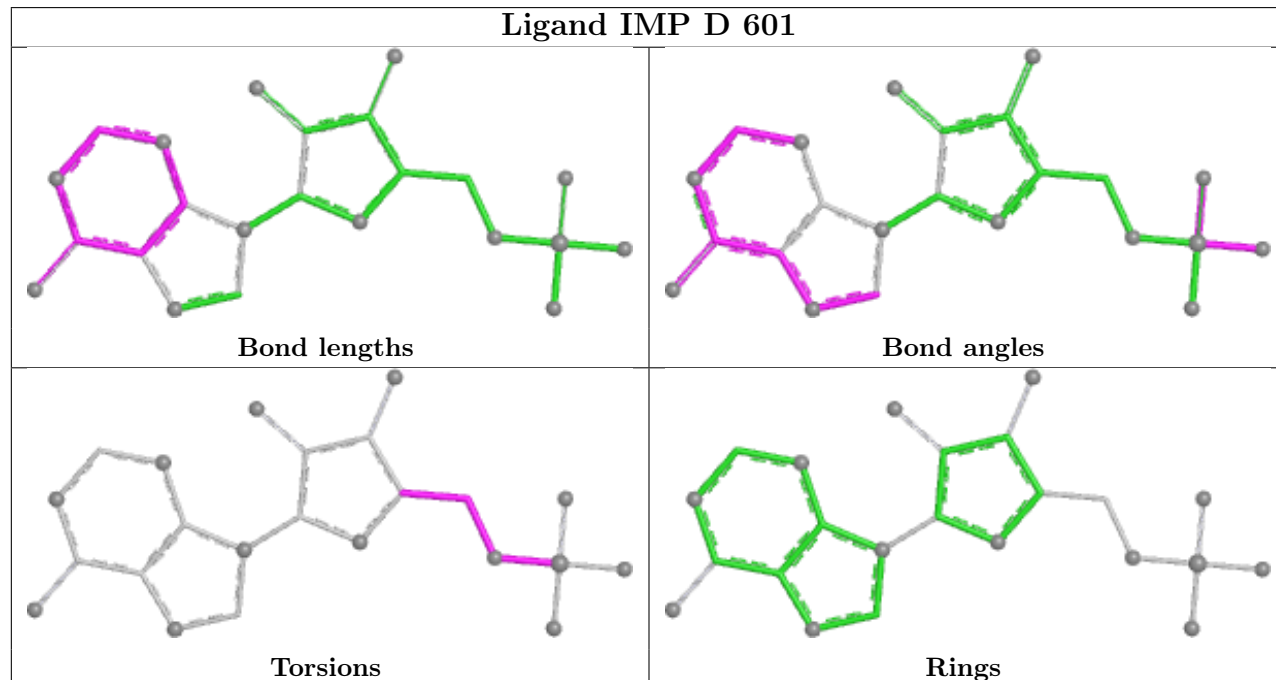




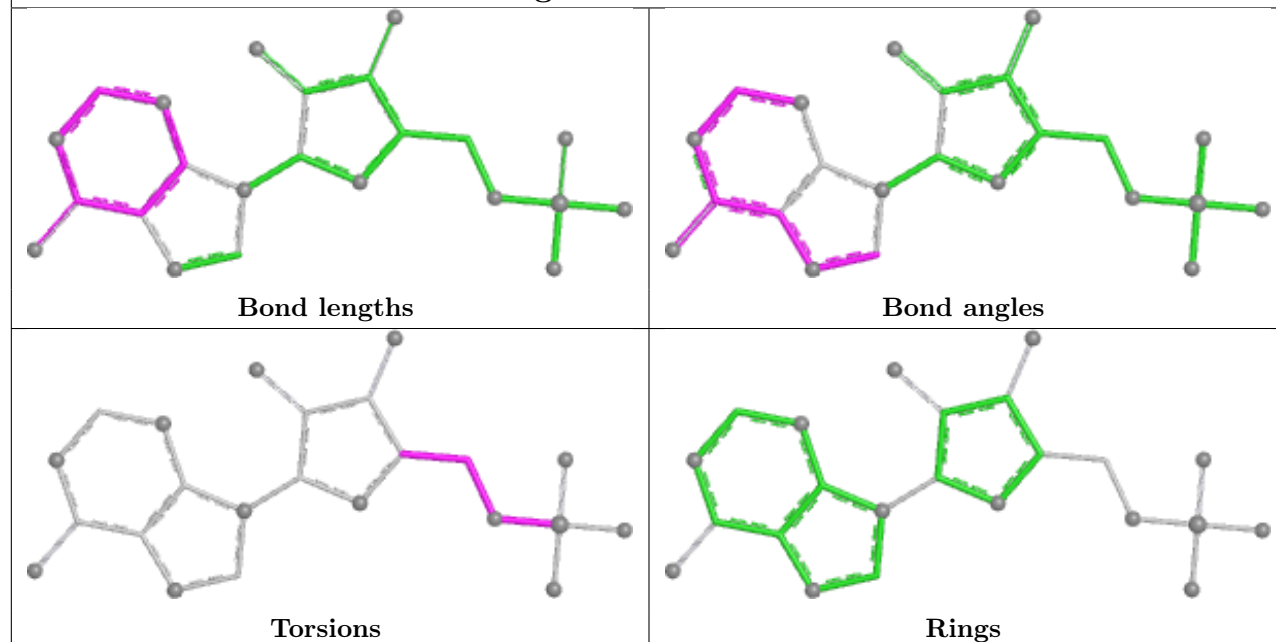
## Ligand GTP E 603



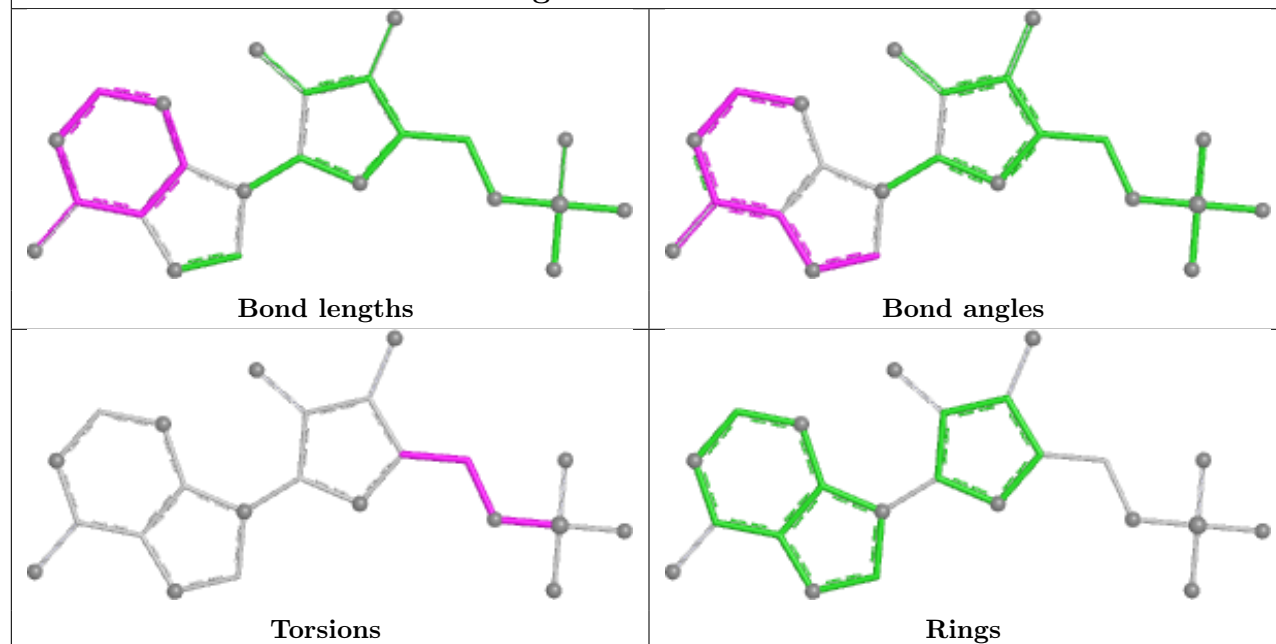
## Ligand IMP D 601

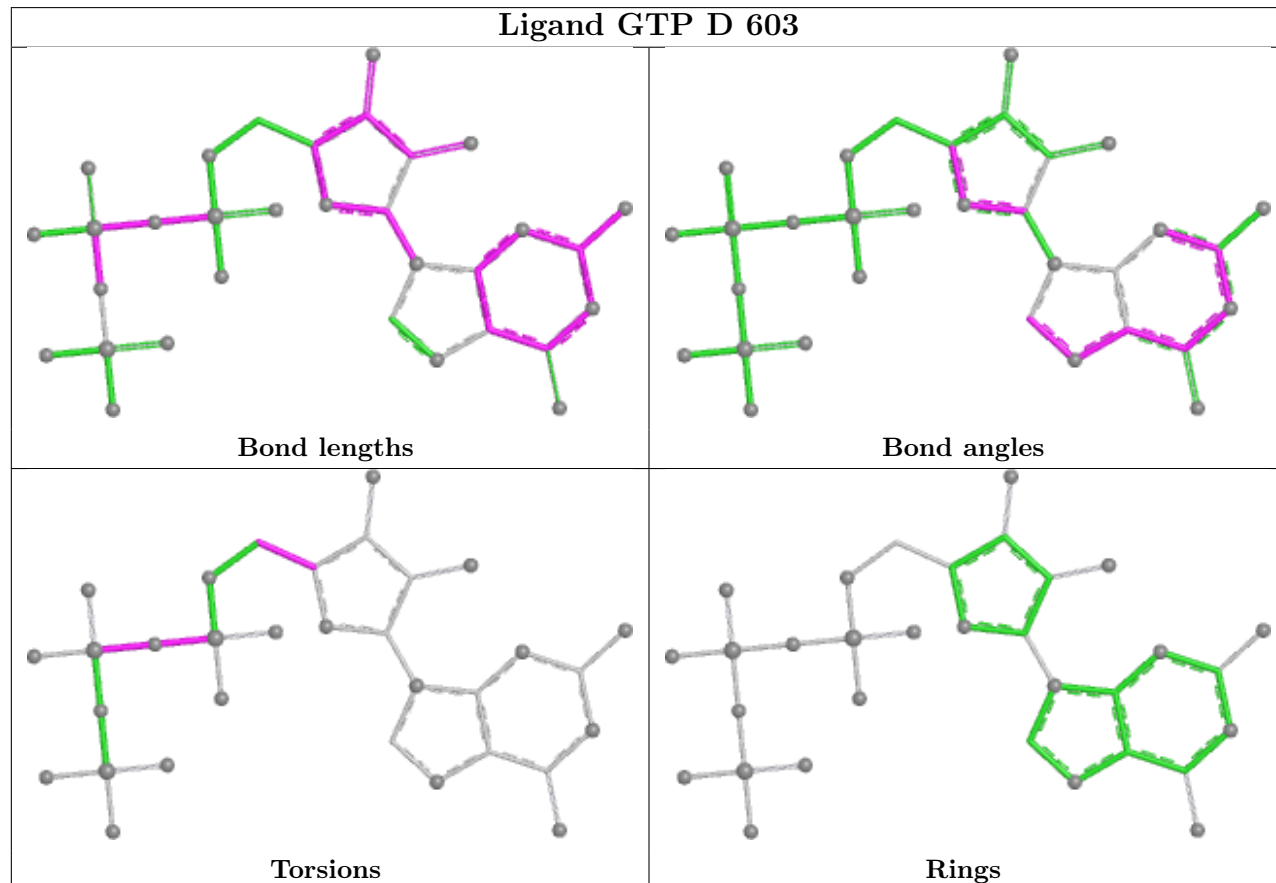
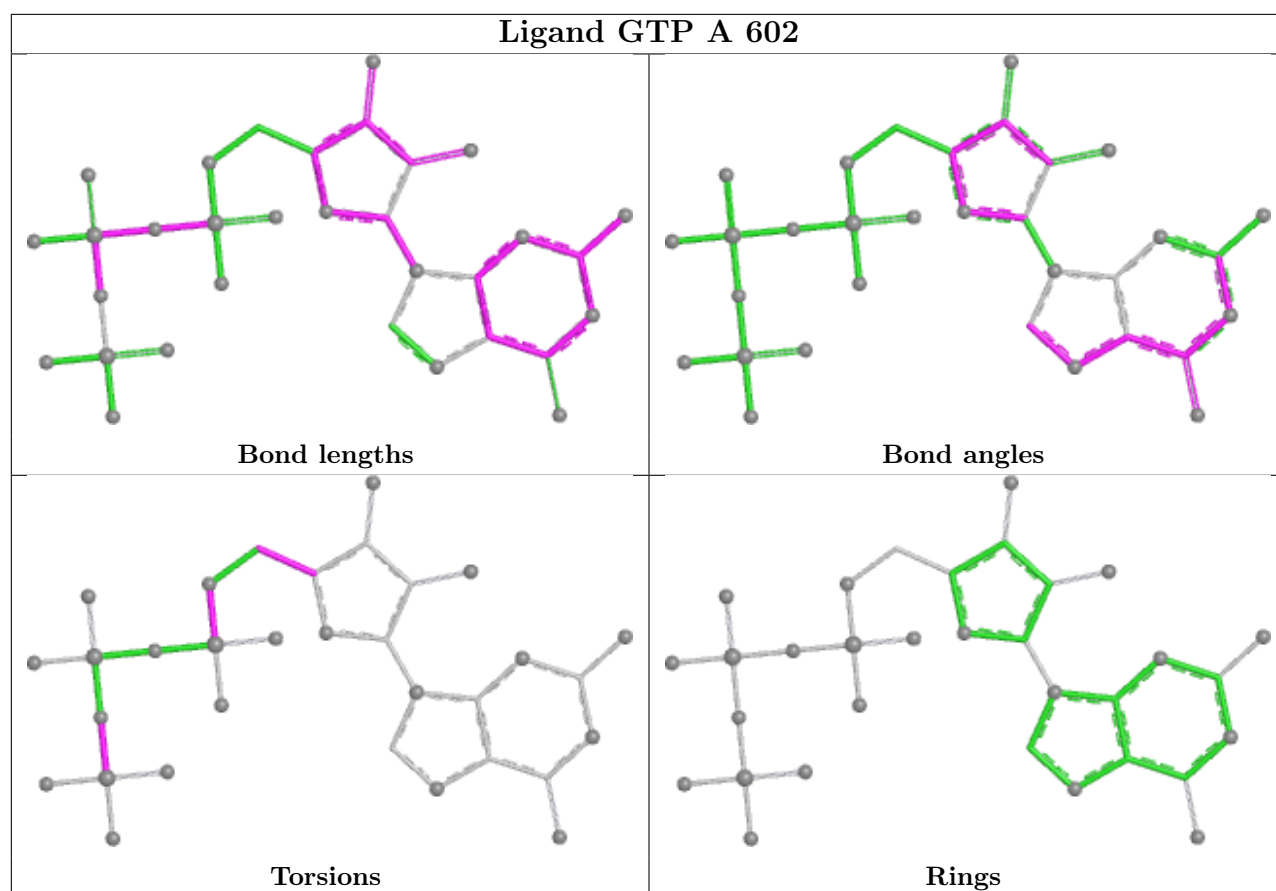


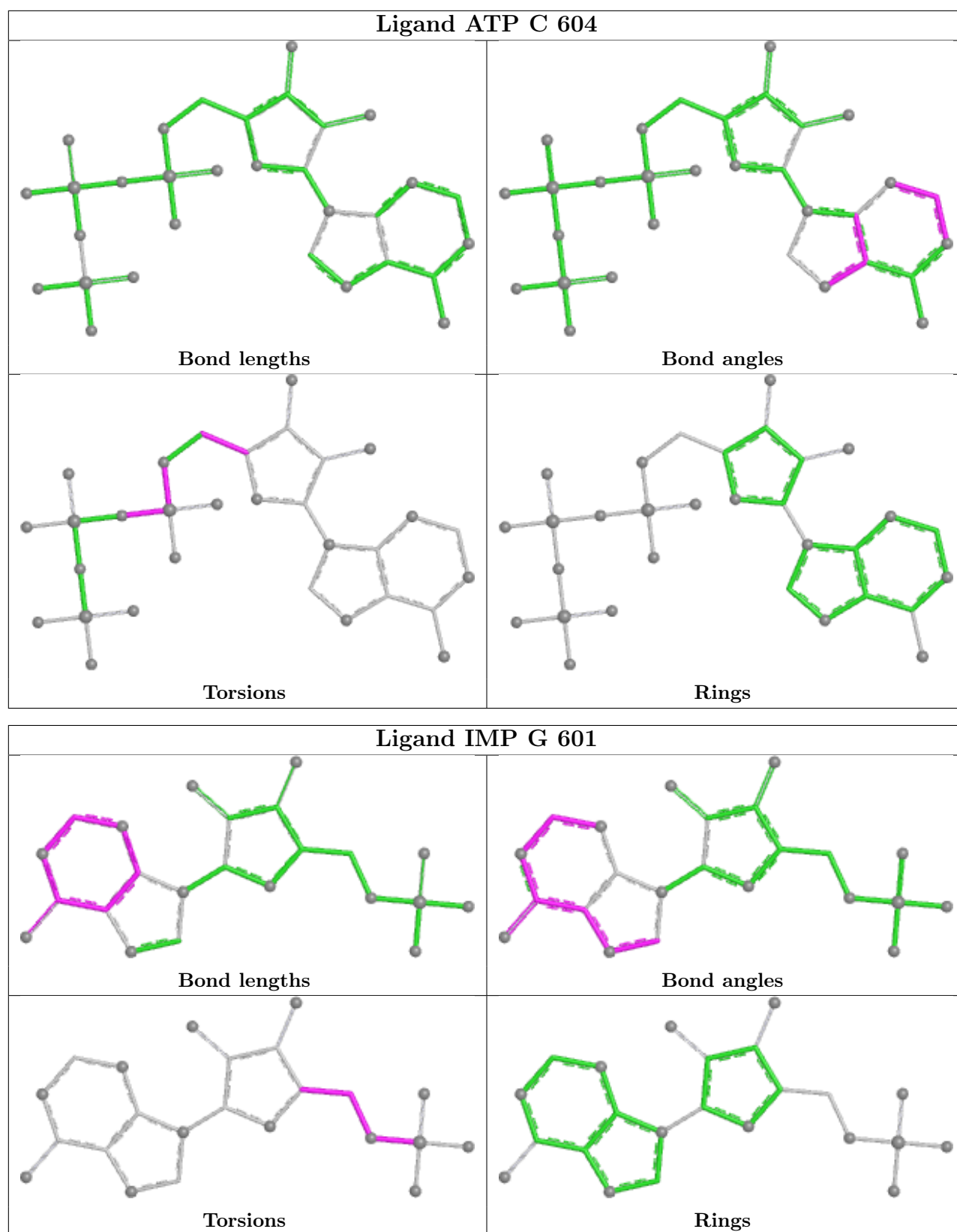
## Ligand IMP E 601



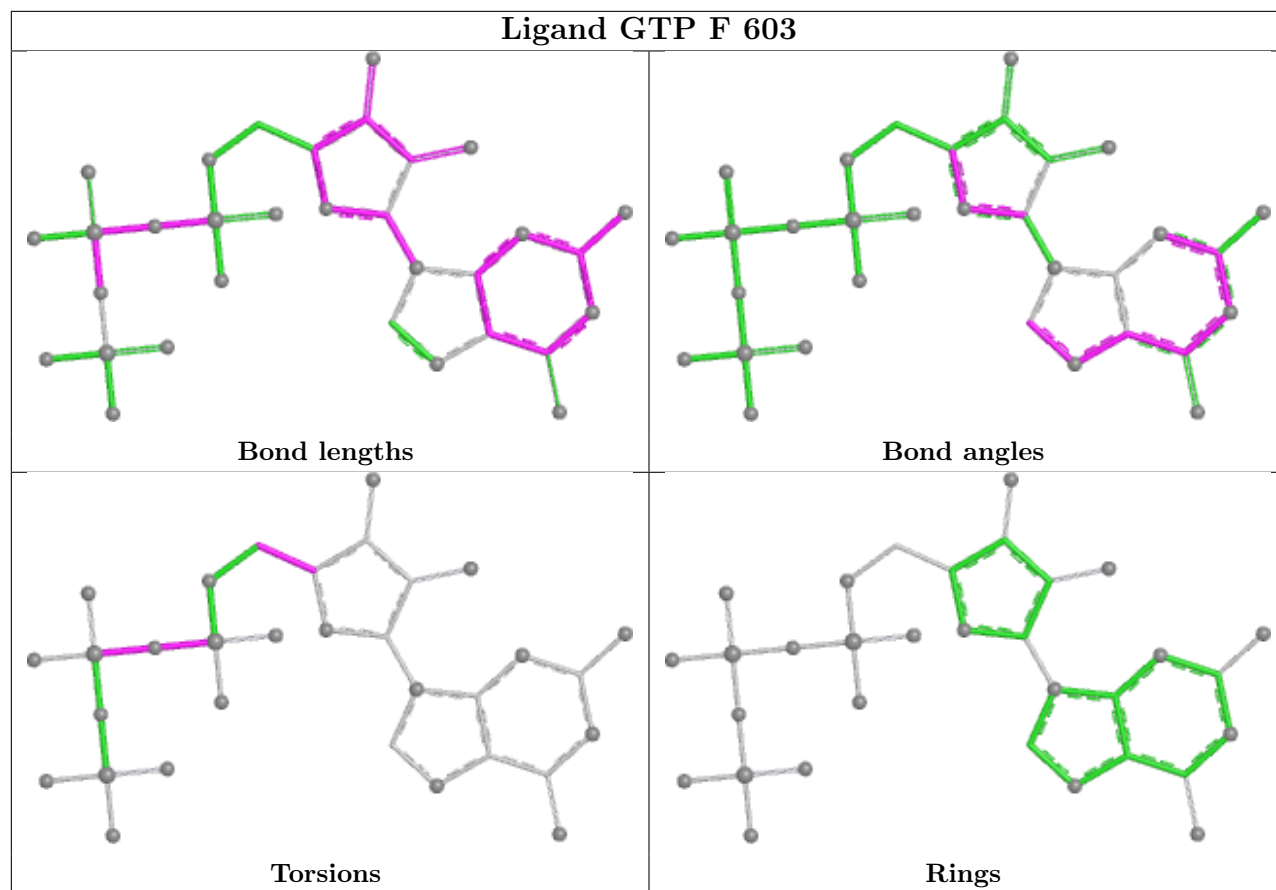
## Ligand IMP H 601

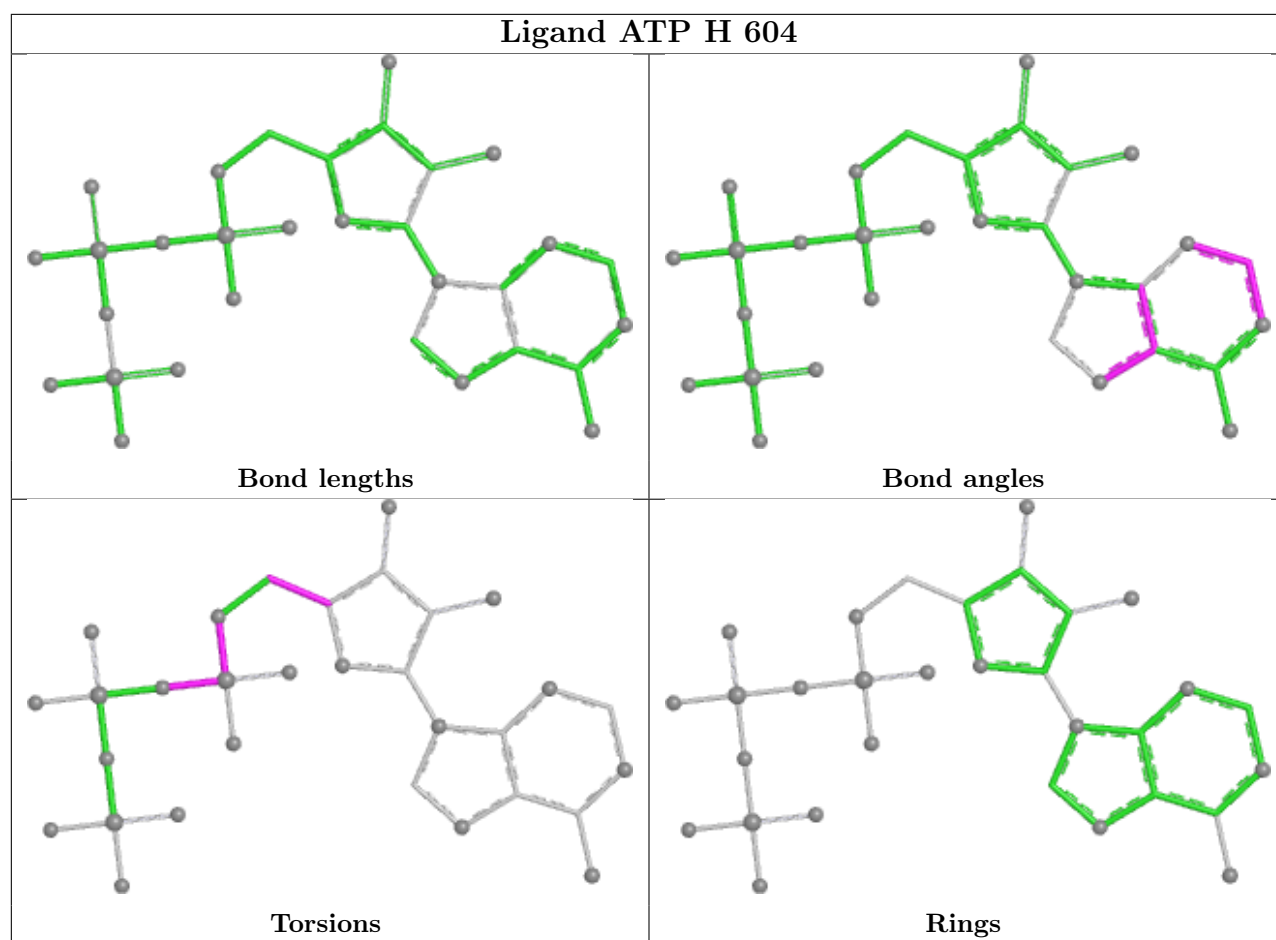


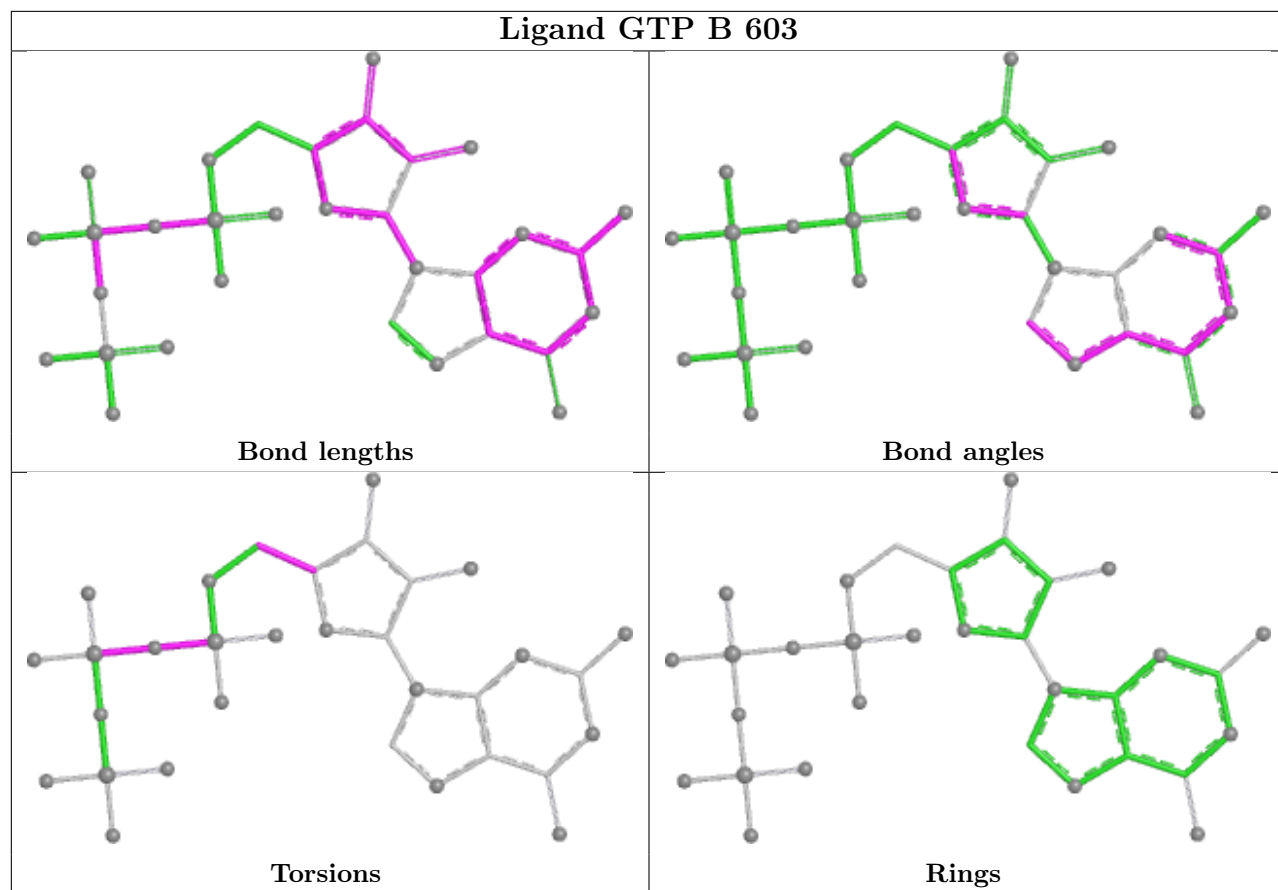


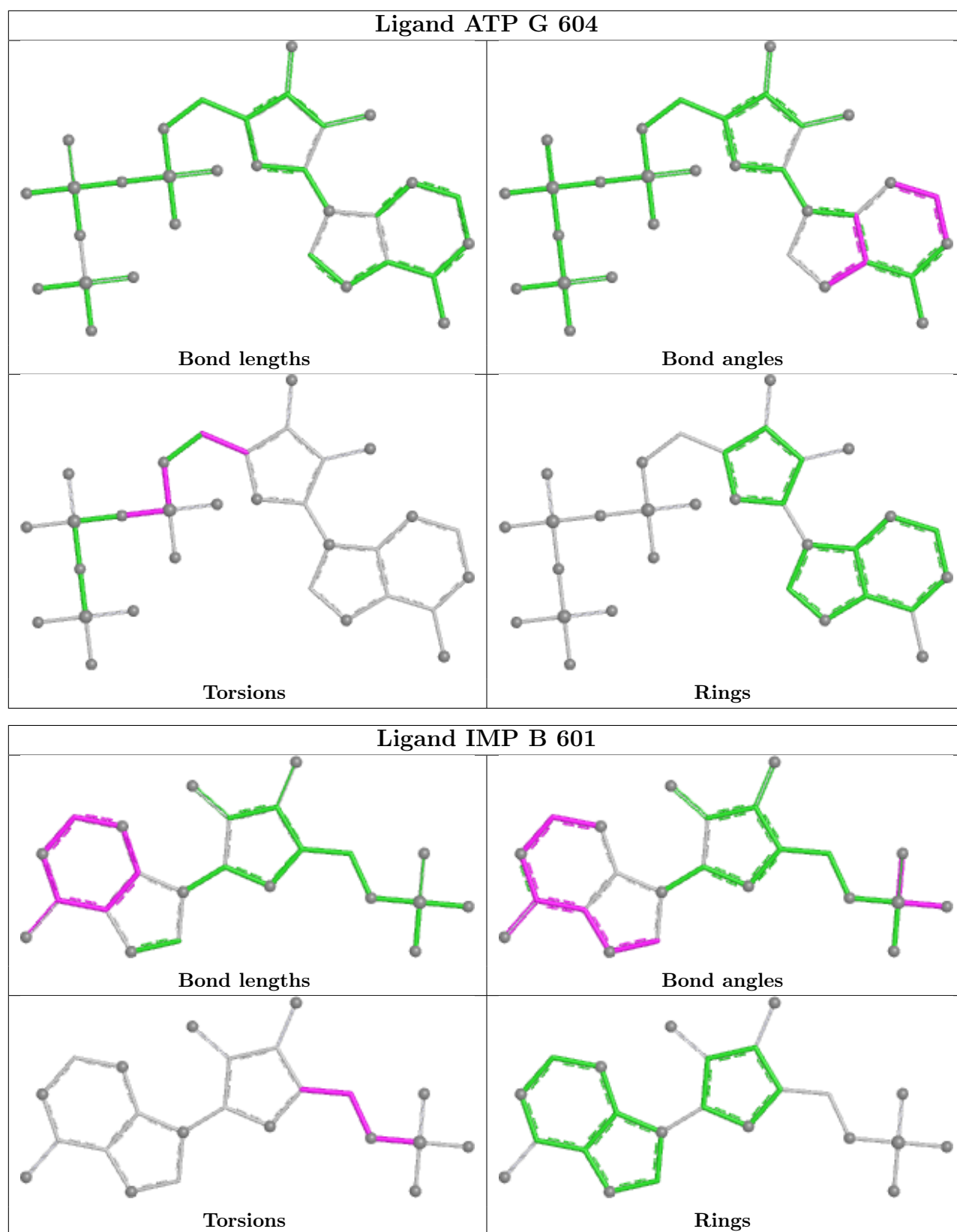




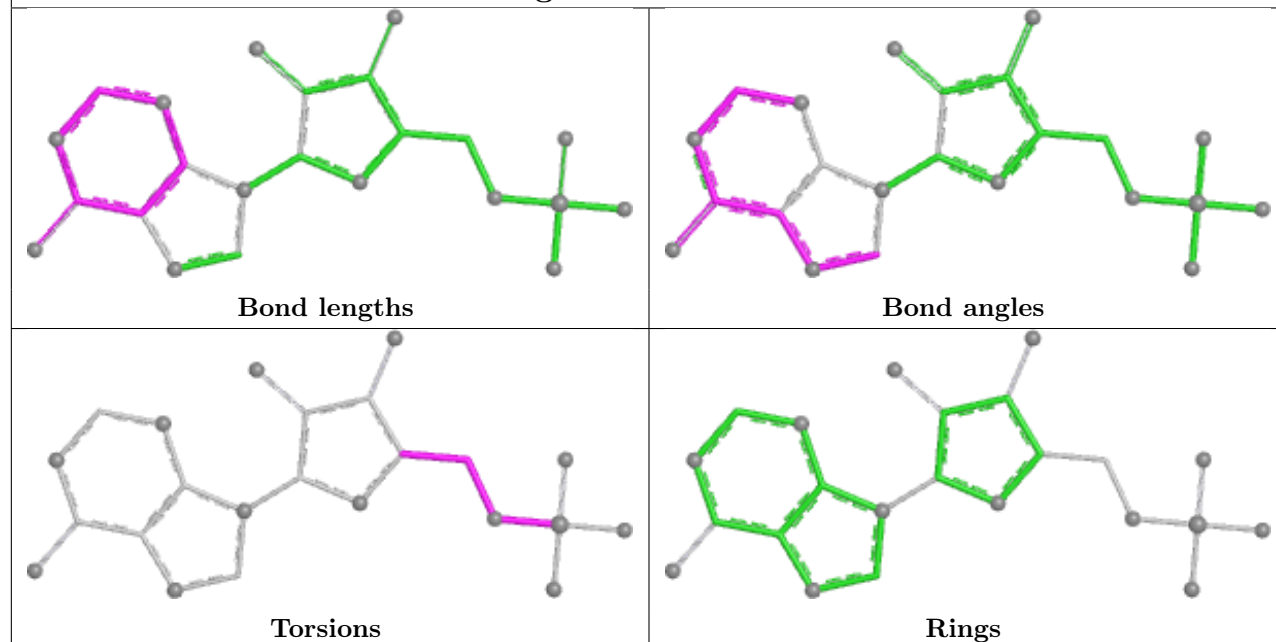




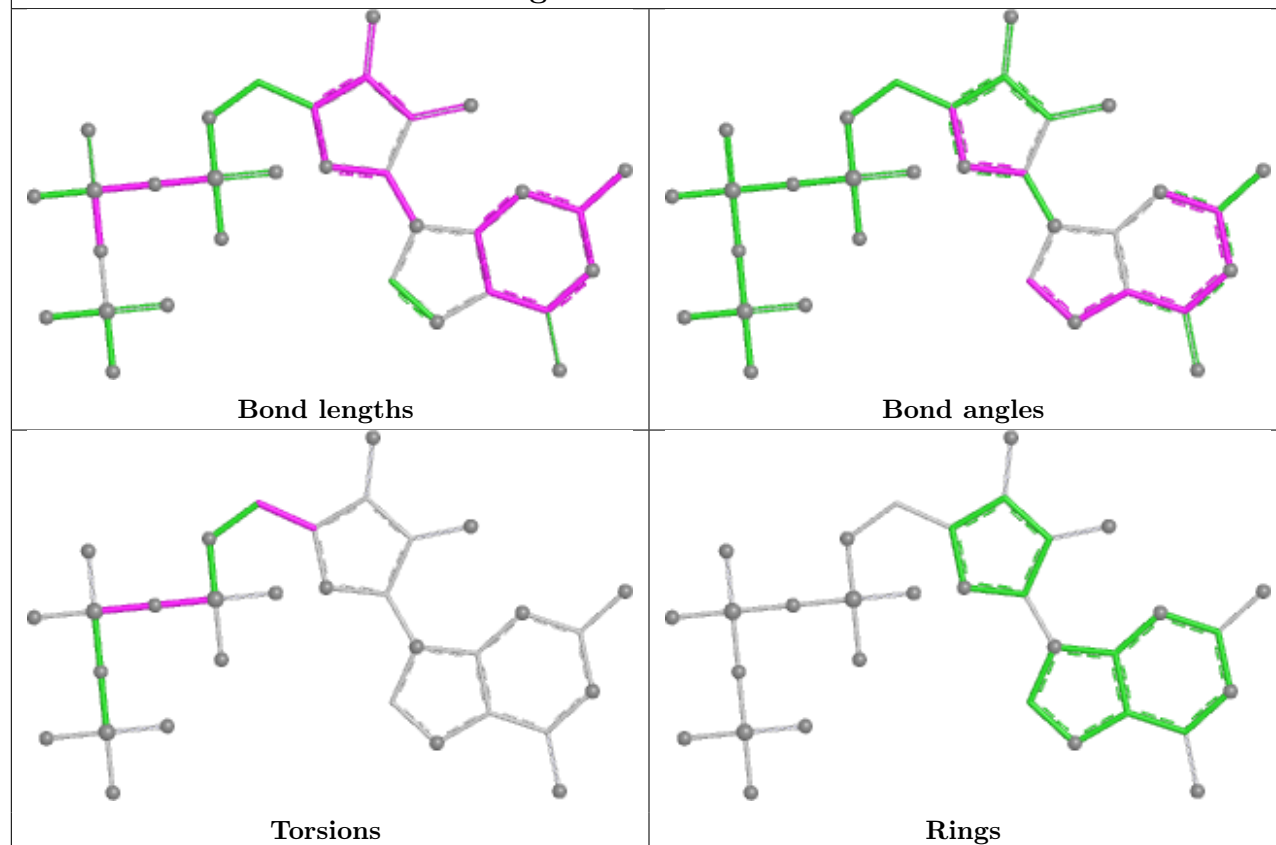


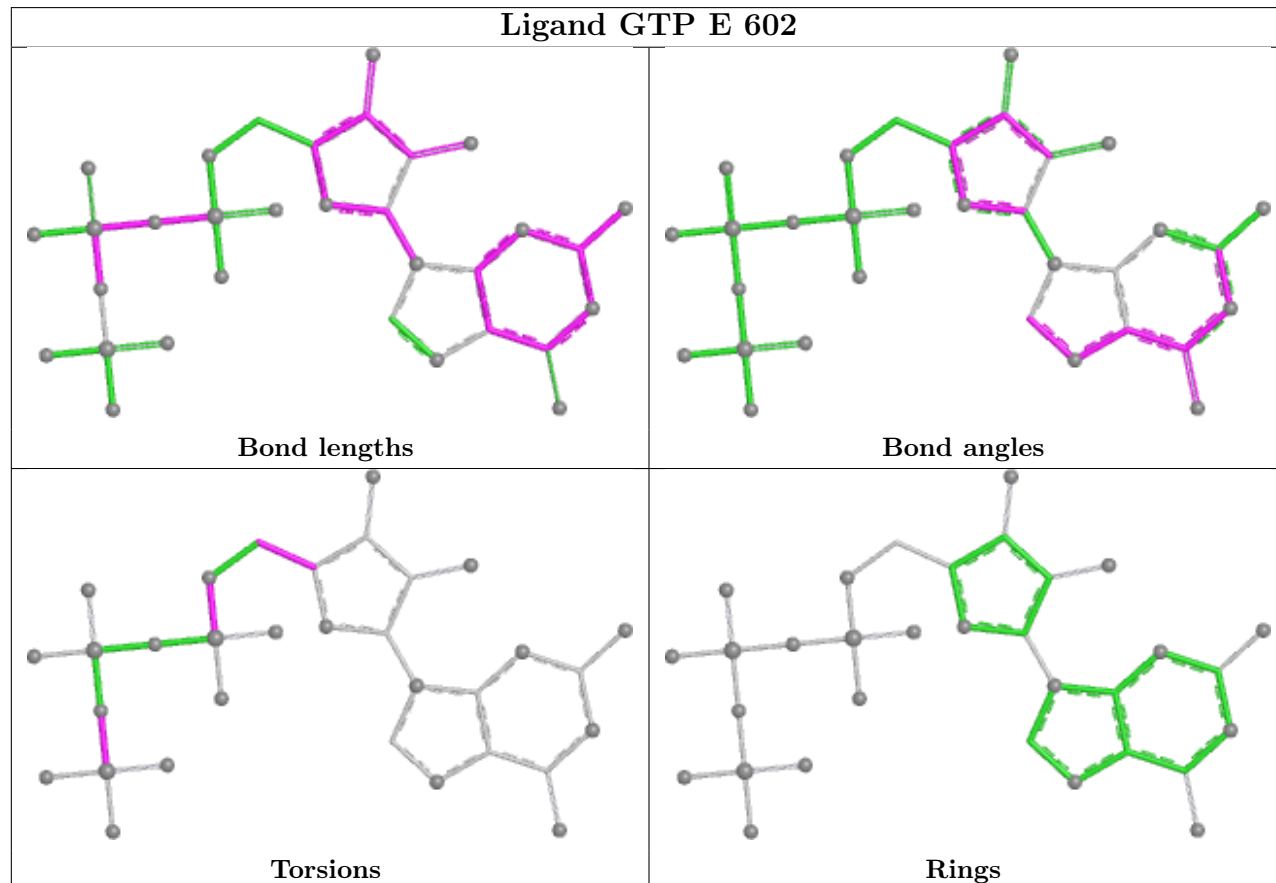
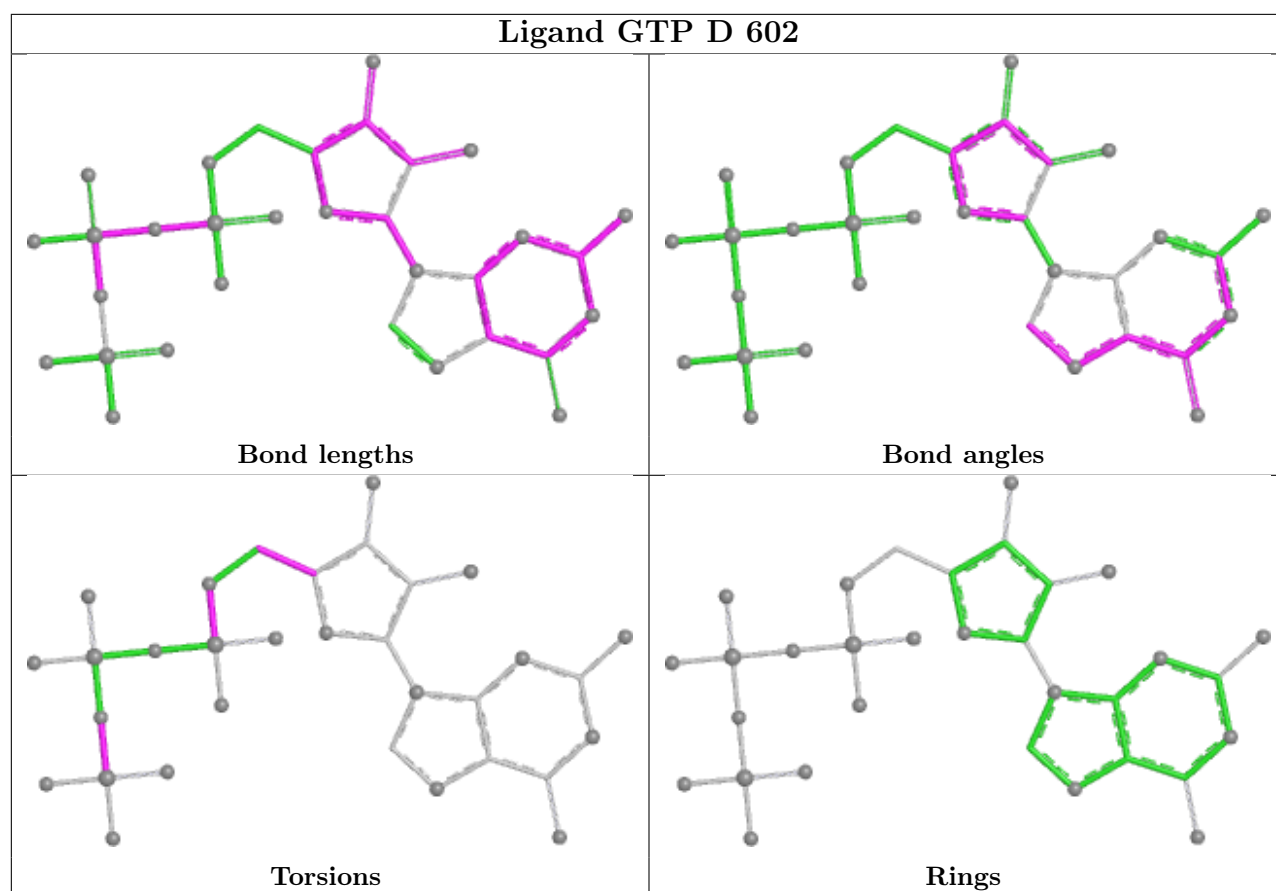


## Ligand IMP F 601

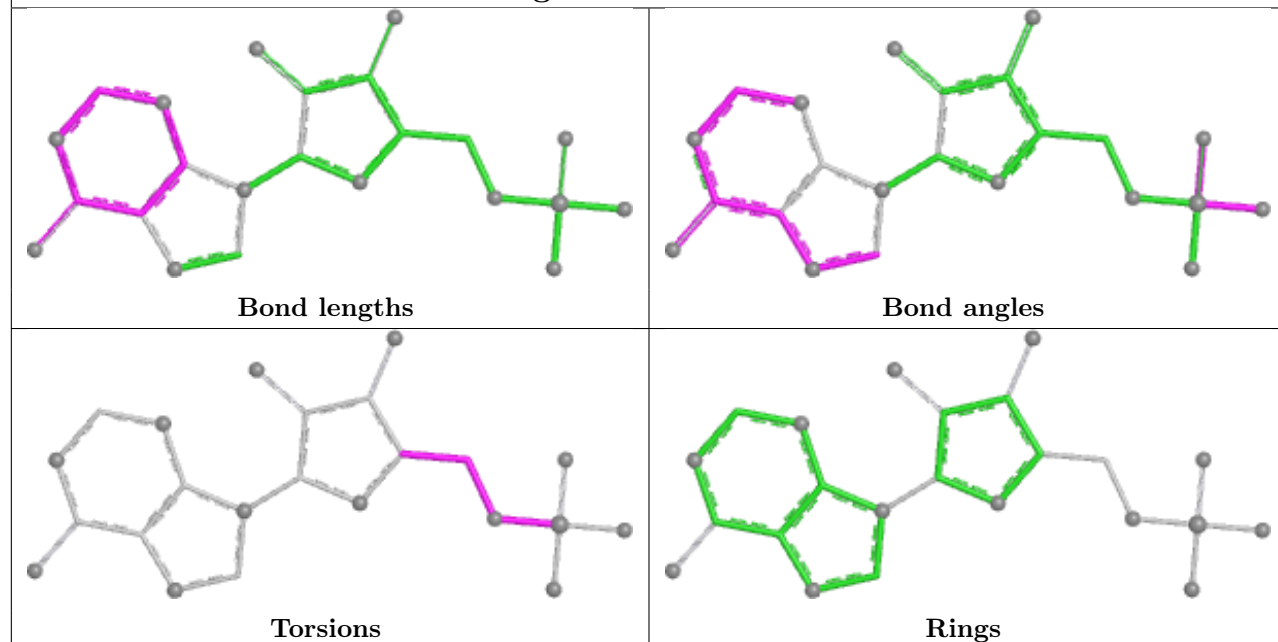


## Ligand GTP G 603

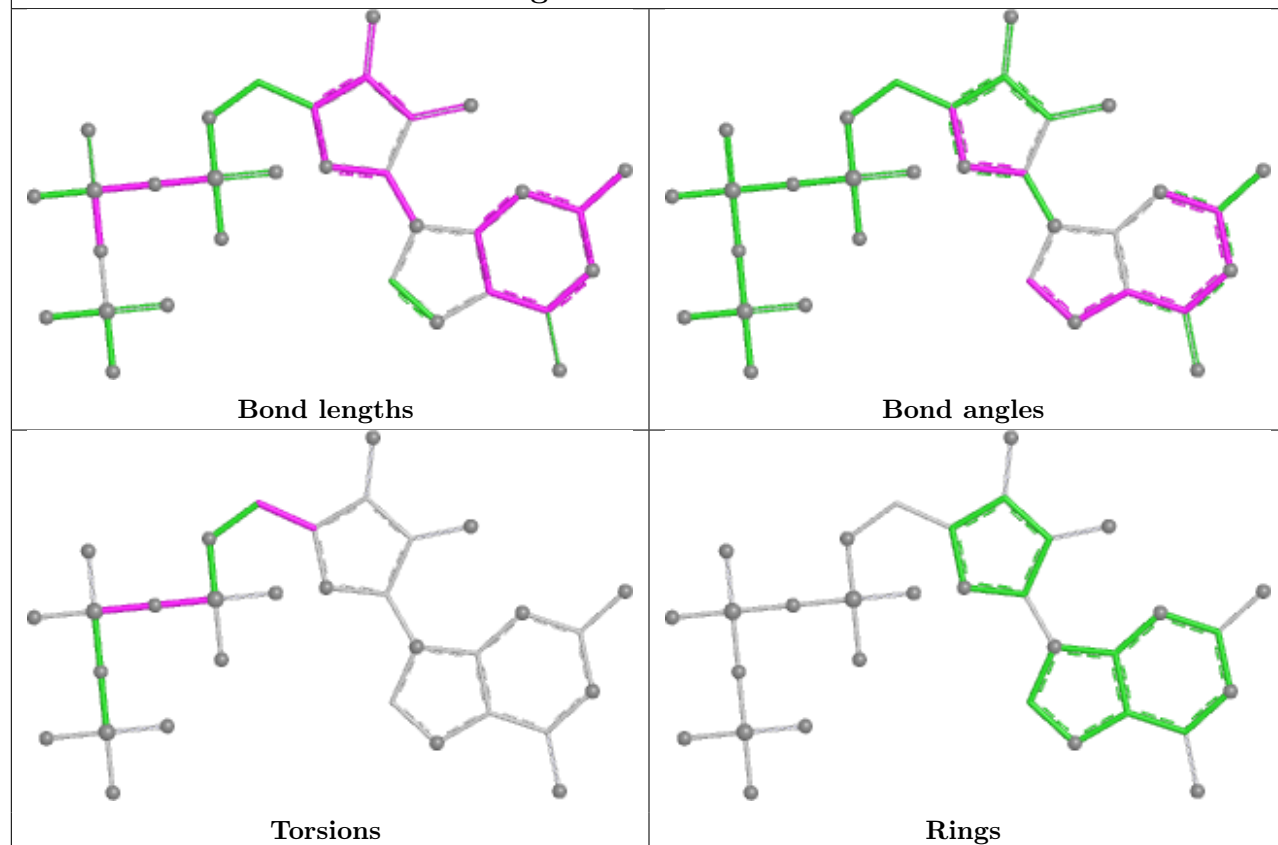


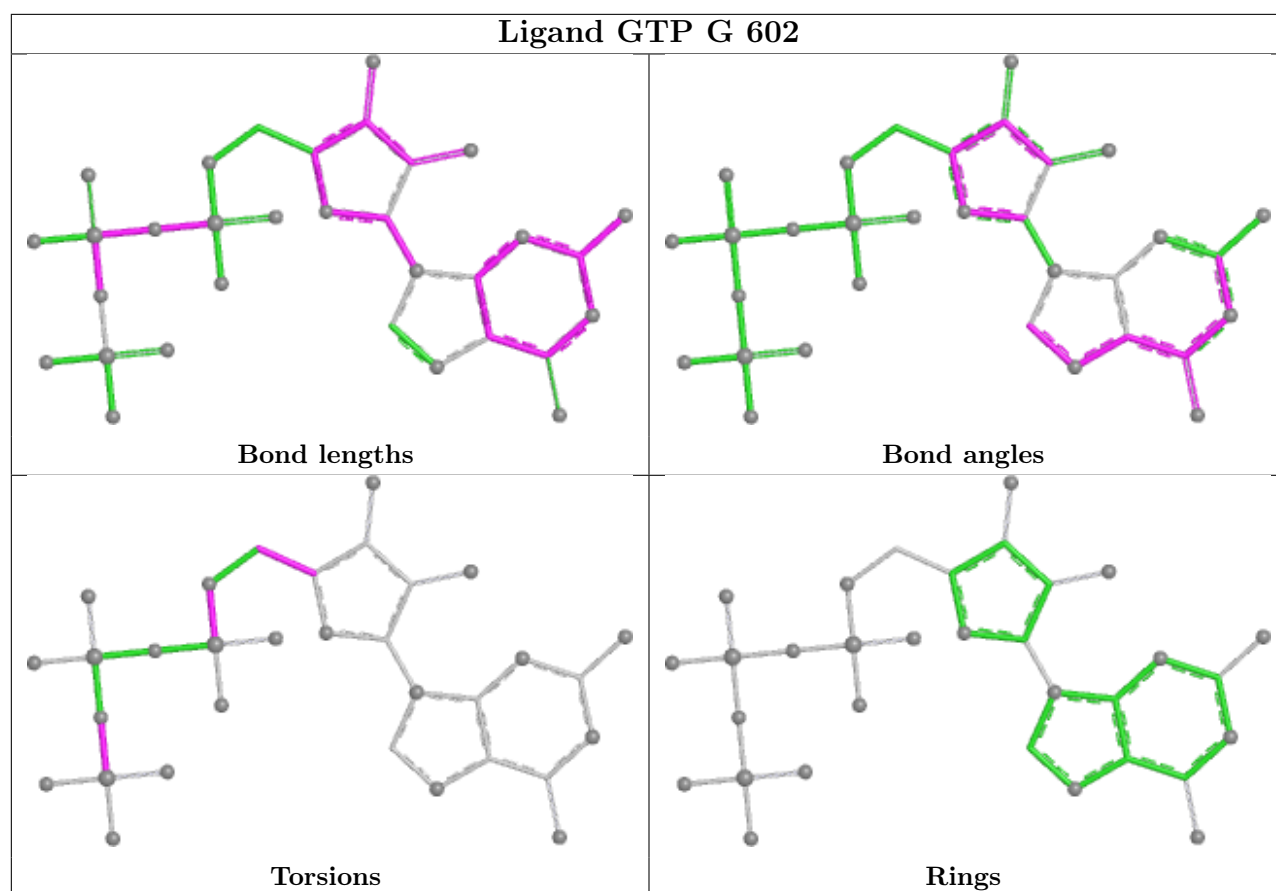


## Ligand IMP A 601



## Ligand GTP C 603





## 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.



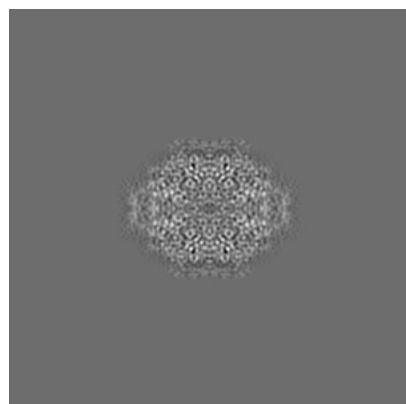
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20741. These allow visual inspection of the internal detail of the map and identification of artifacts.

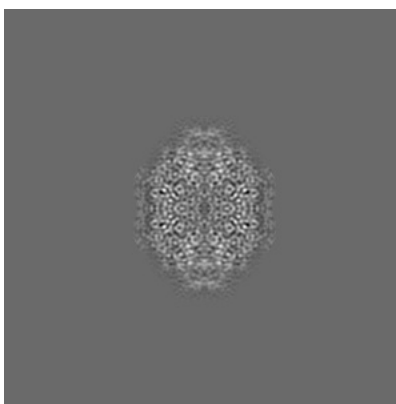
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

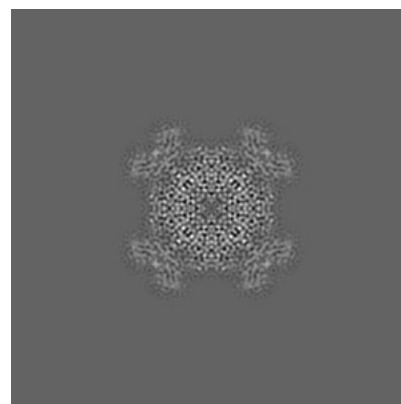
#### 6.1.1 Primary map



X

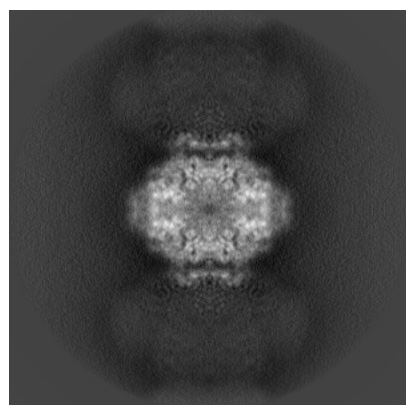


Y

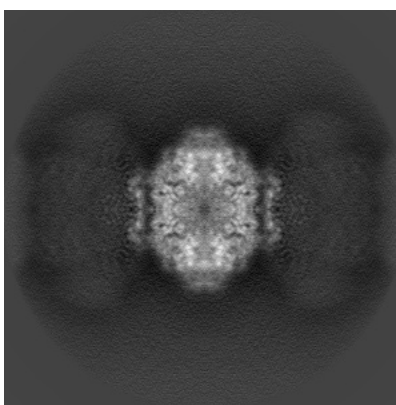


Z

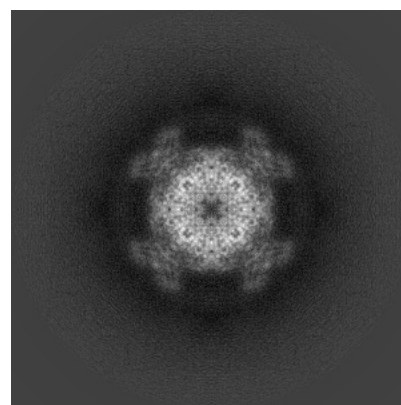
#### 6.1.2 Raw map



X



Y

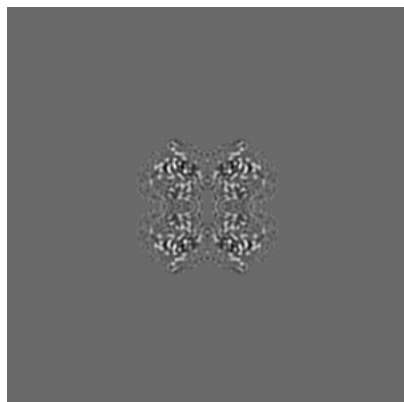


Z

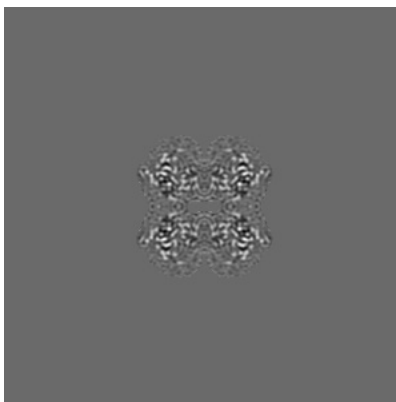
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

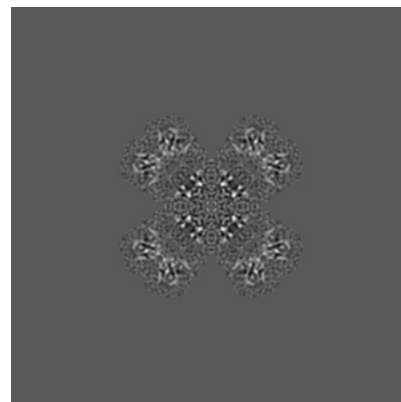
### 6.2.1 Primary map



X Index: 200

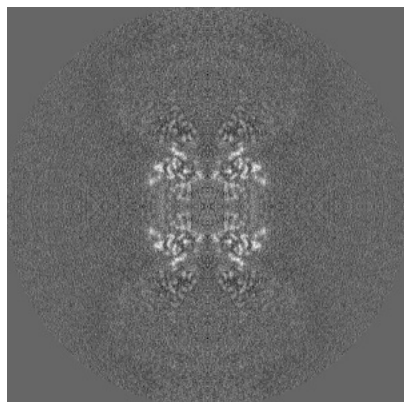


Y Index: 200

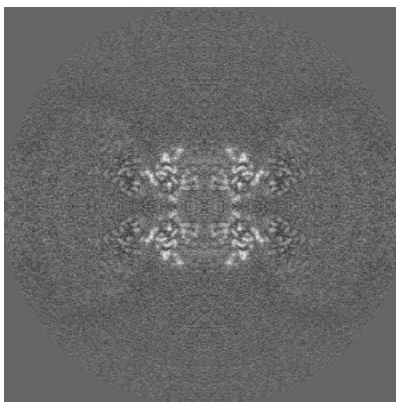


Z Index: 200

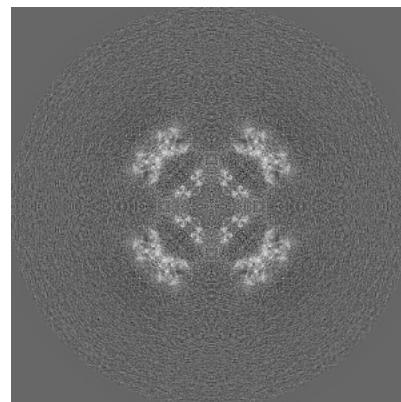
### 6.2.2 Raw map



X Index: 200



Y Index: 200

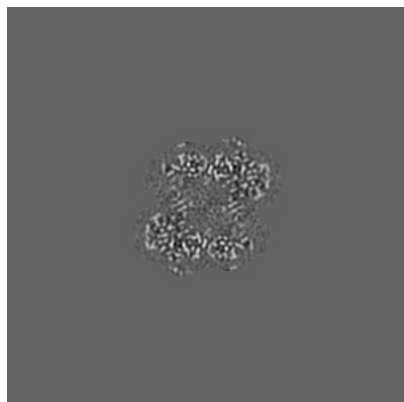


Z Index: 200

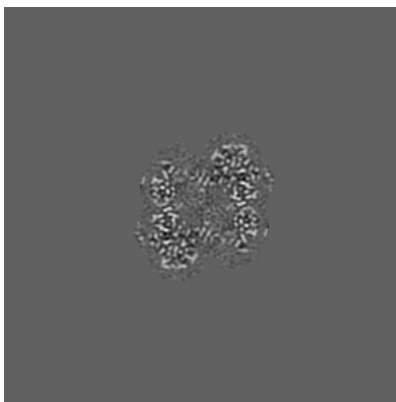
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

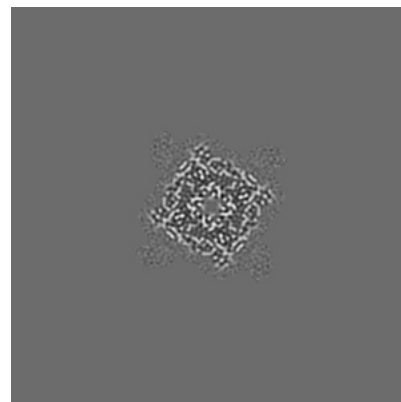
### 6.3.1 Primary map



X Index: 188

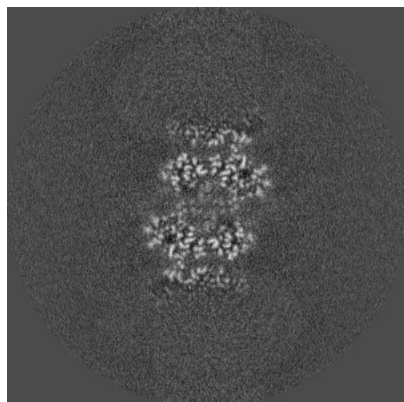


Y Index: 212

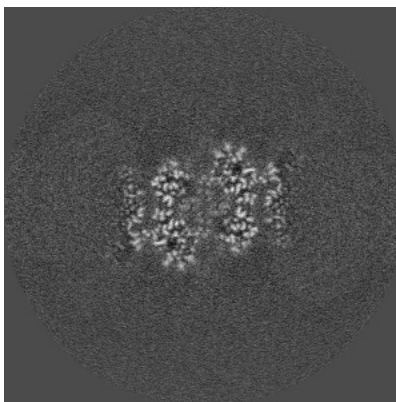


Z Index: 235

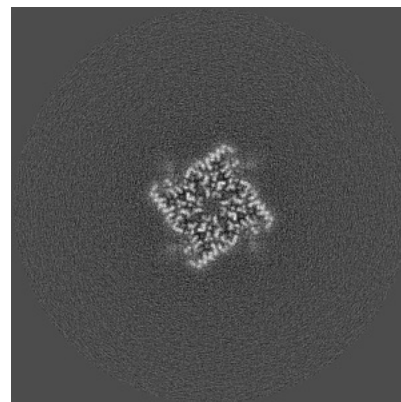
### 6.3.2 Raw map



X Index: 181



Y Index: 219

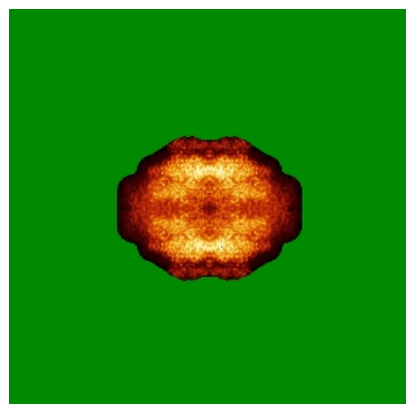


Z Index: 161

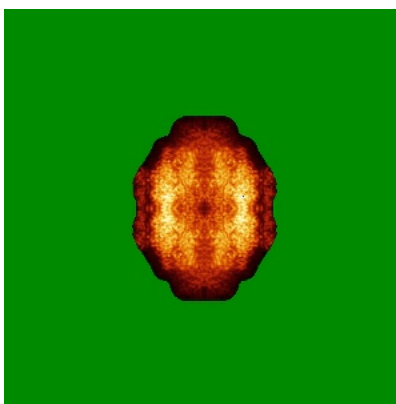
The images above show the largest variance slices of the map in three orthogonal directions.

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

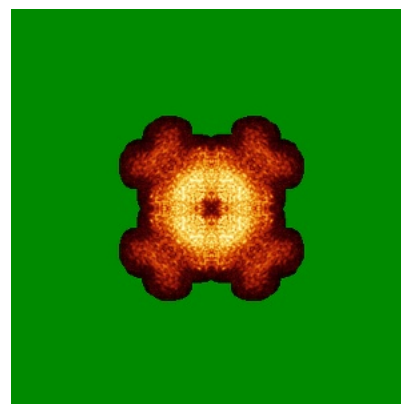
### 6.4.1 Primary map



X

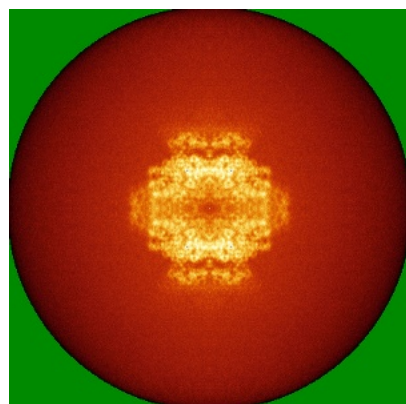


Y

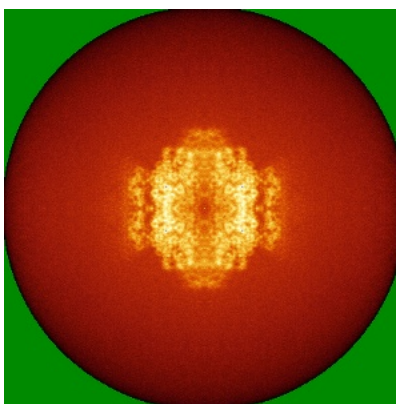


Z

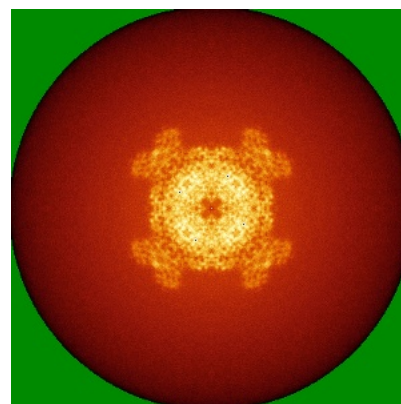
### 6.4.2 Raw map



X



Y

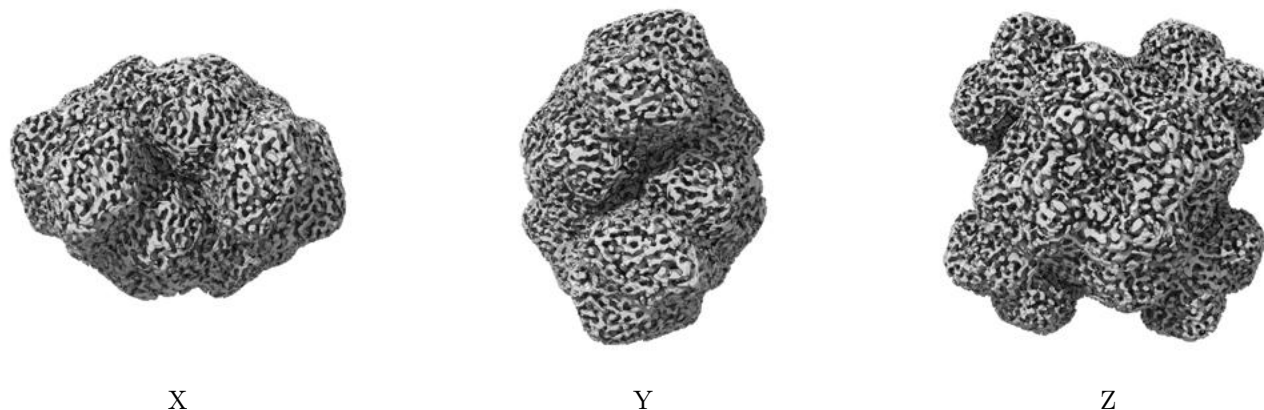


Z

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.

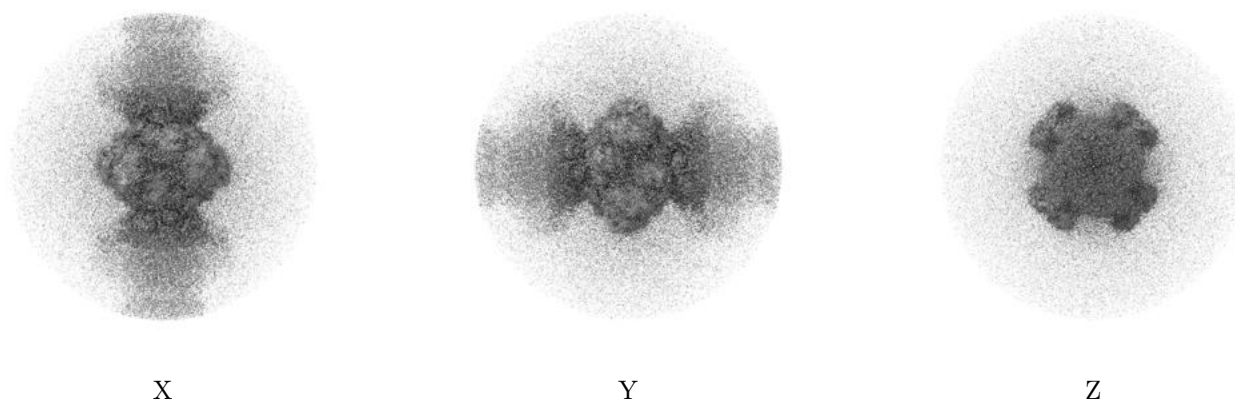
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.



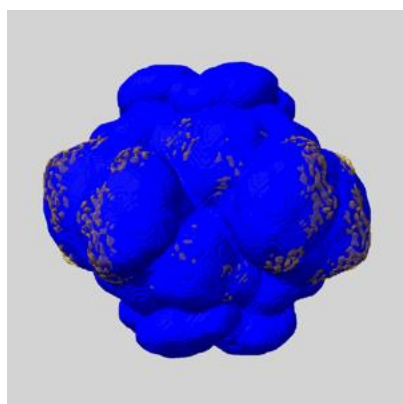
## 6.6 Mask visualisation [i](#)

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

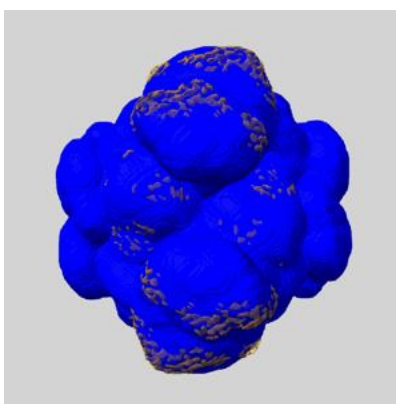
A mask typically either:

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

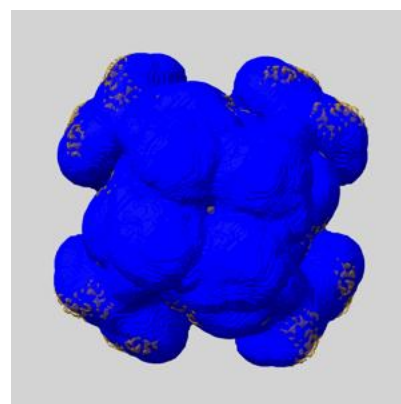
### 6.6.1 emd\_20741\_msk\_1.map [i](#)



X



Y

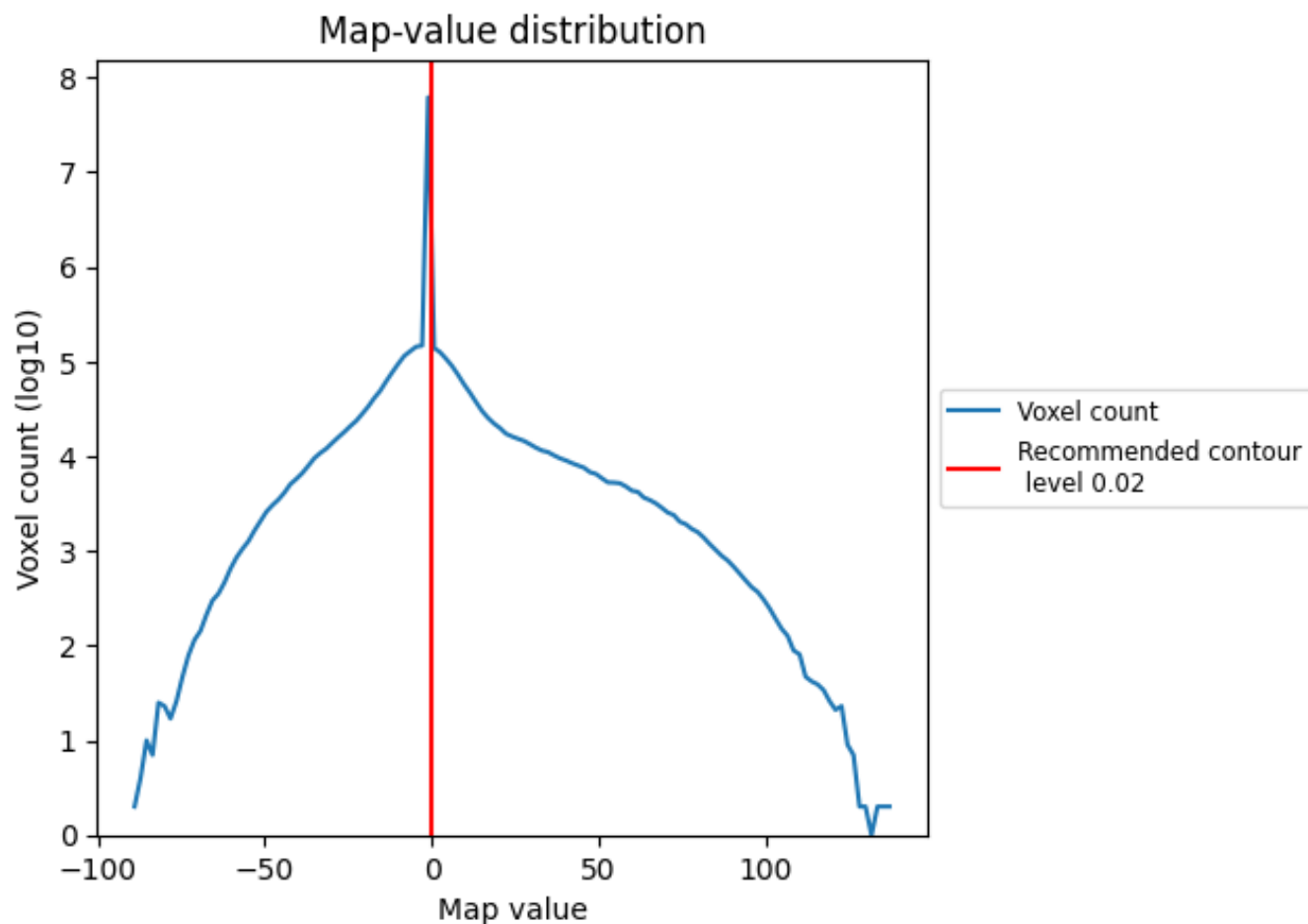


Z

## 7 Map analysis [i](#)

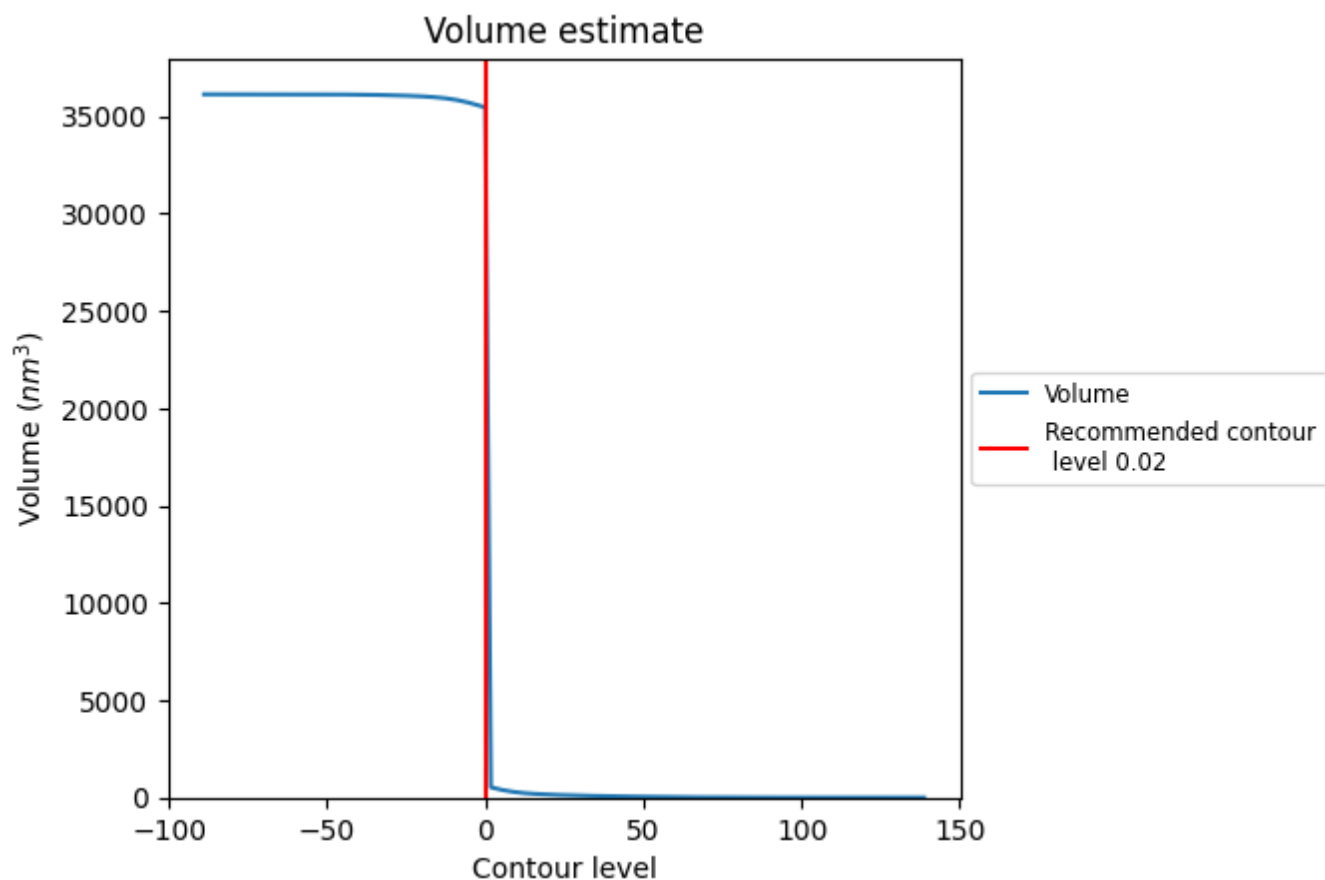
This section contains the results of statistical analysis of the map.

### 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](#)

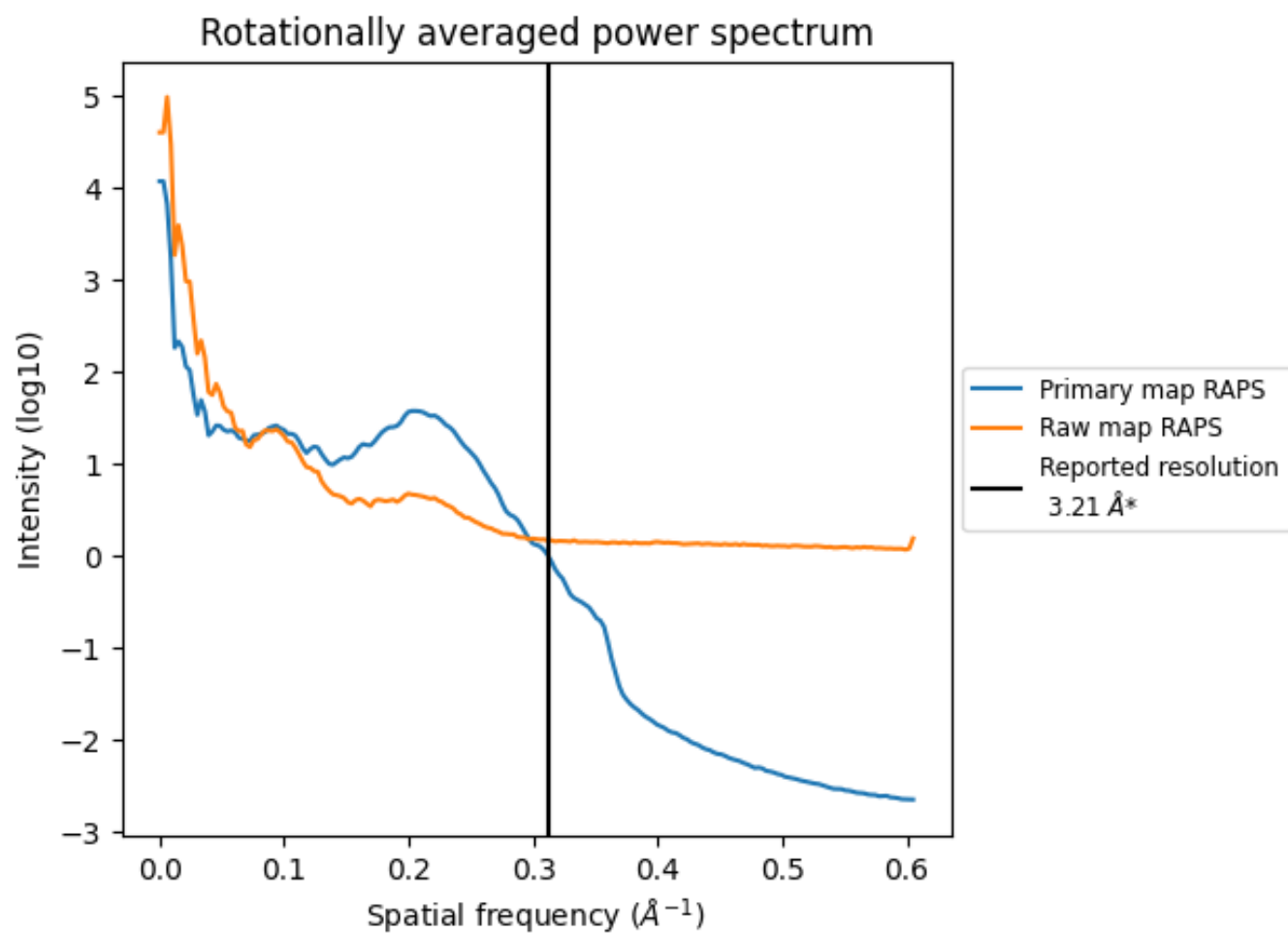


The volume at the recommended contour level is 34772 nm<sup>3</sup>; this corresponds to an approximate mass of 31411 kDa.

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 [i](#)

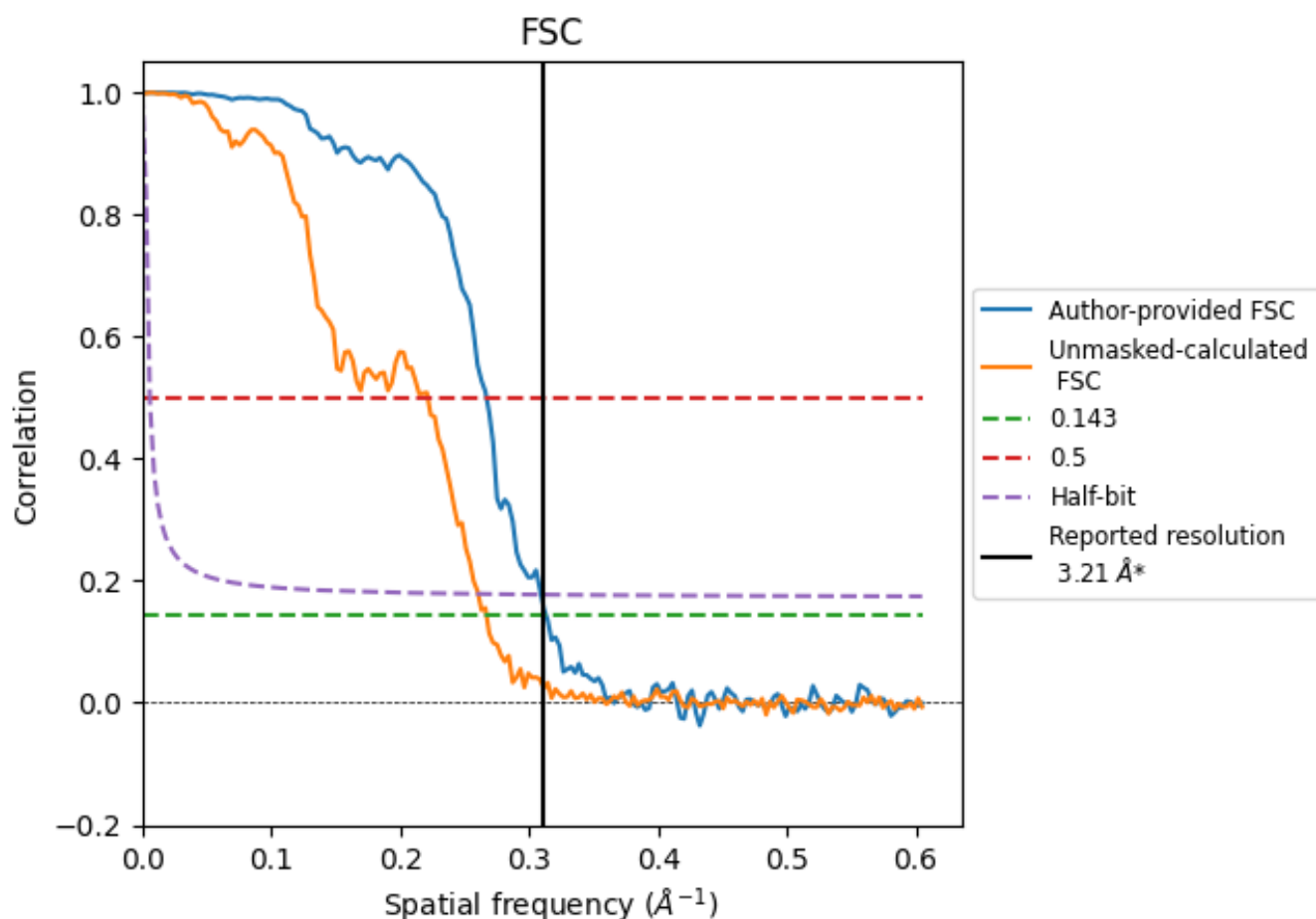


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

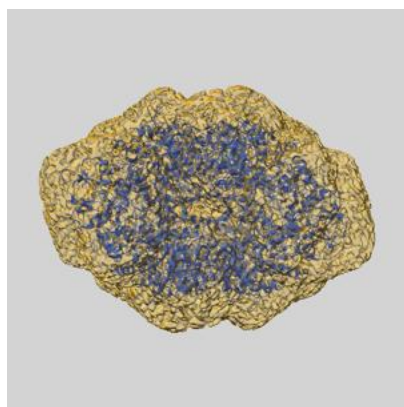
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.19	3.74	3.23
Unmasked-calculated*	3.74	4.51	3.84

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 3.21 by more than 10 %

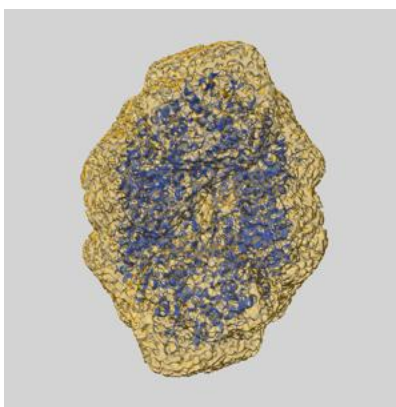
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20741 and PDB model 6UDO. Per-residue inclusion information can be found in section [3](#) on page [10](#).

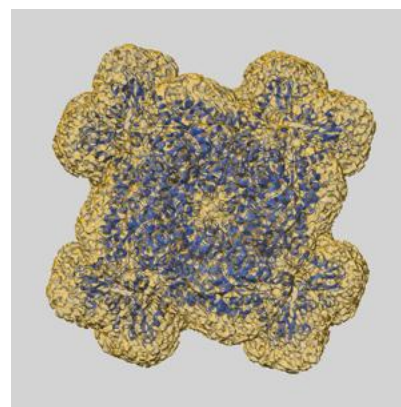
### 9.1 Map-model overlay [i](#)



X



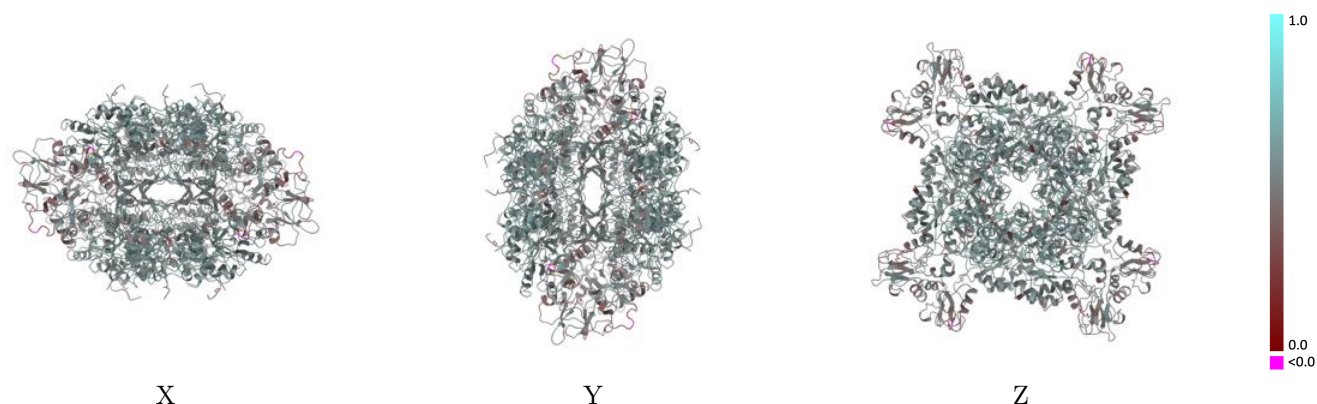
Y



Z

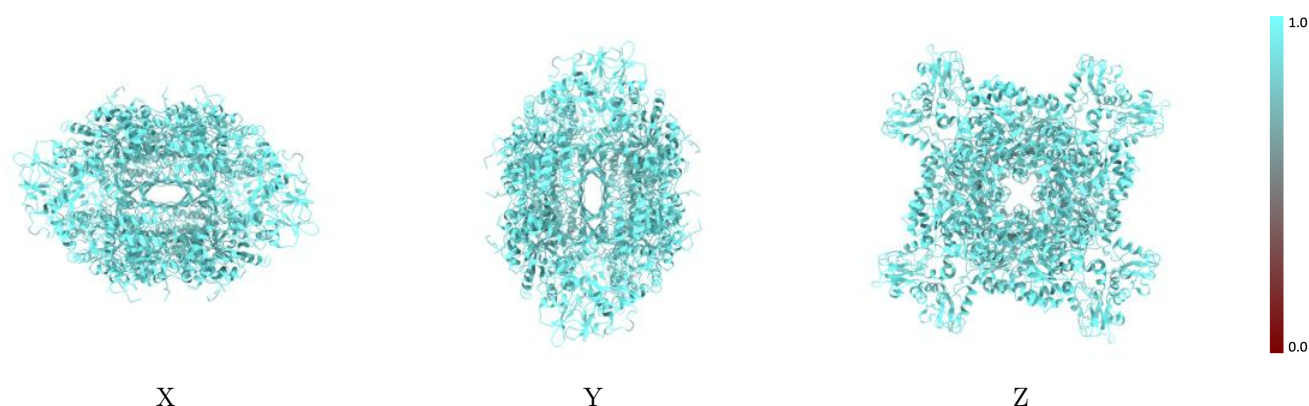
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



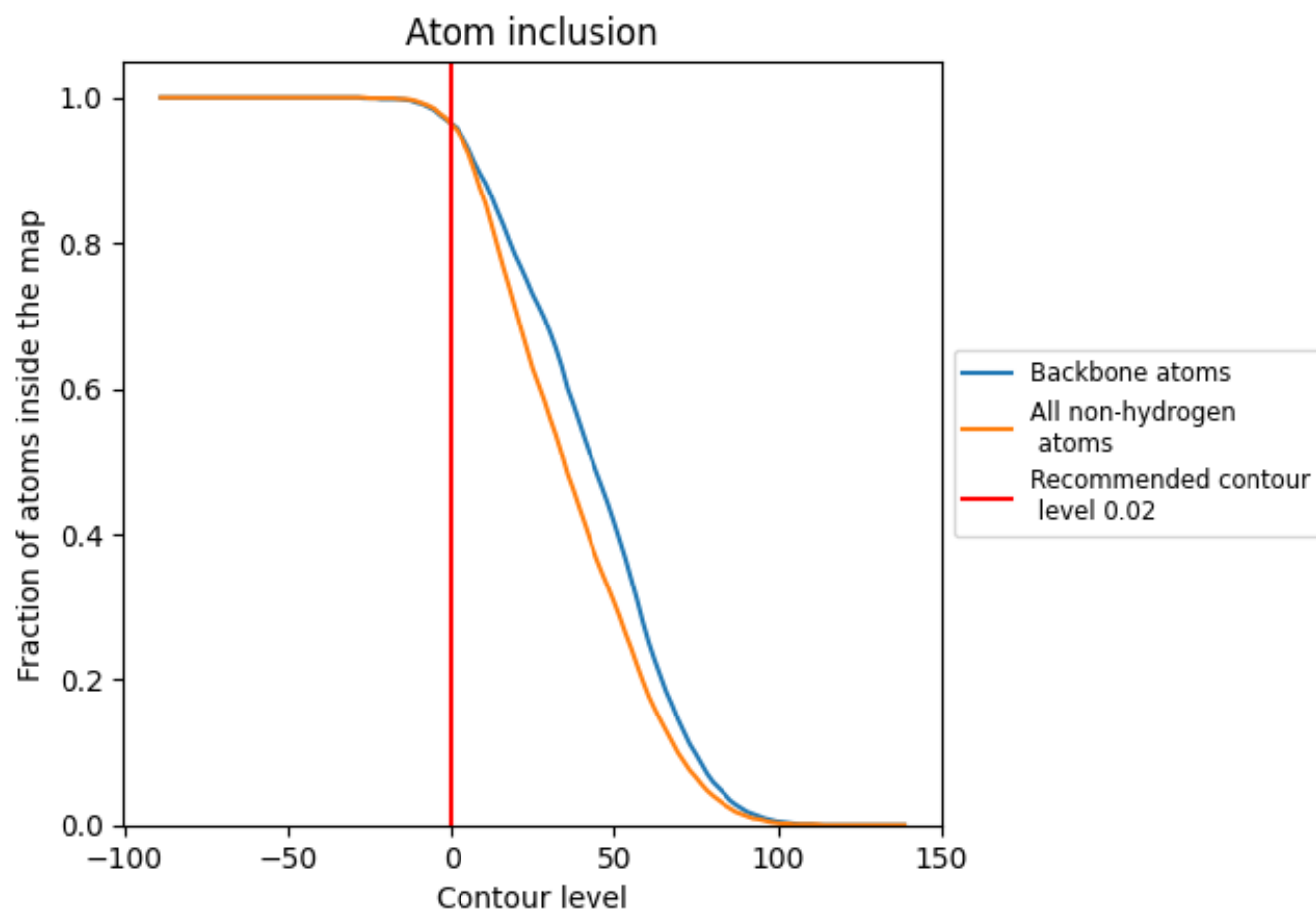
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9630	<div><div></div></div> 0.5100
A	<div><div></div></div> 0.9640	<div><div></div></div> 0.5120
B	<div><div></div></div> 0.9630	<div><div></div></div> 0.5120
C	<div><div></div></div> 0.9640	<div><div></div></div> 0.5110
D	<div><div></div></div> 0.9630	<div><div></div></div> 0.5110
E	<div><div></div></div> 0.9630	<div><div></div></div> 0.5110
F	<div><div></div></div> 0.9630	<div><div></div></div> 0.5120
G	<div><div></div></div> 0.9640	<div><div></div></div> 0.5120
H	<div><div></div></div> 0.9630	<div><div></div></div> 0.5120
I	<div><div></div></div> 0.9500	<div><div></div></div> 0.4760
J	<div><div></div></div> 0.9300	<div><div></div></div> 0.4570
K	<div><div></div></div> 0.9500	<div><div></div></div> 0.4660
L	<div><div></div></div> 0.9400	<div><div></div></div> 0.4650
M	<div><div></div></div> 0.9500	<div><div></div></div> 0.4730
N	<div><div></div></div> 0.9400	<div><div></div></div> 0.4780
O	<div><div></div></div> 0.9500	<div><div></div></div> 0.4660
P	<div><div></div></div> 0.9500	<div><div></div></div> 0.4790

1.0

0.0

<0.0