



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 10:45 AM EST

PDB ID : 7RGD  
EMDB ID : EMD-24448  
Title : HUMAN RETINAL VARIANT IMPDH1(595) TREATED WITH GTP, ATP, IMP, NAD+, OCTAMER-CENTERED  
Authors : Burrell, A.L.; Kollman, J.M.  
Deposited on : 2021-07-15  
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation 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:

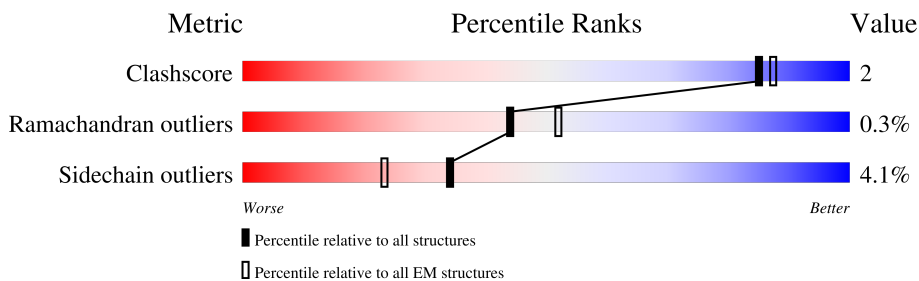
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	595	
1	B	595	
1	C	595	
1	D	595	
1	E	595	
1	F	595	
1	G	595	
1	H	595	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 65008 atoms, of which 32424 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 Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	519	7891	2473	3980	670	743	25	0	0
1	B	519	7891	2473	3980	670	743	25	0	0
1	C	519	7891	2473	3980	670	743	25	0	0
1	D	519	7891	2473	3980	670	743	25	0	0
1	E	519	7891	2473	3980	670	743	25	0	0
1	F	519	7891	2473	3980	670	743	25	0	0
1	G	519	7891	2473	3980	670	743	25	0	0
1	H	519	7891	2473	3980	670	743	25	0	0

There are 504 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P20839-5
A	?	-	CYS	deletion	UNP P20839-5
A	?	-	PHE	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	GLU	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	SER	deletion	UNP P20839-5
A	?	-	SER	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	ALA	deletion	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	GLY	deletion	UNP P20839-5
A	?	-	VAL	deletion	UNP P20839-5
A	?	-	GLN	deletion	UNP P20839-5
A	?	-	MET	deletion	UNP P20839-5
A	?	-	ASP	deletion	UNP P20839-5
A	?	-	ARG	deletion	UNP P20839-5
A	?	-	LEU	deletion	UNP P20839-5
A	?	-	ARG	deletion	UNP P20839-5
A	?	-	ARG	deletion	UNP P20839-5
A	?	-	ALA	deletion	UNP P20839-5
A	510	THR	-	expression tag	UNP P20839-5
A	511	PHE	-	expression tag	UNP P20839-5
A	512	LEU	-	expression tag	UNP P20839-5
A	513	PRO	-	expression tag	UNP P20839-5
A	514	PHE	-	expression tag	UNP P20839-5
A	515	THR	-	expression tag	UNP P20839-5
A	516	LYS	-	expression tag	UNP P20839-5
A	517	SER	-	expression tag	UNP P20839-5
A	518	GLY	-	expression tag	UNP P20839-5
A	519	CYS	-	expression tag	UNP P20839-5
A	520	THR	-	expression tag	UNP P20839-5
A	521	GLU	-	expression tag	UNP P20839-5
A	522	ASP	-	expression tag	UNP P20839-5
A	523	SER	-	expression tag	UNP P20839-5
A	524	GLY	-	expression tag	UNP P20839-5
A	525	GLY	-	expression tag	UNP P20839-5
A	526	GLY	-	expression tag	UNP P20839-5
A	527	ARG	-	expression tag	UNP P20839-5
A	528	GLY	-	expression tag	UNP P20839-5
A	529	GLY	-	expression tag	UNP P20839-5
A	530	GLY	-	expression tag	UNP P20839-5
A	531	GLY	-	expression tag	UNP P20839-5
A	532	ASP	-	expression tag	UNP P20839-5
A	533	ALA	-	expression tag	UNP P20839-5
A	534	PRO	-	expression tag	UNP P20839-5
A	535	GLN	-	expression tag	UNP P20839-5
A	536	CYS	-	expression tag	UNP P20839-5
A	537	PRO	-	expression tag	UNP P20839-5
A	538	LEU	-	expression tag	UNP P20839-5
A	539	LEU	-	expression tag	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	540	GLY	-	expression tag	UNP P20839-5
A	541	THR	-	expression tag	UNP P20839-5
A	542	ALA	-	expression tag	UNP P20839-5
A	543	SER	-	expression tag	UNP P20839-5
A	544	LEU	-	expression tag	UNP P20839-5
A	545	HIS	-	expression tag	UNP P20839-5
A	546	ASN	-	expression tag	UNP P20839-5
B	?	-	SER	deletion	UNP P20839-5
B	?	-	CYS	deletion	UNP P20839-5
B	?	-	PHE	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	GLU	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	SER	deletion	UNP P20839-5
B	?	-	SER	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	ALA	deletion	UNP P20839-5
B	?	-	GLY	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	GLY	deletion	UNP P20839-5
B	?	-	VAL	deletion	UNP P20839-5
B	?	-	GLN	deletion	UNP P20839-5
B	?	-	MET	deletion	UNP P20839-5
B	?	-	ASP	deletion	UNP P20839-5
B	?	-	ARG	deletion	UNP P20839-5
B	?	-	LEU	deletion	UNP P20839-5
B	?	-	ARG	deletion	UNP P20839-5
B	?	-	ARG	deletion	UNP P20839-5
B	?	-	ALA	deletion	UNP P20839-5
B	510	THR	-	expression tag	UNP P20839-5
B	511	PHE	-	expression tag	UNP P20839-5
B	512	LEU	-	expression tag	UNP P20839-5
B	513	PRO	-	expression tag	UNP P20839-5
B	514	PHE	-	expression tag	UNP P20839-5
B	515	THR	-	expression tag	UNP P20839-5
B	516	LYS	-	expression tag	UNP P20839-5
B	517	SER	-	expression tag	UNP P20839-5
B	518	GLY	-	expression tag	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	519	CYS	-	expression tag	UNP P20839-5
B	520	THR	-	expression tag	UNP P20839-5
B	521	GLU	-	expression tag	UNP P20839-5
B	522	ASP	-	expression tag	UNP P20839-5
B	523	SER	-	expression tag	UNP P20839-5
B	524	GLY	-	expression tag	UNP P20839-5
B	525	GLY	-	expression tag	UNP P20839-5
B	526	GLY	-	expression tag	UNP P20839-5
B	527	ARG	-	expression tag	UNP P20839-5
B	528	GLY	-	expression tag	UNP P20839-5
B	529	GLY	-	expression tag	UNP P20839-5
B	530	GLY	-	expression tag	UNP P20839-5
B	531	GLY	-	expression tag	UNP P20839-5
B	532	ASP	-	expression tag	UNP P20839-5
B	533	ALA	-	expression tag	UNP P20839-5
B	534	PRO	-	expression tag	UNP P20839-5
B	535	GLN	-	expression tag	UNP P20839-5
B	536	CYS	-	expression tag	UNP P20839-5
B	537	PRO	-	expression tag	UNP P20839-5
B	538	LEU	-	expression tag	UNP P20839-5
B	539	LEU	-	expression tag	UNP P20839-5
B	540	GLY	-	expression tag	UNP P20839-5
B	541	THR	-	expression tag	UNP P20839-5
B	542	ALA	-	expression tag	UNP P20839-5
B	543	SER	-	expression tag	UNP P20839-5
B	544	LEU	-	expression tag	UNP P20839-5
B	545	HIS	-	expression tag	UNP P20839-5
B	546	ASN	-	expression tag	UNP P20839-5
C	?	-	SER	deletion	UNP P20839-5
C	?	-	CYS	deletion	UNP P20839-5
C	?	-	PHE	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	GLU	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	SER	deletion	UNP P20839-5
C	?	-	SER	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	ALA	deletion	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	GLY	deletion	UNP P20839-5
C	?	-	VAL	deletion	UNP P20839-5
C	?	-	GLN	deletion	UNP P20839-5
C	?	-	MET	deletion	UNP P20839-5
C	?	-	ASP	deletion	UNP P20839-5
C	?	-	ARG	deletion	UNP P20839-5
C	?	-	LEU	deletion	UNP P20839-5
C	?	-	ARG	deletion	UNP P20839-5
C	?	-	ARG	deletion	UNP P20839-5
C	?	-	ALA	deletion	UNP P20839-5
C	510	THR	-	expression tag	UNP P20839-5
C	511	PHE	-	expression tag	UNP P20839-5
C	512	LEU	-	expression tag	UNP P20839-5
C	513	PRO	-	expression tag	UNP P20839-5
C	514	PHE	-	expression tag	UNP P20839-5
C	515	THR	-	expression tag	UNP P20839-5
C	516	LYS	-	expression tag	UNP P20839-5
C	517	SER	-	expression tag	UNP P20839-5
C	518	GLY	-	expression tag	UNP P20839-5
C	519	CYS	-	expression tag	UNP P20839-5
C	520	THR	-	expression tag	UNP P20839-5
C	521	GLU	-	expression tag	UNP P20839-5
C	522	ASP	-	expression tag	UNP P20839-5
C	523	SER	-	expression tag	UNP P20839-5
C	524	GLY	-	expression tag	UNP P20839-5
C	525	GLY	-	expression tag	UNP P20839-5
C	526	GLY	-	expression tag	UNP P20839-5
C	527	ARG	-	expression tag	UNP P20839-5
C	528	GLY	-	expression tag	UNP P20839-5
C	529	GLY	-	expression tag	UNP P20839-5
C	530	GLY	-	expression tag	UNP P20839-5
C	531	GLY	-	expression tag	UNP P20839-5
C	532	ASP	-	expression tag	UNP P20839-5
C	533	ALA	-	expression tag	UNP P20839-5
C	534	PRO	-	expression tag	UNP P20839-5
C	535	GLN	-	expression tag	UNP P20839-5
C	536	CYS	-	expression tag	UNP P20839-5
C	537	PRO	-	expression tag	UNP P20839-5
C	538	LEU	-	expression tag	UNP P20839-5
C	539	LEU	-	expression tag	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	540	GLY	-	expression tag	UNP P20839-5
C	541	THR	-	expression tag	UNP P20839-5
C	542	ALA	-	expression tag	UNP P20839-5
C	543	SER	-	expression tag	UNP P20839-5
C	544	LEU	-	expression tag	UNP P20839-5
C	545	HIS	-	expression tag	UNP P20839-5
C	546	ASN	-	expression tag	UNP P20839-5
D	?	-	SER	deletion	UNP P20839-5
D	?	-	CYS	deletion	UNP P20839-5
D	?	-	PHE	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	GLU	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	SER	deletion	UNP P20839-5
D	?	-	SER	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	ALA	deletion	UNP P20839-5
D	?	-	GLY	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	GLY	deletion	UNP P20839-5
D	?	-	VAL	deletion	UNP P20839-5
D	?	-	GLN	deletion	UNP P20839-5
D	?	-	MET	deletion	UNP P20839-5
D	?	-	ASP	deletion	UNP P20839-5
D	?	-	ARG	deletion	UNP P20839-5
D	?	-	LEU	deletion	UNP P20839-5
D	?	-	ARG	deletion	UNP P20839-5
D	?	-	ARG	deletion	UNP P20839-5
D	?	-	ALA	deletion	UNP P20839-5
D	510	THR	-	expression tag	UNP P20839-5
D	511	PHE	-	expression tag	UNP P20839-5
D	512	LEU	-	expression tag	UNP P20839-5
D	513	PRO	-	expression tag	UNP P20839-5
D	514	PHE	-	expression tag	UNP P20839-5
D	515	THR	-	expression tag	UNP P20839-5
D	516	LYS	-	expression tag	UNP P20839-5
D	517	SER	-	expression tag	UNP P20839-5
D	518	GLY	-	expression tag	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	519	CYS	-	expression tag	UNP P20839-5
D	520	THR	-	expression tag	UNP P20839-5
D	521	GLU	-	expression tag	UNP P20839-5
D	522	ASP	-	expression tag	UNP P20839-5
D	523	SER	-	expression tag	UNP P20839-5
D	524	GLY	-	expression tag	UNP P20839-5
D	525	GLY	-	expression tag	UNP P20839-5
D	526	GLY	-	expression tag	UNP P20839-5
D	527	ARG	-	expression tag	UNP P20839-5
D	528	GLY	-	expression tag	UNP P20839-5
D	529	GLY	-	expression tag	UNP P20839-5
D	530	GLY	-	expression tag	UNP P20839-5
D	531	GLY	-	expression tag	UNP P20839-5
D	532	ASP	-	expression tag	UNP P20839-5
D	533	ALA	-	expression tag	UNP P20839-5
D	534	PRO	-	expression tag	UNP P20839-5
D	535	GLN	-	expression tag	UNP P20839-5
D	536	CYS	-	expression tag	UNP P20839-5
D	537	PRO	-	expression tag	UNP P20839-5
D	538	LEU	-	expression tag	UNP P20839-5
D	539	LEU	-	expression tag	UNP P20839-5
D	540	GLY	-	expression tag	UNP P20839-5
D	541	THR	-	expression tag	UNP P20839-5
D	542	ALA	-	expression tag	UNP P20839-5
D	543	SER	-	expression tag	UNP P20839-5
D	544	LEU	-	expression tag	UNP P20839-5
D	545	HIS	-	expression tag	UNP P20839-5
D	546	ASN	-	expression tag	UNP P20839-5
E	?	-	SER	deletion	UNP P20839-5
E	?	-	CYS	deletion	UNP P20839-5
E	?	-	PHE	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	GLU	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	SER	deletion	UNP P20839-5
E	?	-	SER	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	ALA	deletion	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	GLY	deletion	UNP P20839-5
E	?	-	VAL	deletion	UNP P20839-5
E	?	-	GLN	deletion	UNP P20839-5
E	?	-	MET	deletion	UNP P20839-5
E	?	-	ASP	deletion	UNP P20839-5
E	?	-	ARG	deletion	UNP P20839-5
E	?	-	LEU	deletion	UNP P20839-5
E	?	-	ARG	deletion	UNP P20839-5
E	?	-	ARG	deletion	UNP P20839-5
E	?	-	ALA	deletion	UNP P20839-5
E	510	THR	-	expression tag	UNP P20839-5
E	511	PHE	-	expression tag	UNP P20839-5
E	512	LEU	-	expression tag	UNP P20839-5
E	513	PRO	-	expression tag	UNP P20839-5
E	514	PHE	-	expression tag	UNP P20839-5
E	515	THR	-	expression tag	UNP P20839-5
E	516	LYS	-	expression tag	UNP P20839-5
E	517	SER	-	expression tag	UNP P20839-5
E	518	GLY	-	expression tag	UNP P20839-5
E	519	CYS	-	expression tag	UNP P20839-5
E	520	THR	-	expression tag	UNP P20839-5
E	521	GLU	-	expression tag	UNP P20839-5
E	522	ASP	-	expression tag	UNP P20839-5
E	523	SER	-	expression tag	UNP P20839-5
E	524	GLY	-	expression tag	UNP P20839-5
E	525	GLY	-	expression tag	UNP P20839-5
E	526	GLY	-	expression tag	UNP P20839-5
E	527	ARG	-	expression tag	UNP P20839-5
E	528	GLY	-	expression tag	UNP P20839-5
E	529	GLY	-	expression tag	UNP P20839-5
E	530	GLY	-	expression tag	UNP P20839-5
E	531	GLY	-	expression tag	UNP P20839-5
E	532	ASP	-	expression tag	UNP P20839-5
E	533	ALA	-	expression tag	UNP P20839-5
E	534	PRO	-	expression tag	UNP P20839-5
E	535	GLN	-	expression tag	UNP P20839-5
E	536	CYS	-	expression tag	UNP P20839-5
E	537	PRO	-	expression tag	UNP P20839-5
E	538	LEU	-	expression tag	UNP P20839-5
E	539	LEU	-	expression tag	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	540	GLY	-	expression tag	UNP P20839-5
E	541	THR	-	expression tag	UNP P20839-5
E	542	ALA	-	expression tag	UNP P20839-5
E	543	SER	-	expression tag	UNP P20839-5
E	544	LEU	-	expression tag	UNP P20839-5
E	545	HIS	-	expression tag	UNP P20839-5
E	546	ASN	-	expression tag	UNP P20839-5
F	?	-	SER	deletion	UNP P20839-5
F	?	-	CYS	deletion	UNP P20839-5
F	?	-	PHE	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	GLU	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	SER	deletion	UNP P20839-5
F	?	-	SER	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	ALA	deletion	UNP P20839-5
F	?	-	GLY	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	GLY	deletion	UNP P20839-5
F	?	-	VAL	deletion	UNP P20839-5
F	?	-	GLN	deletion	UNP P20839-5
F	?	-	MET	deletion	UNP P20839-5
F	?	-	ASP	deletion	UNP P20839-5
F	?	-	ARG	deletion	UNP P20839-5
F	?	-	LEU	deletion	UNP P20839-5
F	?	-	ARG	deletion	UNP P20839-5
F	?	-	ARG	deletion	UNP P20839-5
F	?	-	ALA	deletion	UNP P20839-5
F	510	THR	-	expression tag	UNP P20839-5
F	511	PHE	-	expression tag	UNP P20839-5
F	512	LEU	-	expression tag	UNP P20839-5
F	513	PRO	-	expression tag	UNP P20839-5
F	514	PHE	-	expression tag	UNP P20839-5
F	515	THR	-	expression tag	UNP P20839-5
F	516	LYS	-	expression tag	UNP P20839-5
F	517	SER	-	expression tag	UNP P20839-5
F	518	GLY	-	expression tag	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	519	CYS	-	expression tag	UNP P20839-5
F	520	THR	-	expression tag	UNP P20839-5
F	521	GLU	-	expression tag	UNP P20839-5
F	522	ASP	-	expression tag	UNP P20839-5
F	523	SER	-	expression tag	UNP P20839-5
F	524	GLY	-	expression tag	UNP P20839-5
F	525	GLY	-	expression tag	UNP P20839-5
F	526	GLY	-	expression tag	UNP P20839-5
F	527	ARG	-	expression tag	UNP P20839-5
F	528	GLY	-	expression tag	UNP P20839-5
F	529	GLY	-	expression tag	UNP P20839-5
F	530	GLY	-	expression tag	UNP P20839-5
F	531	GLY	-	expression tag	UNP P20839-5
F	532	ASP	-	expression tag	UNP P20839-5
F	533	ALA	-	expression tag	UNP P20839-5
F	534	PRO	-	expression tag	UNP P20839-5
F	535	GLN	-	expression tag	UNP P20839-5
F	536	CYS	-	expression tag	UNP P20839-5
F	537	PRO	-	expression tag	UNP P20839-5
F	538	LEU	-	expression tag	UNP P20839-5
F	539	LEU	-	expression tag	UNP P20839-5
F	540	GLY	-	expression tag	UNP P20839-5
F	541	THR	-	expression tag	UNP P20839-5
F	542	ALA	-	expression tag	UNP P20839-5
F	543	SER	-	expression tag	UNP P20839-5
F	544	LEU	-	expression tag	UNP P20839-5
F	545	HIS	-	expression tag	UNP P20839-5
F	546	ASN	-	expression tag	UNP P20839-5
G	?	-	SER	deletion	UNP P20839-5
G	?	-	CYS	deletion	UNP P20839-5
G	?	-	PHE	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	GLU	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	SER	deletion	UNP P20839-5
G	?	-	SER	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	ALA	deletion	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	GLY	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	GLY	deletion	UNP P20839-5
G	?	-	VAL	deletion	UNP P20839-5
G	?	-	GLN	deletion	UNP P20839-5
G	?	-	MET	deletion	UNP P20839-5
G	?	-	ASP	deletion	UNP P20839-5
G	?	-	ARG	deletion	UNP P20839-5
G	?	-	LEU	deletion	UNP P20839-5
G	?	-	ARG	deletion	UNP P20839-5
G	?	-	ARG	deletion	UNP P20839-5
G	?	-	ALA	deletion	UNP P20839-5
G	510	THR	-	expression tag	UNP P20839-5
G	511	PHE	-	expression tag	UNP P20839-5
G	512	LEU	-	expression tag	UNP P20839-5
G	513	PRO	-	expression tag	UNP P20839-5
G	514	PHE	-	expression tag	UNP P20839-5
G	515	THR	-	expression tag	UNP P20839-5
G	516	LYS	-	expression tag	UNP P20839-5
G	517	SER	-	expression tag	UNP P20839-5
G	518	GLY	-	expression tag	UNP P20839-5
G	519	CYS	-	expression tag	UNP P20839-5
G	520	THR	-	expression tag	UNP P20839-5
G	521	GLU	-	expression tag	UNP P20839-5
G	522	ASP	-	expression tag	UNP P20839-5
G	523	SER	-	expression tag	UNP P20839-5
G	524	GLY	-	expression tag	UNP P20839-5
G	525	GLY	-	expression tag	UNP P20839-5
G	526	GLY	-	expression tag	UNP P20839-5
G	527	ARG	-	expression tag	UNP P20839-5
G	528	GLY	-	expression tag	UNP P20839-5
G	529	GLY	-	expression tag	UNP P20839-5
G	530	GLY	-	expression tag	UNP P20839-5
G	531	GLY	-	expression tag	UNP P20839-5
G	532	ASP	-	expression tag	UNP P20839-5
G	533	ALA	-	expression tag	UNP P20839-5
G	534	PRO	-	expression tag	UNP P20839-5
G	535	GLN	-	expression tag	UNP P20839-5
G	536	CYS	-	expression tag	UNP P20839-5
G	537	PRO	-	expression tag	UNP P20839-5
G	538	LEU	-	expression tag	UNP P20839-5
G	539	LEU	-	expression tag	UNP P20839-5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	540	GLY	-	expression tag	UNP P20839-5
G	541	THR	-	expression tag	UNP P20839-5
G	542	ALA	-	expression tag	UNP P20839-5
G	543	SER	-	expression tag	UNP P20839-5
G	544	LEU	-	expression tag	UNP P20839-5
G	545	HIS	-	expression tag	UNP P20839-5
G	546	ASN	-	expression tag	UNP P20839-5
H	?	-	SER	deletion	UNP P20839-5
H	?	-	CYS	deletion	UNP P20839-5
H	?	-	PHE	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	GLU	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	SER	deletion	UNP P20839-5
H	?	-	SER	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	ALA	deletion	UNP P20839-5
H	?	-	GLY	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	GLY	deletion	UNP P20839-5
H	?	-	VAL	deletion	UNP P20839-5
H	?	-	GLN	deletion	UNP P20839-5
H	?	-	MET	deletion	UNP P20839-5
H	?	-	ASP	deletion	UNP P20839-5
H	?	-	ARG	deletion	UNP P20839-5
H	?	-	LEU	deletion	UNP P20839-5
H	?	-	ARG	deletion	UNP P20839-5
H	?	-	ARG	deletion	UNP P20839-5
H	?	-	ALA	deletion	UNP P20839-5
H	510	THR	-	expression tag	UNP P20839-5
H	511	PHE	-	expression tag	UNP P20839-5
H	512	LEU	-	expression tag	UNP P20839-5
H	513	PRO	-	expression tag	UNP P20839-5
H	514	PHE	-	expression tag	UNP P20839-5
H	515	THR	-	expression tag	UNP P20839-5
H	516	LYS	-	expression tag	UNP P20839-5
H	517	SER	-	expression tag	UNP P20839-5
H	518	GLY	-	expression tag	UNP P20839-5

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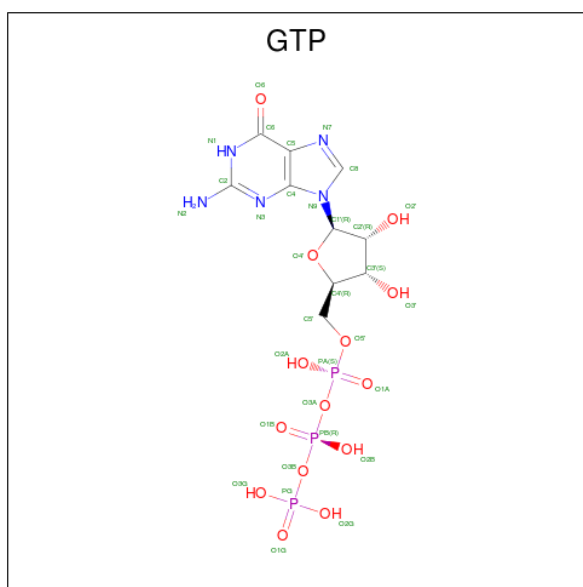


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Chain	Residue	Modelled	Actual	Comment	Reference
H	519	CYS	-	expression tag	UNP P20839-5
H	520	THR	-	expression tag	UNP P20839-5
H	521	GLU	-	expression tag	UNP P20839-5
H	522	ASP	-	expression tag	UNP P20839-5
H	523	SER	-	expression tag	UNP P20839-5
H	524	GLY	-	expression tag	UNP P20839-5
H	525	GLY	-	expression tag	UNP P20839-5
H	526	GLY	-	expression tag	UNP P20839-5
H	527	ARG	-	expression tag	UNP P20839-5
H	528	GLY	-	expression tag	UNP P20839-5
H	529	GLY	-	expression tag	UNP P20839-5
H	530	GLY	-	expression tag	UNP P20839-5
H	531	GLY	-	expression tag	UNP P20839-5
H	532	ASP	-	expression tag	UNP P20839-5
H	533	ALA	-	expression tag	UNP P20839-5
H	534	PRO	-	expression tag	UNP P20839-5
H	535	GLN	-	expression tag	UNP P20839-5
H	536	CYS	-	expression tag	UNP P20839-5
H	537	PRO	-	expression tag	UNP P20839-5
H	538	LEU	-	expression tag	UNP P20839-5
H	539	LEU	-	expression tag	UNP P20839-5
H	540	GLY	-	expression tag	UNP P20839-5
H	541	THR	-	expression tag	UNP P20839-5
H	542	ALA	-	expression tag	UNP P20839-5
H	543	SER	-	expression tag	UNP P20839-5
H	544	LEU	-	expression tag	UNP P20839-5
H	545	HIS	-	expression tag	UNP P20839-5
H	546	ASN	-	expression tag	UNP P20839-5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





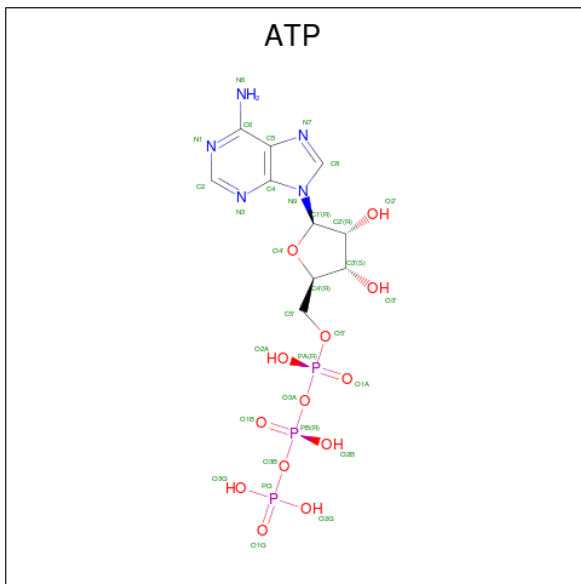
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	A	1	Total 88	20	24	10	28	6	0
2	A	1	Total 88	20	24	10	28	6	0
2	B	1	Total 88	20	24	10	28	6	0
2	B	1	Total 88	20	24	10	28	6	0
2	C	1	Total 88	20	24	10	28	6	0
2	C	1	Total 88	20	24	10	28	6	0
2	D	1	Total 88	20	24	10	28	6	0
2	D	1	Total 88	20	24	10	28	6	0
2	E	1	Total 88	20	24	10	28	6	0
2	E	1	Total 88	20	24	10	28	6	0
2	F	1	Total 88	20	24	10	28	6	0
2	F	1	Total 88	20	24	10	28	6	0
2	G	1	Total 88	20	24	10	28	6	0
2	G	1	Total 88	20	24	10	28	6	0

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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	H	1	Total	C	H	N	O	P	0
			88	20	24	10	28	6	
2	H	1	Total	C	H	N	O	P	0
			88	20	24	10	28	6	

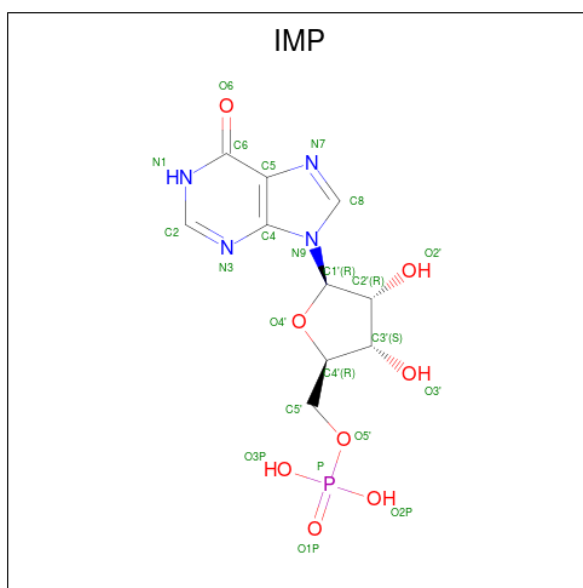
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
3	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	G	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	H	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

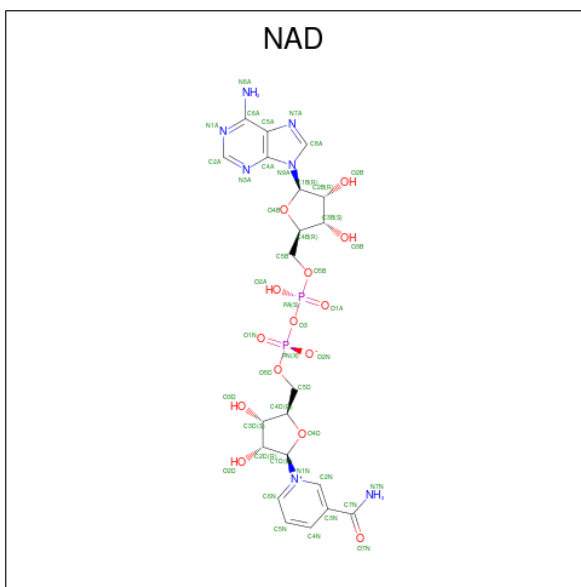
- Molecule 4 is INOSINIC ACID (three-letter code: IMP) (formula:  $C_{10}H_{13}N_4O_8P$ ) (labeled

as "Ligand of Interest" by depositor).



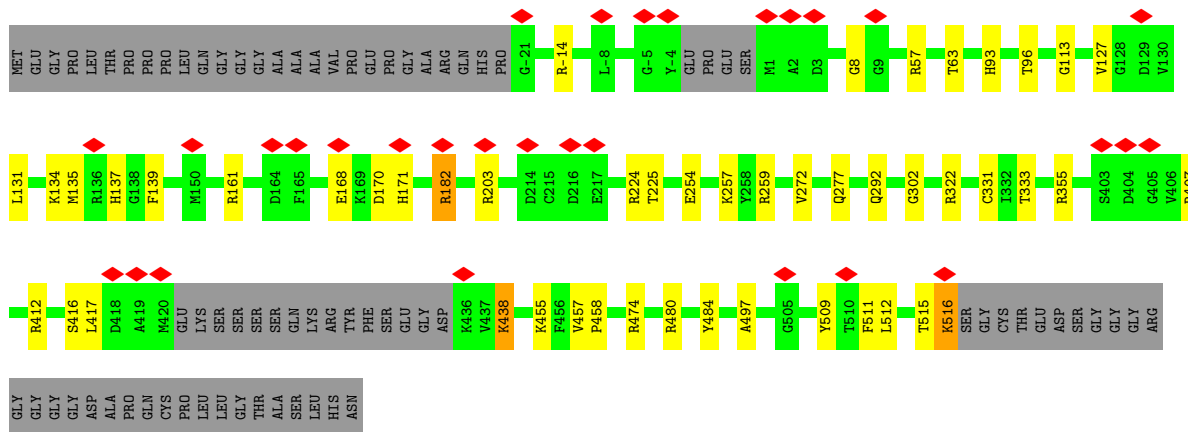
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
4	A	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	
4	B	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	
4	C	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	
4	D	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	
4	E	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	
4	F	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	
4	G	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	
4	H	1	Total	C	H	N	O	P	0
			34	10	11	4	8	1	

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

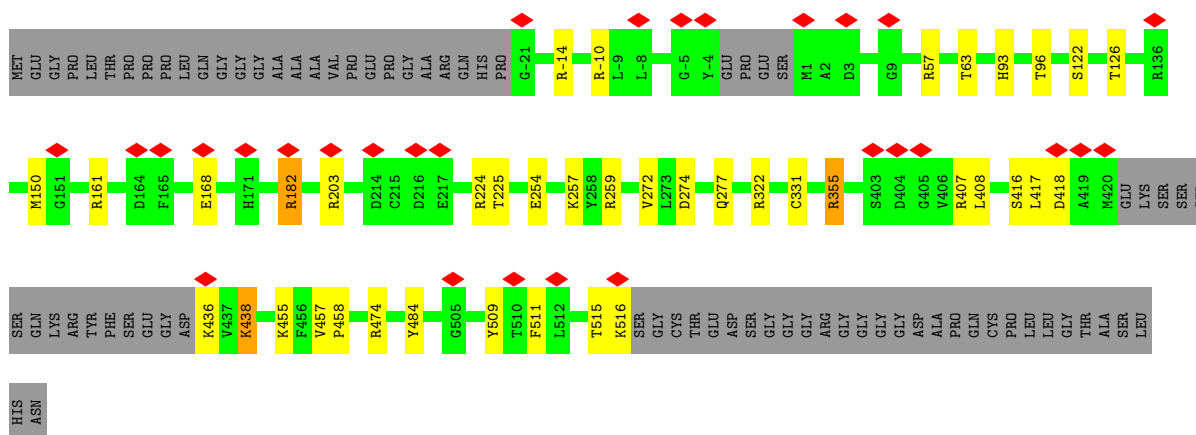
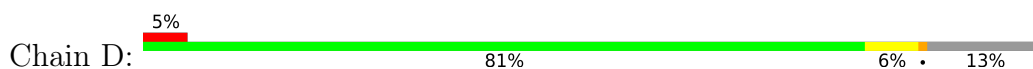


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
5	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
5	B	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
5	C	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
5	D	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
5	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
5	F	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
5	G	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
5	H	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

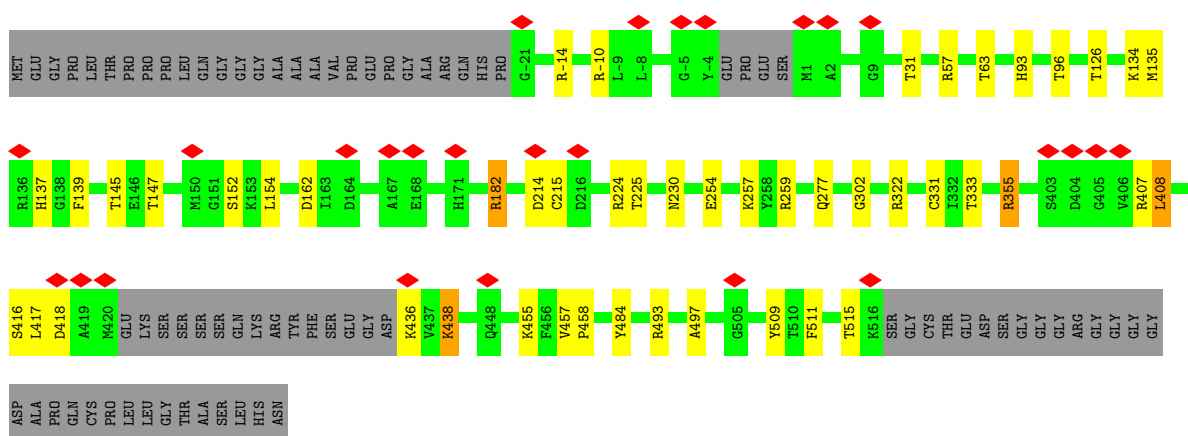
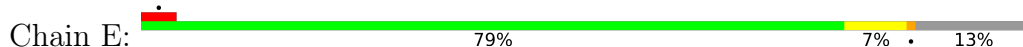




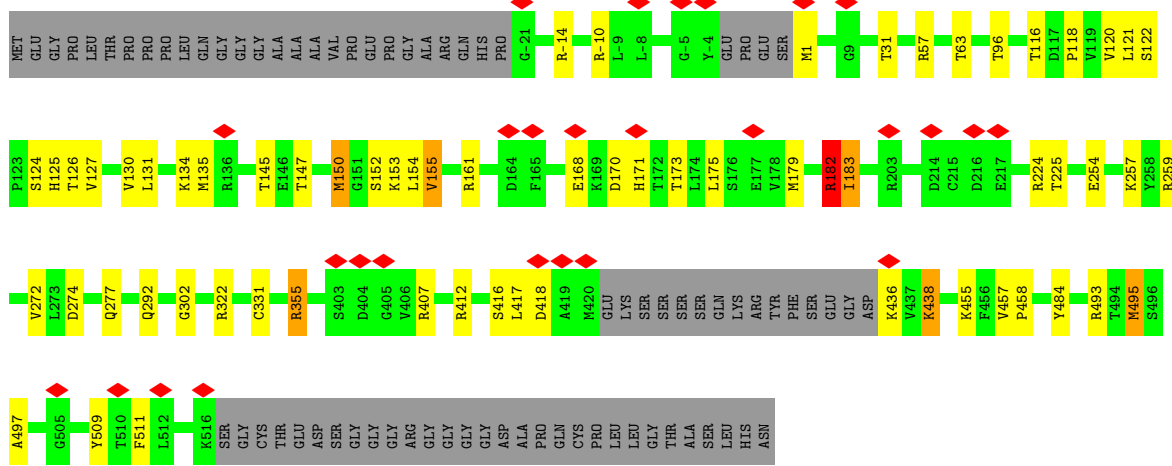
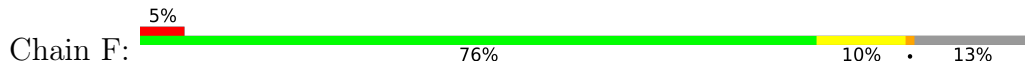
• Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



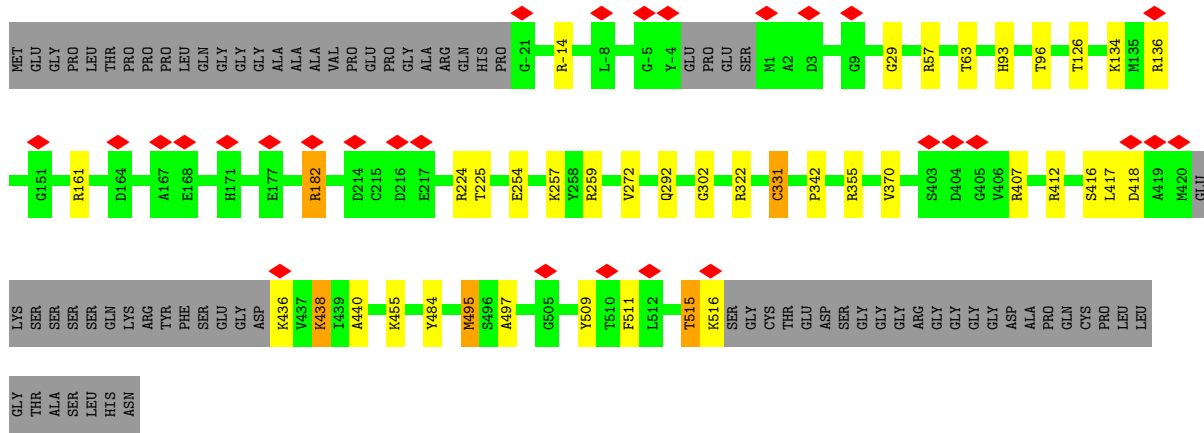
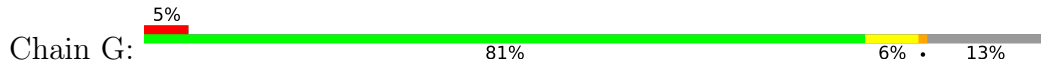
• Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



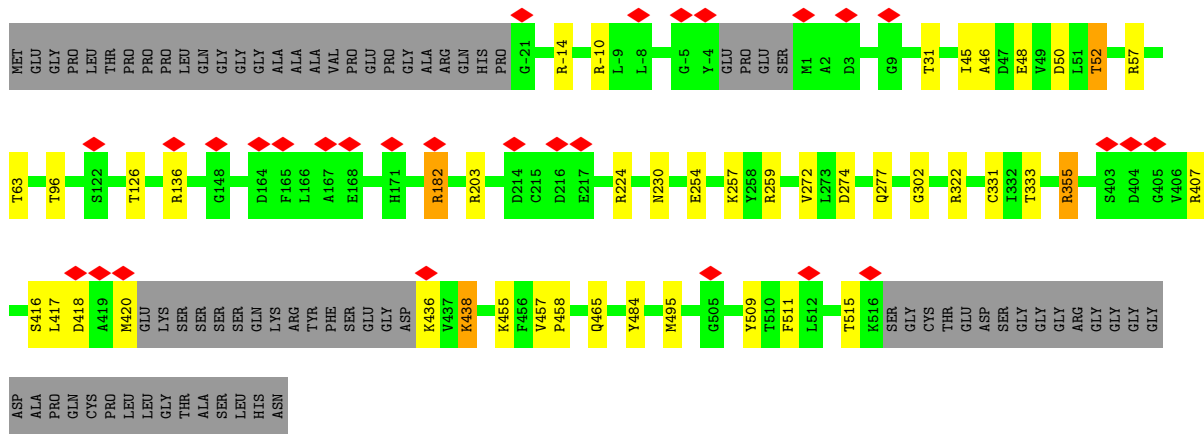
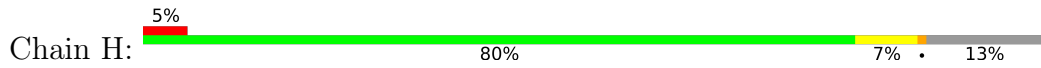
• Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



• Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1



• Molecule 1: Isoform 5 of Inosine-5'-monophosphate dehydrogenase 1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95415	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 ( $e^-/\text{\AA}^2$ )	50	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	12.157	Depositor
Minimum map value	-6.421	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.305	Depositor
Recommended contour level	1.24	Depositor
Map size (Å)	337.2, 337.2, 337.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84300005, 0.84300005, 0.84300005	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, IMP, NAD, 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	0.60	0/3972	0.97	9/5363 (0.2%)
1	B	0.60	0/3972	0.97	11/5363 (0.2%)
1	C	0.61	0/3972	0.96	11/5363 (0.2%)
1	D	0.60	0/3972	0.97	11/5363 (0.2%)
1	E	0.60	0/3972	0.95	9/5363 (0.2%)
1	F	0.60	0/3972	0.94	11/5363 (0.2%)
1	G	0.62	1/3972 (0.0%)	0.97	8/5363 (0.1%)
1	H	0.61	0/3972	0.96	10/5363 (0.2%)
All	All	0.60	1/31776 (0.0%)	0.96	80/42904 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	331	CYS	CB-SG	-6.58	1.71	1.82

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	A	407	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	H	407	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	F	407	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	D	407	ARG	NE-CZ-NH2	7.35	123.98	120.30
1	E	407	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	B	259	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	H	259	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	G	-14	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	G	407	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	E	-14	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	259	ARG	NE-CZ-NH1	7.13	123.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-14	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	-14	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	G	136	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	C	259	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	F	259	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	407	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	D	259	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	F	-14	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	-10	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	H	-10	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	H	-14	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	-14	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	G	161	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	C	-14	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	H	136	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	G	259	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	E	259	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	182	ARG	NE-CZ-NH2	6.35	123.48	120.30
1	A	136	ARG	NE-CZ-NH2	6.19	123.40	120.30
1	G	57	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	C	161	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	474	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	G	182	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	E	224	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	H	182	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	D	474	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	B	161	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	182	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	B	224	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	182	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	F	182	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	57	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	E	182	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	D	57	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	F	183	ILE	O-C-N	-5.81	113.41	122.70
1	A	224	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	G	224	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	57	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	D	-10	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	-10	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	A	182	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	161	ARG	NE-CZ-NH1	5.65	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	161	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	F	493	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	-10	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	57	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	D	224	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	F	-10	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	E	493	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	H	224	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	412	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	57	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	F	355	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	H	355	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	C	224	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	H	57	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	B	355	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	F	224	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	D	355	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	C	57	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	161	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	480	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	D	203	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	493	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	H	203	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	341	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	203	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	355	ARG	NE-CZ-NH2	5.04	122.82	120.30

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	3911	3980	3983	8	0
1	B	3911	3980	3983	16	0
1	C	3911	3980	3983	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3911	3980	3983	13	0
1	E	3911	3980	3983	21	0
1	F	3911	3980	3983	38	0
1	G	3911	3980	3983	17	0
1	H	3911	3980	3983	20	0
2	A	64	24	24	1	0
2	B	64	24	24	0	0
2	C	64	24	24	1	0
2	D	64	24	24	0	0
2	E	64	24	24	2	0
2	F	64	24	24	0	0
2	G	64	24	24	1	0
2	H	64	24	24	1	0
3	A	31	12	12	0	0
3	B	31	12	12	0	0
3	C	31	12	12	0	0
3	D	31	12	12	0	0
3	E	31	12	12	0	0
3	F	31	12	12	0	0
3	G	31	12	12	0	0
3	H	31	12	12	0	0
4	A	23	11	11	0	0
4	B	23	11	11	1	0
4	C	23	11	11	1	0
4	D	23	11	11	1	0
4	E	23	11	11	1	0
4	F	23	11	11	1	0
4	G	23	11	11	1	0
4	H	23	11	11	1	0
5	A	44	26	26	0	0
5	B	44	26	26	0	0
5	C	44	26	26	0	0
5	D	44	26	26	0	0
5	E	44	26	26	0	0
5	F	44	26	26	0	0
5	G	44	26	26	0	0
5	H	44	26	26	0	0
All	All	32584	32424	32448	144	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 2.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:VAL:O	1:F:131:LEU:HD12	1.82	0.78
1:E:147:THR:HG23	1:E:152:SER:OG	1.85	0.75
1:F:147:THR:HG23	1:F:152:SER:OG	1.85	0.75
1:F:175:LEU:O	1:F:179:MET:HG2	1.87	0.75
1:H:45:ILE:HG13	1:H:48:GLU:HG3	1.67	0.74
1:E:134:LYS:HD3	1:E:134:LYS:O	1.89	0.72
1:B:134:LYS:O	1:B:134:LYS:HD3	1.90	0.72
1:F:134:LYS:O	1:F:134:LYS:HD3	1.90	0.71
1:C:134:LYS:O	1:C:134:LYS:HD3	1.90	0.70
1:D:436:LYS:HE2	1:D:436:LYS:N	2.06	0.70
1:H:45:ILE:CG1	1:H:48:GLU:HG3	2.23	0.68
1:G:417:LEU:HD12	1:G:440:ALA:HB2	1.76	0.67
1:F:126:THR:HA	1:F:173:THR:O	1.94	0.66
1:H:495:MET:CE	1:H:495:MET:H	2.10	0.65
1:C:170:ASP:OD1	1:C:171:HIS:N	2.30	0.65
1:B:170:ASP:OD1	1:B:171:HIS:N	2.30	0.64
1:F:170:ASP:OD1	1:F:171:HIS:N	2.30	0.64
1:F:150:MET:SD	1:F:150:MET:N	2.62	0.63
1:F:130:VAL:CG2	1:F:175:LEU:HD21	2.29	0.63
1:F:145:THR:HB	1:F:152:SER:HB3	1.80	0.62
1:C:225:THR:HG21	2:C:601:GTP:H3'	1.82	0.62
1:C:416:SER:O	1:C:417:LEU:HB2	2.00	0.61
1:F:153:LYS:NZ	1:F:153:LYS:HB2	2.16	0.60
1:E:145:THR:HB	1:E:152:SER:HB3	1.83	0.60
1:G:495:MET:HE3	1:G:495:MET:H	1.66	0.60
1:C:127:VAL:O	1:C:131:LEU:HD12	2.02	0.59
1:E:254:GLU:OE1	1:E:257:LYS:NZ	2.34	0.59
1:D:254:GLU:OE1	1:D:257:LYS:NZ	2.34	0.59
1:G:495:MET:H	1:G:495:MET:CE	2.16	0.59
1:H:416:SER:O	1:H:417:LEU:HB2	2.02	0.58
1:F:130:VAL:HG21	1:F:175:LEU:HD21	1.86	0.58
1:D:416:SER:O	1:D:417:LEU:HB2	2.03	0.57
1:B:127:VAL:O	1:B:131:LEU:HD12	2.03	0.57
1:E:436:LYS:HA	1:E:436:LYS:HE2	1.87	0.57
1:H:254:GLU:OE1	1:H:257:LYS:NZ	2.36	0.57
1:C:254:GLU:OE1	1:C:257:LYS:NZ	2.37	0.56
1:E:436:LYS:N	1:E:436:LYS:HD2	2.20	0.56
1:D:417:LEU:HD21	1:D:438:LYS:HG3	1.88	0.55
1:F:254:GLU:OE1	1:F:257:LYS:NZ	2.36	0.55
1:G:254:GLU:OE1	1:G:257:LYS:NZ	2.35	0.55
1:F:155:VAL:C	1:F:179:MET:HE3	2.28	0.55
1:G:495:MET:SD	1:G:495:MET:N	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:THR:HG22	1:E:154:LEU:HA	1.91	0.52
1:G:29:GLY:HA3	1:G:342:PRO:HG2	1.92	0.52
1:E:147:THR:OG1	1:E:152:SER:HB2	2.09	0.51
1:F:147:THR:OG1	1:F:152:SER:HB2	2.11	0.51
1:D:436:LYS:HE2	1:D:436:LYS:CA	2.41	0.51
1:C:331:CYS:SG	4:C:604:IMP:H2	2.51	0.50
1:H:50:ASP:CG	1:H:52:THR:HG22	2.32	0.50
1:F:118:PRO:HD2	1:F:150:MET:HE2	1.94	0.50
1:H:50:ASP:OD2	1:H:52:THR:HG22	2.12	0.49
1:H:457:VAL:N	1:H:458:PRO:HD2	2.28	0.49
1:D:457:VAL:N	1:D:458:PRO:HD2	2.28	0.49
1:F:145:THR:HG22	1:F:154:LEU:HA	1.93	0.49
1:H:495:MET:SD	1:H:495:MET:N	2.85	0.49
1:A:457:VAL:N	1:A:458:PRO:HD2	2.28	0.49
1:D:168:GLU:OE1	1:D:168:GLU:HA	2.13	0.48
1:E:457:VAL:N	1:E:458:PRO:HD2	2.28	0.48
1:F:457:VAL:N	1:F:458:PRO:HD2	2.28	0.48
1:B:457:VAL:N	1:B:458:PRO:HD2	2.28	0.48
1:C:457:VAL:N	1:C:458:PRO:HD2	2.28	0.48
1:H:331:CYS:SG	4:H:604:IMP:H2	2.54	0.48
1:E:417:LEU:HD23	1:E:417:LEU:HA	1.72	0.48
1:B:331:CYS:SG	4:B:604:IMP:H2	2.54	0.48
1:F:126:THR:HG22	1:F:173:THR:O	2.14	0.48
1:B:436:LYS:N	1:B:436:LYS:HD2	2.29	0.47
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.74	0.47
1:E:331:CYS:SG	4:E:604:IMP:H2	2.53	0.47
1:C:168:GLU:HA	1:C:168:GLU:OE1	2.14	0.47
1:F:168:GLU:HA	1:F:168:GLU:OE1	2.14	0.47
1:B:168:GLU:HA	1:B:168:GLU:OE1	2.14	0.47
1:H:417:LEU:HD21	1:H:438:LYS:HG3	1.97	0.47
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.76	0.47
1:C:417:LEU:HA	1:C:417:LEU:HD23	1.72	0.47
1:G:355:ARG:HD2	1:G:484:TYR:CZ	2.50	0.46
1:D:331:CYS:SG	4:D:604:IMP:H2	2.55	0.46
1:G:416:SER:C	1:G:418:ASP:H	2.18	0.46
1:H:50:ASP:OD1	1:H:52:THR:HG22	2.15	0.46
1:F:331:CYS:SG	4:F:604:IMP:H2	2.55	0.46
1:G:438:LYS:HD3	1:G:438:LYS:HA	1.84	0.46
1:E:416:SER:C	1:E:418:ASP:H	2.19	0.46
1:E:230:ASN:ND2	2:E:602:GTP:C8	2.83	0.46
1:G:331:CYS:SG	4:G:604:IMP:H2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:436:LYS:N	1:H:436:LYS:HD2	2.31	0.46
1:B:122:SER:H	1:B:125:HIS:HD2	1.64	0.46
1:G:495:MET:HE3	1:G:495:MET:N	2.31	0.46
1:H:46:ALA:O	1:H:465:GLN:HB3	2.16	0.46
1:F:436:LYS:N	1:F:436:LYS:HD2	2.32	0.45
1:H:417:LEU:HD23	1:H:417:LEU:HA	1.74	0.45
1:F:168:GLU:OE1	1:F:168:GLU:CA	2.64	0.45
1:B:168:GLU:OE1	1:B:168:GLU:CA	2.65	0.45
1:C:355:ARG:HD2	1:C:484:TYR:CZ	2.51	0.45
1:B:355:ARG:HD2	1:B:484:TYR:CZ	2.51	0.45
1:C:168:GLU:OE1	1:C:168:GLU:CA	2.65	0.45
1:D:355:ARG:HD2	1:D:484:TYR:CZ	2.53	0.44
1:G:417:LEU:HD21	1:G:438:LYS:HG3	1.98	0.44
1:H:495:MET:HB3	1:H:495:MET:HE3	1.88	0.44
1:D:438:LYS:HD3	1:D:438:LYS:HA	1.83	0.44
1:A:436:LYS:N	1:A:436:LYS:HD2	2.32	0.44
1:F:127:VAL:HG12	1:F:131:LEU:CD1	2.48	0.44
1:C:438:LYS:HD3	1:C:438:LYS:HA	1.85	0.43
1:E:214:ASP:N	1:E:214:ASP:OD1	2.51	0.43
1:G:436:LYS:HD2	1:G:436:LYS:N	2.33	0.43
1:D:168:GLU:OE1	1:D:168:GLU:CA	2.64	0.43
1:A:417:LEU:HD21	1:A:438:LYS:HG3	2.00	0.43
1:F:417:LEU:HD22	1:G:515:THR:HG22	2.00	0.43
1:H:230:ASN:ND2	2:H:602:GTP:C8	2.86	0.43
1:F:355:ARG:HD2	1:F:484:TYR:CZ	2.52	0.43
1:E:497:ALA:HA	1:H:31:THR:HG21	2.01	0.43
1:F:135:MET:O	1:F:135:MET:HG2	2.18	0.43
1:B:135:MET:HG2	1:B:135:MET:O	2.18	0.43
1:A:355:ARG:HD2	1:A:484:TYR:CZ	2.53	0.43
1:C:516:LYS:HD3	1:C:516:LYS:HA	1.77	0.43
1:F:416:SER:C	1:F:418:ASP:H	2.22	0.43
1:H:416:SER:C	1:H:418:ASP:H	2.23	0.43
1:C:135:MET:O	1:C:135:MET:HG2	2.18	0.43
1:D:416:SER:C	1:D:418:ASP:H	2.22	0.42
1:D:417:LEU:HA	1:D:417:LEU:HD23	1.75	0.42
1:A:230:ASN:ND2	2:A:602:GTP:C8	2.88	0.42
1:F:438:LYS:HD3	1:F:438:LYS:HA	1.85	0.42
1:F:183:ILE:HG13	1:F:183:ILE:O	2.19	0.42
1:B:31:THR:HG21	1:C:497:ALA:HA	2.01	0.42
1:G:225:THR:HG23	2:G:601:GTP:H3'	2.01	0.42
1:G:516:LYS:HD3	1:G:516:LYS:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LEU:HD21	1:B:438:LYS:HG3	2.02	0.41
1:C:137:HIS:HB3	1:C:139:PHE:CE2	2.55	0.41
1:A:31:THR:HG21	1:B:497:ALA:HA	2.03	0.41
1:E:31:THR:HG21	1:F:497:ALA:HA	2.02	0.41
1:F:120:VAL:O	1:F:121:LEU:HD23	2.21	0.41
1:H:355:ARG:HD2	1:H:484:TYR:CZ	2.55	0.41
1:B:121:LEU:HD23	1:B:121:LEU:HA	1.86	0.41
1:E:135:MET:HG2	1:E:135:MET:O	2.19	0.41
1:A:438:LYS:HD3	1:A:438:LYS:HA	1.88	0.41
1:E:225:THR:CG2	2:E:601:GTP:H3'	2.51	0.41
1:E:137:HIS:HB3	1:E:139:PHE:CE2	2.55	0.41
1:F:31:THR:HG21	1:G:497:ALA:HA	2.02	0.41
1:F:116:THR:C	1:F:118:PRO:HD3	2.41	0.41
1:E:355:ARG:HD2	1:E:484:TYR:CZ	2.55	0.41
1:F:122:SER:H	1:F:125:HIS:HD2	1.68	0.41
1:F:153:LYS:NZ	1:F:153:LYS:CB	2.84	0.41
1:E:438:LYS:HD3	1:E:438:LYS:HA	1.88	0.41
1:F:155:VAL:O	1:F:182:ARG:N	2.54	0.41
1:F:495:MET:N	1:F:495:MET:CE	2.84	0.41
1:F:121:LEU:HD23	1:F:121:LEU:HA	1.88	0.40

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	513/595 (86%)	474 (92%)	38 (7%)	1 (0%)	47 82
1	B	513/595 (86%)	479 (93%)	33 (6%)	1 (0%)	47 82
1	C	513/595 (86%)	480 (94%)	30 (6%)	3 (1%)	25 64
1	D	513/595 (86%)	484 (94%)	28 (6%)	1 (0%)	47 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	513/595 (86%)	474 (92%)	37 (7%)	2 (0%)	34	72
1	F	513/595 (86%)	475 (93%)	36 (7%)	2 (0%)	34	72
1	G	513/595 (86%)	478 (93%)	34 (7%)	1 (0%)	47	82
1	H	513/595 (86%)	476 (93%)	35 (7%)	2 (0%)	34	72
All	All	4104/4760 (86%)	3820 (93%)	271 (7%)	13 (0%)	44	76

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	408	LEU
1	C	302	GLY
1	E	302	GLY
1	F	302	GLY
1	H	302	GLY
1	E	408	LEU
1	D	274	ASP
1	F	274	ASP
1	H	274	ASP
1	A	303	ASN
1	C	8	GLY
1	G	302	GLY
1	C	113	GLY

### 5.3.2 Protein sidechains [i](#)

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	419/474 (88%)	402 (96%)	17 (4%)	30	67
1	B	419/474 (88%)	398 (95%)	21 (5%)	24	60
1	C	419/474 (88%)	403 (96%)	16 (4%)	33	69
1	D	419/474 (88%)	401 (96%)	18 (4%)	29	66
1	E	419/474 (88%)	403 (96%)	16 (4%)	33	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	419/474 (88%)	401 (96%)	18 (4%)	29	66
1	G	419/474 (88%)	402 (96%)	17 (4%)	30	67
1	H	419/474 (88%)	404 (96%)	15 (4%)	35	70
All	All	3352/3792 (88%)	3214 (96%)	138 (4%)	34	67

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	93	HIS
1	A	134	LYS
1	A	162	ASP
1	A	169	LYS
1	A	182	ARG
1	A	225	THR
1	A	272	VAL
1	A	277	GLN
1	A	292	GLN
1	A	322	ARG
1	A	438	LYS
1	A	455	LYS
1	A	509	TYR
1	A	510	THR
1	A	511	PHE
1	A	515	THR
1	B	-20	HIS
1	B	1	MET
1	B	63	THR
1	B	93	HIS
1	B	96	THR
1	B	124	SER
1	B	182	ARG
1	B	272	VAL
1	B	277	GLN
1	B	322	ARG
1	B	333	THR
1	B	408	LEU
1	B	412	ARG
1	B	420	MET
1	B	438	LYS
1	B	455	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	495	MET
1	B	509	TYR
1	B	511	PHE
1	B	515	THR
1	B	516	LYS
1	C	63	THR
1	C	93	HIS
1	C	96	THR
1	C	182	ARG
1	C	272	VAL
1	C	277	GLN
1	C	292	GLN
1	C	322	ARG
1	C	333	THR
1	C	438	LYS
1	C	455	LYS
1	C	509	TYR
1	C	511	PHE
1	C	512	LEU
1	C	515	THR
1	C	516	LYS
1	D	63	THR
1	D	93	HIS
1	D	96	THR
1	D	122	SER
1	D	126	THR
1	D	150	MET
1	D	182	ARG
1	D	225	THR
1	D	272	VAL
1	D	277	GLN
1	D	322	ARG
1	D	408	LEU
1	D	438	LYS
1	D	455	LYS
1	D	509	TYR
1	D	511	PHE
1	D	515	THR
1	D	516	LYS
1	E	63	THR
1	E	93	HIS
1	E	96	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	126	THR
1	E	162	ASP
1	E	182	ARG
1	E	215	CYS
1	E	277	GLN
1	E	322	ARG
1	E	333	THR
1	E	408	LEU
1	E	438	LYS
1	E	455	LYS
1	E	509	TYR
1	E	511	PHE
1	E	515	THR
1	F	1	MET
1	F	63	THR
1	F	96	THR
1	F	124	SER
1	F	150	MET
1	F	155	VAL
1	F	182	ARG
1	F	225	THR
1	F	272	VAL
1	F	277	GLN
1	F	292	GLN
1	F	322	ARG
1	F	412	ARG
1	F	438	LYS
1	F	455	LYS
1	F	495	MET
1	F	509	TYR
1	F	511	PHE
1	G	63	THR
1	G	93	HIS
1	G	96	THR
1	G	126	THR
1	G	134	LYS
1	G	182	ARG
1	G	272	VAL
1	G	292	GLN
1	G	322	ARG
1	G	370	VAL
1	G	412	ARG

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Mol	Chain	Res	Type
1	G	438	LYS
1	G	455	LYS
1	G	495	MET
1	G	509	TYR
1	G	511	PHE
1	G	515	THR
1	H	52	THR
1	H	63	THR
1	H	96	THR
1	H	126	THR
1	H	182	ARG
1	H	272	VAL
1	H	277	GLN
1	H	322	ARG
1	H	333	THR
1	H	420	MET
1	H	438	LYS
1	H	455	LYS
1	H	509	TYR
1	H	511	PHE
1	H	515	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	HIS
1	B	283	GLN
1	C	-20	HIS
1	C	100	GLN
1	D	100	GLN
1	E	-20	HIS
1	E	100	GLN
1	E	283	GLN
1	F	-20	HIS
1	F	100	GLN
1	F	125	HIS
1	G	-20	HIS
1	H	100	GLN
1	H	498	GLN



### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

40 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
5	NAD	C	605	-	42,48,48	1.26	1 (2%)	50,73,73	1.30	5 (10%)
3	ATP	C	603	-	26,33,33	1.03	2 (7%)	31,52,52	1.39	6 (19%)
4	IMP	G	604	-	21,25,25	1.29	2 (9%)	24,38,38	1.03	1 (4%)
2	GTP	D	601	-	26,34,34	1.15	3 (11%)	32,54,54	1.54	4 (12%)
4	IMP	B	604	-	21,25,25	1.25	2 (9%)	24,38,38	1.05	2 (8%)
4	IMP	H	604	-	21,25,25	1.29	2 (9%)	24,38,38	1.07	2 (8%)
2	GTP	C	601	-	26,34,34	1.17	4 (15%)	32,54,54	1.51	5 (15%)
2	GTP	D	602	-	26,34,34	1.17	3 (11%)	32,54,54	1.35	5 (15%)
2	GTP	G	601	-	26,34,34	1.20	4 (15%)	32,54,54	1.44	4 (12%)
2	GTP	C	602	-	26,34,34	1.14	2 (7%)	32,54,54	1.45	5 (15%)
5	NAD	G	605	-	42,48,48	1.26	2 (4%)	50,73,73	1.29	5 (10%)
3	ATP	E	603	-	26,33,33	1.03	2 (7%)	31,52,52	1.38	6 (19%)
2	GTP	G	602	-	26,34,34	1.18	2 (7%)	32,54,54	1.33	5 (15%)
2	GTP	E	602	-	26,34,34	1.13	2 (7%)	32,54,54	1.42	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAD	B	605	-	42,48,48	1.22	1 (2%)	50,73,73	1.33	5 (10%)
2	GTP	B	602	-	26,34,34	1.15	2 (7%)	32,54,54	1.32	5 (15%)
2	GTP	H	602	-	26,34,34	1.17	2 (7%)	32,54,54	1.33	5 (15%)
4	IMP	E	604	-	21,25,25	1.25	2 (9%)	24,38,38	1.02	1 (4%)
5	NAD	A	605	-	42,48,48	1.26	1 (2%)	50,73,73	1.24	4 (8%)
4	IMP	F	604	-	21,25,25	1.26	2 (9%)	24,38,38	1.08	2 (8%)
3	ATP	A	603	-	26,33,33	1.04	2 (7%)	31,52,52	1.52	7 (22%)
5	NAD	E	605	-	42,48,48	1.26	1 (2%)	50,73,73	1.25	4 (8%)
4	IMP	A	604	-	21,25,25	1.23	2 (9%)	24,38,38	1.05	2 (8%)
2	GTP	B	601	-	26,34,34	1.16	3 (11%)	32,54,54	1.44	4 (12%)
5	NAD	F	605	-	42,48,48	1.27	1 (2%)	50,73,73	1.29	4 (8%)
3	ATP	F	603	-	26,33,33	1.00	1 (3%)	31,52,52	1.48	7 (22%)
5	NAD	D	605	-	42,48,48	1.25	2 (4%)	50,73,73	1.28	4 (8%)
2	GTP	E	601	-	26,34,34	1.21	2 (7%)	32,54,54	1.49	4 (12%)
3	ATP	G	603	-	26,33,33	1.05	2 (7%)	31,52,52	1.39	6 (19%)
2	GTP	A	602	-	26,34,34	1.17	2 (7%)	32,54,54	1.31	4 (12%)
2	GTP	F	601	-	26,34,34	1.20	3 (11%)	32,54,54	1.55	4 (12%)
2	GTP	H	601	-	26,34,34	1.16	3 (11%)	32,54,54	1.55	4 (12%)
4	IMP	D	604	-	21,25,25	1.27	2 (9%)	24,38,38	1.04	1 (4%)
5	NAD	H	605	-	42,48,48	1.24	1 (2%)	50,73,73	1.29	5 (10%)
2	GTP	A	601	-	26,34,34	1.18	3 (11%)	32,54,54	1.53	4 (12%)
4	IMP	C	604	-	21,25,25	1.29	2 (9%)	24,38,38	1.09	1 (4%)
3	ATP	H	603	-	26,33,33	1.04	2 (7%)	31,52,52	1.45	7 (22%)
2	GTP	F	602	-	26,34,34	1.17	2 (7%)	32,54,54	1.38	4 (12%)
3	ATP	B	603	-	26,33,33	1.03	2 (7%)	31,52,52	1.39	6 (19%)
3	ATP	D	603	-	26,33,33	1.00	1 (3%)	31,52,52	1.45	6 (19%)

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
5	NAD	C	605	-	-	6/26/62/62	0/5/5/5
3	ATP	C	603	-	-	0/18/38/38	0/3/3/3
4	IMP	G	604	-	-	0/6/26/26	0/3/3/3

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

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	NAD	C3N-C7N	-6.02	1.41	1.50
5	F	605	NAD	C3N-C7N	-5.93	1.41	1.50
5	E	605	NAD	C3N-C7N	-5.91	1.41	1.50
5	G	605	NAD	C3N-C7N	-5.83	1.41	1.50
5	C	605	NAD	C3N-C7N	-5.79	1.41	1.50
5	D	605	NAD	C3N-C7N	-5.79	1.41	1.50
5	H	605	NAD	C3N-C7N	-5.62	1.42	1.50
5	B	605	NAD	C3N-C7N	-5.54	1.42	1.50
4	C	604	IMP	O4'-C1'	3.06	1.45	1.41
4	G	604	IMP	O4'-C1'	3.04	1.45	1.41
4	D	604	IMP	O4'-C1'	2.99	1.45	1.41
4	H	604	IMP	O4'-C1'	2.93	1.45	1.41
4	E	604	IMP	O4'-C1'	2.89	1.45	1.41
4	A	604	IMP	C5-C4	-2.86	1.35	1.43
2	A	602	GTP	C8-N7	-2.84	1.30	1.35
4	A	604	IMP	O4'-C1'	2.82	1.45	1.41
4	G	604	IMP	C5-C4	-2.80	1.35	1.43
2	H	602	GTP	C8-N7	-2.79	1.30	1.35
4	F	604	IMP	O4'-C1'	2.76	1.44	1.41
4	B	604	IMP	O4'-C1'	2.76	1.44	1.41
4	D	604	IMP	C5-C4	-2.74	1.36	1.43
4	H	604	IMP	C5-C4	-2.73	1.36	1.43
4	F	604	IMP	C5-C4	-2.71	1.36	1.43
4	C	604	IMP	C5-C4	-2.68	1.36	1.43
4	B	604	IMP	C5-C4	-2.68	1.36	1.43
4	E	604	IMP	C5-C4	-2.67	1.36	1.43
2	F	602	GTP	C8-N7	-2.61	1.30	1.35
2	E	601	GTP	C5-C4	-2.58	1.36	1.43
2	B	602	GTP	C8-N7	-2.54	1.30	1.35
2	G	602	GTP	C8-N7	-2.54	1.30	1.35
2	D	602	GTP	C8-N7	-2.51	1.30	1.35
2	G	601	GTP	C5-C4	-2.47	1.36	1.43
2	C	601	GTP	C5-C4	-2.47	1.36	1.43
2	A	601	GTP	C5-C4	-2.47	1.36	1.43
2	D	602	GTP	C5-C4	-2.45	1.36	1.43
2	C	602	GTP	C8-N7	-2.45	1.30	1.35
2	G	602	GTP	C5-C4	-2.44	1.36	1.43
2	B	601	GTP	C5-C4	-2.43	1.36	1.43
2	C	602	GTP	C5-C4	-2.43	1.36	1.43
2	F	601	GTP	C8-N7	-2.42	1.30	1.35
2	E	602	GTP	C5-C4	-2.41	1.36	1.43
2	F	601	GTP	C5-C4	-2.41	1.36	1.43
2	D	601	GTP	C5-C4	-2.40	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	GTP	C5-C4	-2.39	1.37	1.43
2	E	601	GTP	C8-N7	-2.33	1.31	1.35
2	B	602	GTP	C5-C4	-2.33	1.37	1.43
2	G	601	GTP	C8-N7	-2.32	1.31	1.35
2	E	602	GTP	C8-N7	-2.31	1.31	1.35
2	A	602	GTP	C5-C4	-2.31	1.37	1.43
2	F	602	GTP	C5-C4	-2.31	1.37	1.43
3	G	603	ATP	O4'-C1'	2.30	1.44	1.41
2	A	601	GTP	C8-N7	-2.30	1.31	1.35
2	H	602	GTP	C5-C4	-2.29	1.37	1.43
2	D	601	GTP	C8-N7	-2.26	1.31	1.35
3	C	603	ATP	O4'-C1'	2.23	1.44	1.41
2	H	601	GTP	C8-N7	-2.23	1.31	1.35
2	B	601	GTP	C8-N7	-2.20	1.31	1.35
2	C	601	GTP	C8-N7	-2.19	1.31	1.35
3	H	603	ATP	O4'-C1'	2.17	1.44	1.41
3	E	603	ATP	O4'-C1'	2.16	1.44	1.41
3	B	603	ATP	O4'-C1'	2.14	1.44	1.41
3	A	603	ATP	O4'-C1'	2.11	1.44	1.41
2	C	601	GTP	PG-O3G	-2.07	1.46	1.54
3	G	603	ATP	C5-C4	-2.06	1.35	1.40
2	G	601	GTP	PG-O2G	-2.06	1.46	1.54
3	D	603	ATP	C5-C4	-2.05	1.35	1.40
3	C	603	ATP	C5-C4	-2.05	1.35	1.40
3	A	603	ATP	C5-C4	-2.05	1.35	1.40
2	A	601	GTP	PG-O3G	-2.04	1.47	1.54
2	D	601	GTP	PG-O3G	-2.03	1.47	1.54
2	G	601	GTP	PG-O3G	-2.03	1.47	1.54
3	E	603	ATP	C5-C4	-2.03	1.35	1.40
2	F	601	GTP	PG-O3G	-2.02	1.47	1.54
2	B	601	GTP	PG-O2G	-2.02	1.47	1.54
5	D	605	NAD	C2N-C3N	2.02	1.42	1.39
3	B	603	ATP	C5-C4	-2.02	1.35	1.40
5	G	605	NAD	C2N-C3N	2.02	1.42	1.39
2	H	601	GTP	PG-O3G	-2.01	1.47	1.54
3	F	603	ATP	C5-C4	-2.01	1.35	1.40
3	H	603	ATP	C5-C4	-2.01	1.35	1.40
2	D	602	GTP	C5-C6	-2.01	1.43	1.47
2	C	601	GTP	PG-O2G	-2.00	1.47	1.54

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	605	NAD	PN-O3-PA	-4.81	116.31	132.83
5	D	605	NAD	PN-O3-PA	-4.77	116.47	132.83
5	F	605	NAD	PN-O3-PA	-4.75	116.52	132.83
5	C	605	NAD	PN-O3-PA	-4.74	116.55	132.83
5	G	605	NAD	PN-O3-PA	-4.73	116.59	132.83
2	H	601	GTP	PA-O3A-PB	-4.58	117.10	132.83
5	E	605	NAD	PN-O3-PA	-4.54	117.24	132.83
2	D	601	GTP	PA-O3A-PB	-4.50	117.39	132.83
5	A	605	NAD	PN-O3-PA	-4.40	117.73	132.83
5	B	605	NAD	PN-O3-PA	-4.31	118.02	132.83
3	F	603	ATP	C4-C5-N7	4.26	113.83	109.40
2	A	601	GTP	PB-O3B-PG	-4.21	118.38	132.83
2	E	601	GTP	O6-C6-N1	-4.19	115.70	120.65
3	A	603	ATP	C4-C5-N7	4.13	113.71	109.40
3	G	603	ATP	C4-C5-N7	4.13	113.71	109.40
2	F	601	GTP	O6-C6-N1	-4.09	115.81	120.65
2	F	601	GTP	PA-O3A-PB	-4.09	118.79	132.83
3	D	603	ATP	C4-C5-N7	4.08	113.66	109.40
3	C	603	ATP	C4-C5-N7	4.08	113.65	109.40
3	E	603	ATP	C4-C5-N7	4.07	113.64	109.40
2	F	601	GTP	PB-O3B-PG	-4.05	118.93	132.83
3	H	603	ATP	C4-C5-N7	4.02	113.59	109.40
2	E	601	GTP	PA-O3A-PB	-4.02	119.04	132.83
2	G	601	GTP	PB-O3B-PG	-4.01	119.05	132.83
3	B	603	ATP	C4-C5-N7	3.90	113.47	109.40
2	A	601	GTP	O6-C6-N1	-3.84	116.11	120.65
2	B	601	GTP	PA-O3A-PB	-3.84	119.65	132.83
2	C	602	GTP	PB-O3B-PG	-3.84	119.66	132.83
2	C	602	GTP	PA-O3A-PB	-3.82	119.72	132.83
2	H	601	GTP	O6-C6-N1	-3.77	116.20	120.65
2	C	601	GTP	PA-O3A-PB	-3.73	120.04	132.83
2	D	601	GTP	PB-O3B-PG	-3.72	120.07	132.83
2	G	601	GTP	O6-C6-N1	-3.71	116.27	120.65
2	E	601	GTP	PB-O3B-PG	-3.71	120.11	132.83
2	H	601	GTP	PB-O3B-PG	-3.69	120.17	132.83
2	F	602	GTP	PB-O3B-PG	-3.68	120.18	132.83
2	B	601	GTP	O6-C6-N1	-3.67	116.32	120.65
5	B	605	NAD	C5A-C6A-N6A	3.66	125.92	120.35
2	D	601	GTP	O6-C6-N1	-3.65	116.33	120.65
5	C	605	NAD	C5A-C6A-N6A	3.64	125.88	120.35
2	C	601	GTP	O6-C6-N1	-3.59	116.41	120.65
2	E	602	GTP	O6-C6-N1	-3.57	116.43	120.65
2	B	601	GTP	PB-O3B-PG	-3.57	120.59	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	602	GTP	PB-O3B-PG	-3.54	120.69	132.83
5	E	605	NAD	C5A-C6A-N6A	3.53	125.71	120.35
5	A	605	NAD	C5A-C6A-N6A	3.51	125.69	120.35
2	F	602	GTP	PA-O3A-PB	-3.50	120.83	132.83
5	H	605	NAD	C5A-C6A-N6A	3.49	125.66	120.35
5	D	605	NAD	C5A-C6A-N6A	3.48	125.64	120.35
5	G	605	NAD	C5A-C6A-N6A	3.48	125.64	120.35
2	C	601	GTP	PB-O3B-PG	-3.46	120.96	132.83
5	F	605	NAD	C5A-C6A-N6A	3.44	125.58	120.35
2	D	602	GTP	PB-O3B-PG	-3.43	121.05	132.83
2	B	602	GTP	PB-O3B-PG	-3.43	121.07	132.83
2	E	602	GTP	PB-O3B-PG	-3.38	121.22	132.83
2	H	602	GTP	PB-O3B-PG	-3.38	121.24	132.83
2	A	601	GTP	PA-O3A-PB	-3.34	121.36	132.83
2	G	601	GTP	PA-O3A-PB	-3.34	121.37	132.83
2	A	602	GTP	PB-O3B-PG	-3.33	121.40	132.83
2	D	602	GTP	O6-C6-N1	-3.30	116.76	120.65
3	B	603	ATP	PB-O3B-PG	-3.23	121.76	132.83
2	F	602	GTP	O6-C6-N1	-3.20	116.86	120.65
2	B	602	GTP	O6-C6-N1	-3.15	116.93	120.65
3	D	603	ATP	PA-O3A-PB	-3.11	122.16	132.83
2	C	602	GTP	O6-C6-N1	-3.08	117.01	120.65
3	G	603	ATP	PB-O3B-PG	-3.08	122.27	132.83
2	A	602	GTP	PA-O3A-PB	-3.06	122.32	132.83
3	F	603	ATP	PA-O3A-PB	-3.05	122.35	132.83
2	H	602	GTP	O6-C6-N1	-3.05	117.05	120.65
2	B	602	GTP	PA-O3A-PB	-3.02	122.47	132.83
2	G	602	GTP	O6-C6-N1	-3.01	117.09	120.65
2	H	602	GTP	PA-O3A-PB	-2.98	122.59	132.83
2	F	601	GTP	O6-C6-C5	2.98	130.19	124.37
3	C	603	ATP	PB-O3B-PG	-2.96	122.66	132.83
3	D	603	ATP	PB-O3B-PG	-2.95	122.72	132.83
3	A	603	ATP	PA-O3A-PB	-2.90	122.88	132.83
2	G	602	GTP	PA-O3A-PB	-2.89	122.89	132.83
2	A	602	GTP	O6-C6-N1	-2.87	117.25	120.65
4	A	604	IMP	O4'-C4'-C3'	-2.86	99.46	105.11
2	E	602	GTP	PA-O3A-PB	-2.86	123.02	132.83
4	H	604	IMP	O4'-C4'-C3'	-2.83	99.51	105.11
4	C	604	IMP	O4'-C4'-C3'	-2.83	99.52	105.11
2	D	602	GTP	PA-O3A-PB	-2.81	123.19	132.83
2	F	602	GTP	O6-C6-C5	2.80	129.85	124.37
5	B	605	NAD	N6A-C6A-N1A	-2.80	112.76	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	GTP	O6-C6-C5	2.78	129.80	124.37
5	C	605	NAD	N6A-C6A-N1A	-2.76	112.84	118.57
2	A	601	GTP	O6-C6-C5	2.76	129.76	124.37
4	G	604	IMP	O4'-C4'-C3'	-2.75	99.67	105.11
4	F	604	IMP	O4'-C4'-C3'	-2.75	99.67	105.11
5	A	605	NAD	N6A-C6A-N1A	-2.74	112.89	118.57
5	B	605	NAD	C6N-N1N-C2N	-2.73	119.49	121.97
2	E	602	GTP	O6-C6-C5	2.72	129.68	124.37
3	F	603	ATP	O3G-PG-O3B	2.71	113.74	104.64
2	B	602	GTP	O6-C6-C5	2.70	129.65	124.37
4	E	604	IMP	O4'-C4'-C3'	-2.69	99.78	105.11
2	H	601	GTP	O6-C6-C5	2.68	129.60	124.37
5	E	605	NAD	N6A-C6A-N1A	-2.68	113.02	118.57
3	E	603	ATP	PA-O3A-PB	-2.67	123.66	132.83
4	D	604	IMP	O4'-C4'-C3'	-2.66	99.86	105.11
2	D	601	GTP	O6-C6-C5	2.65	129.55	124.37
2	G	601	GTP	O6-C6-C5	2.65	129.54	124.37
2	B	601	GTP	O6-C6-C5	2.64	129.54	124.37
3	H	603	ATP	PA-O3A-PB	-2.63	123.79	132.83
2	C	601	GTP	O6-C6-C5	2.63	129.52	124.37
2	D	602	GTP	O6-C6-C5	2.63	129.51	124.37
3	H	603	ATP	PB-O3B-PG	-2.62	123.83	132.83
2	H	602	GTP	O6-C6-C5	2.60	129.46	124.37
5	F	605	NAD	N6A-C6A-N1A	-2.60	113.19	118.57
3	E	603	ATP	PB-O3B-PG	-2.59	123.93	132.83
5	H	605	NAD	N6A-C6A-N1A	-2.59	113.20	118.57
2	G	602	GTP	O6-C6-C5	2.58	129.42	124.37
3	H	603	ATP	O3G-PG-O3B	2.58	113.29	104.64
2	A	602	GTP	O6-C6-C5	2.58	129.41	124.37
5	D	605	NAD	N6A-C6A-N1A	-2.57	113.24	118.57
3	A	603	ATP	PB-O3B-PG	-2.57	124.02	132.83
2	C	602	GTP	O6-C6-C5	2.56	129.37	124.37
5	G	605	NAD	N6A-C6A-N1A	-2.56	113.27	118.57
4	B	604	IMP	O4'-C4'-C3'	-2.54	100.09	105.11
3	A	603	ATP	O3G-PG-O3B	2.53	113.13	104.64
3	F	603	ATP	PB-O3B-PG	-2.53	124.14	132.83
3	D	603	ATP	O2G-PG-O3B	2.52	113.10	104.64
3	G	603	ATP	PA-O3A-PB	-2.48	124.33	132.83
3	C	603	ATP	PA-O3A-PB	-2.47	124.36	132.83
3	B	603	ATP	PA-O3A-PB	-2.46	124.40	132.83
5	B	605	NAD	O7N-C7N-N7N	-2.43	119.12	122.58
5	F	605	NAD	C6N-N1N-C2N	-2.43	119.76	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	ATP	O3G-PG-O3B	2.38	112.61	104.64
5	E	605	NAD	C6N-N1N-C2N	-2.37	119.81	121.97
3	A	603	ATP	O2G-PG-O3B	2.36	112.55	104.64
5	G	605	NAD	C6N-N1N-C2N	-2.33	119.85	121.97
3	G	603	ATP	O3G-PG-O3B	2.30	112.35	104.64
5	C	605	NAD	C6N-N1N-C2N	-2.29	119.88	121.97
3	B	603	ATP	O2G-PG-O3B	2.29	112.32	104.64
5	H	605	NAD	C6N-N1N-C2N	-2.22	119.95	121.97
3	H	603	ATP	C5-C6-N6	2.22	123.73	120.35
5	D	605	NAD	C6N-N1N-C2N	-2.21	119.96	121.97
5	A	605	NAD	C6N-N1N-C2N	-2.21	119.96	121.97
2	C	602	GTP	O3B-PG-O1G	-2.21	98.93	111.19
3	A	603	ATP	C5-C6-N6	2.21	123.71	120.35
3	F	603	ATP	C5-C6-N6	2.21	123.71	120.35
3	C	603	ATP	C5-C6-N6	2.20	123.69	120.35
3	G	603	ATP	C5-C6-N6	2.17	123.65	120.35
3	B	603	ATP	C5-C6-N6	2.17	123.64	120.35
3	A	603	ATP	N6-C6-N1	-2.16	114.08	118.57
3	F	603	ATP	O4'-C1'-C2'	-2.16	103.78	106.93
3	C	603	ATP	N6-C6-N1	-2.15	114.10	118.57
2	D	602	GTP	O5'-C5'-C4'	2.15	116.40	108.99
3	H	603	ATP	N6-C6-N1	-2.13	114.15	118.57
3	G	603	ATP	N6-C6-N1	-2.12	114.18	118.57
2	C	601	GTP	O3G-PG-O3B	2.11	111.73	104.64
3	B	603	ATP	N6-C6-N1	-2.10	114.21	118.57
3	D	603	ATP	C5-C6-N6	2.10	123.54	120.35
4	A	604	IMP	O2P-P-O5'	2.09	112.30	106.73
2	G	602	GTP	O5'-C5'-C4'	2.08	116.16	108.99
2	H	602	GTP	O5'-C5'-C4'	2.08	116.15	108.99
3	F	603	ATP	N6-C6-N1	-2.07	114.27	118.57
5	H	605	NAD	O7N-C7N-N7N	-2.07	119.64	122.58
2	E	602	GTP	O3G-PG-O2G	2.07	115.54	107.64
3	D	603	ATP	N6-C6-N1	-2.05	114.32	118.57
5	C	605	NAD	O7N-C7N-N7N	-2.05	119.67	122.58
4	F	604	IMP	O5'-P-O1P	2.05	112.22	106.47
3	H	603	ATP	O2G-PG-O3B	2.04	111.46	104.64
4	B	604	IMP	O2P-P-O5'	2.03	112.14	106.73
3	E	603	ATP	N6-C6-N1	-2.03	114.36	118.57
5	G	605	NAD	O7N-C7N-N7N	-2.03	119.69	122.58
2	B	602	GTP	O5'-C5'-C4'	2.03	115.97	108.99
3	E	603	ATP	O2G-PG-O3B	2.03	111.44	104.64
4	H	604	IMP	O5'-P-O1P	2.02	112.14	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	603	ATP	C5-C6-N6	2.01	123.40	120.35

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GTP	PB-O3B-PG-O3G
2	E	602	GTP	PB-O3B-PG-O3G
2	G	601	GTP	PB-O3A-PA-O5'
2	H	601	GTP	C5'-O5'-PA-O3A
2	H	602	GTP	PB-O3B-PG-O3G
5	B	605	NAD	C5D-O5D-PN-O3
5	C	605	NAD	C5B-O5B-PA-O1A
5	C	605	NAD	C5B-O5B-PA-O2A
5	D	605	NAD	C5B-O5B-PA-O2A
5	F	605	NAD	C5B-O5B-PA-O1A
5	F	605	NAD	C5B-O5B-PA-O2A
5	G	605	NAD	C5B-O5B-PA-O3
5	H	605	NAD	C5B-O5B-PA-O2A
2	A	602	GTP	O4'-C4'-C5'-O5'
2	B	602	GTP	O4'-C4'-C5'-O5'
2	D	602	GTP	O4'-C4'-C5'-O5'
2	F	602	GTP	O4'-C4'-C5'-O5'
2	G	602	GTP	O4'-C4'-C5'-O5'
2	H	601	GTP	O4'-C4'-C5'-O5'
2	H	601	GTP	C3'-C4'-C5'-O5'
2	H	602	GTP	O4'-C4'-C5'-O5'
5	C	605	NAD	O4B-C4B-C5B-O5B
5	D	605	NAD	O4B-C4B-C5B-O5B
5	F	605	NAD	O4B-C4B-C5B-O5B
5	G	605	NAD	O4B-C4B-C5B-O5B
5	H	605	NAD	O4B-C4B-C5B-O5B
5	C	605	NAD	C3B-C4B-C5B-O5B
5	F	605	NAD	C3B-C4B-C5B-O5B
5	D	605	NAD	C3B-C4B-C5B-O5B
2	E	602	GTP	PB-O3A-PA-O1A
2	B	602	GTP	C3'-C4'-C5'-O5'
2	F	602	GTP	C3'-C4'-C5'-O5'
5	H	605	NAD	C3B-C4B-C5B-O5B
5	G	605	NAD	C3B-C4B-C5B-O5B
2	B	601	GTP	PB-O3A-PA-O5'
2	C	601	GTP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
2	E	601	GTP	PB-O3A-PA-O5'
2	F	601	GTP	PB-O3A-PA-O5'
5	A	605	NAD	PN-O3-PA-O5B
5	B	605	NAD	PA-O3-PN-O5D
5	C	605	NAD	PN-O3-PA-O5B
5	D	605	NAD	PN-O3-PA-O5B
5	E	605	NAD	PN-O3-PA-O5B
5	F	605	NAD	PN-O3-PA-O5B
5	G	605	NAD	PN-O3-PA-O5B
5	H	605	NAD	PN-O3-PA-O5B
2	C	602	GTP	O4'-C4'-C5'-O5'
2	E	602	GTP	PB-O3B-PG-O1G
2	C	602	GTP	C5'-O5'-PA-O3A
2	D	601	GTP	PG-O3B-PB-O1B
2	F	602	GTP	PB-O3A-PA-O2A
5	B	605	NAD	C5D-O5D-PN-O1N
5	D	605	NAD	C5B-O5B-PA-O1A
5	G	605	NAD	C5B-O5B-PA-O1A
5	H	605	NAD	C5B-O5B-PA-O1A
2	G	602	GTP	C3'-C4'-C5'-O5'
2	D	602	GTP	C3'-C4'-C5'-O5'
2	E	602	GTP	O4'-C4'-C5'-O5'
2	H	602	GTP	PB-O3B-PG-O1G
4	F	604	IMP	C5'-O5'-P-O1P
5	B	605	NAD	C4D-C5D-O5D-PN
2	F	601	GTP	PA-O3A-PB-O3B
2	E	602	GTP	PB-O3A-PA-O2A
2	H	602	GTP	PB-O3A-PA-O1A
5	B	605	NAD	PN-O3-PA-O2A
2	E	602	GTP	C4'-C5'-O5'-PA
2	A	602	GTP	PB-O3A-PA-O1A
2	B	602	GTP	PB-O3A-PA-O1A
2	C	602	GTP	C3'-C4'-C5'-O5'
2	A	602	GTP	PB-O3B-PG-O1G
2	C	601	GTP	PB-O3B-PG-O1G
2	F	602	GTP	PB-O3B-PG-O2G
2	B	601	GTP	C5'-O5'-PA-O3A
5	C	605	NAD	C5B-O5B-PA-O3
5	D	605	NAD	C5B-O5B-PA-O3
5	F	605	NAD	C5B-O5B-PA-O3
5	H	605	NAD	C5B-O5B-PA-O3
2	A	601	GTP	C3'-C4'-C5'-O5'

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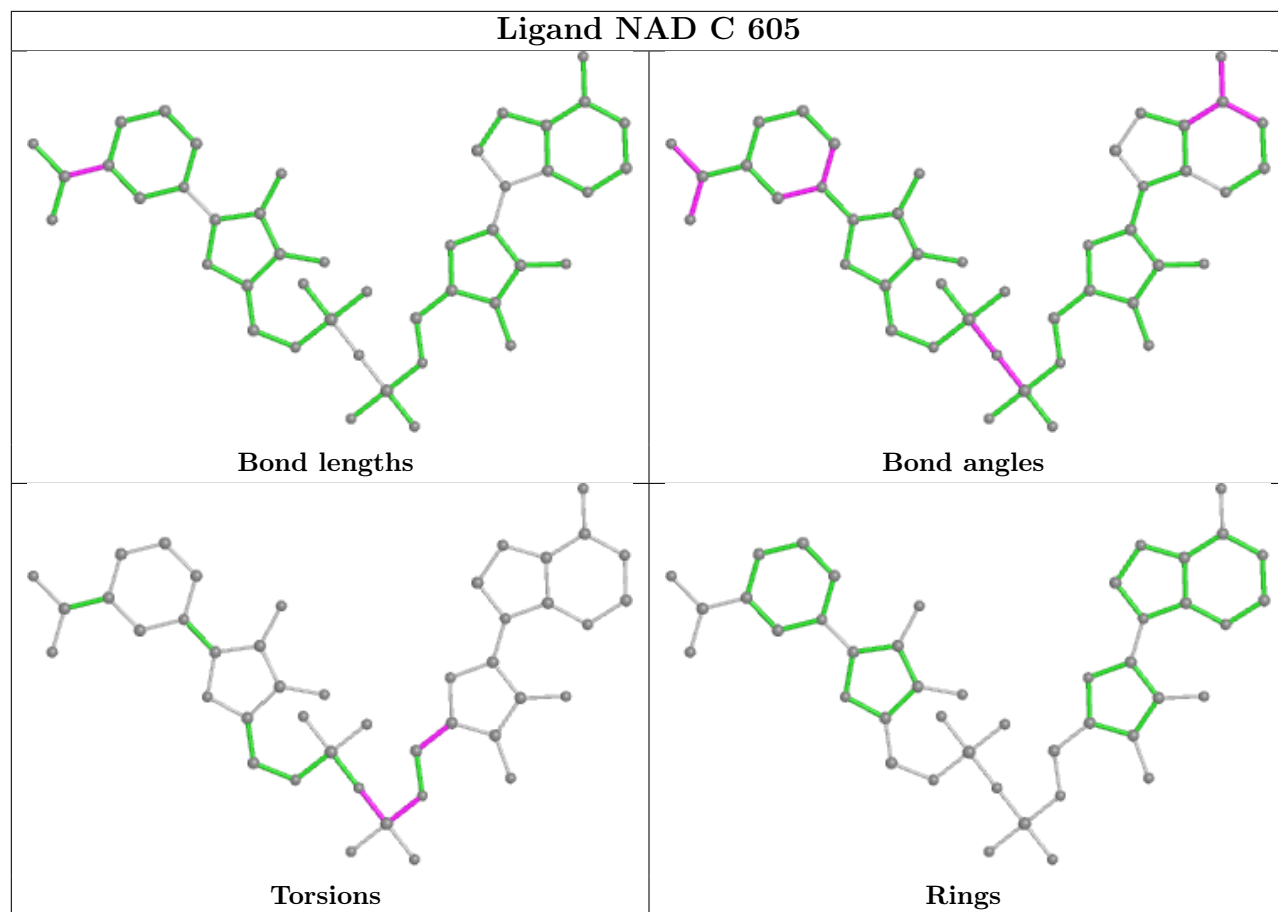
Mol	Chain	Res	Type	Atoms
2	A	602	GTP	PB-O3A-PA-O2A
2	B	602	GTP	PB-O3A-PA-O2A
2	D	602	GTP	PB-O3A-PA-O2A
2	F	601	GTP	PA-O3A-PB-O1B
2	G	602	GTP	PB-O3A-PA-O2A
2	H	602	GTP	PB-O3A-PA-O2A
3	E	603	ATP	PG-O3B-PB-O2B
3	G	603	ATP	PA-O3A-PB-O2B
5	B	605	NAD	PN-O3-PA-O1A

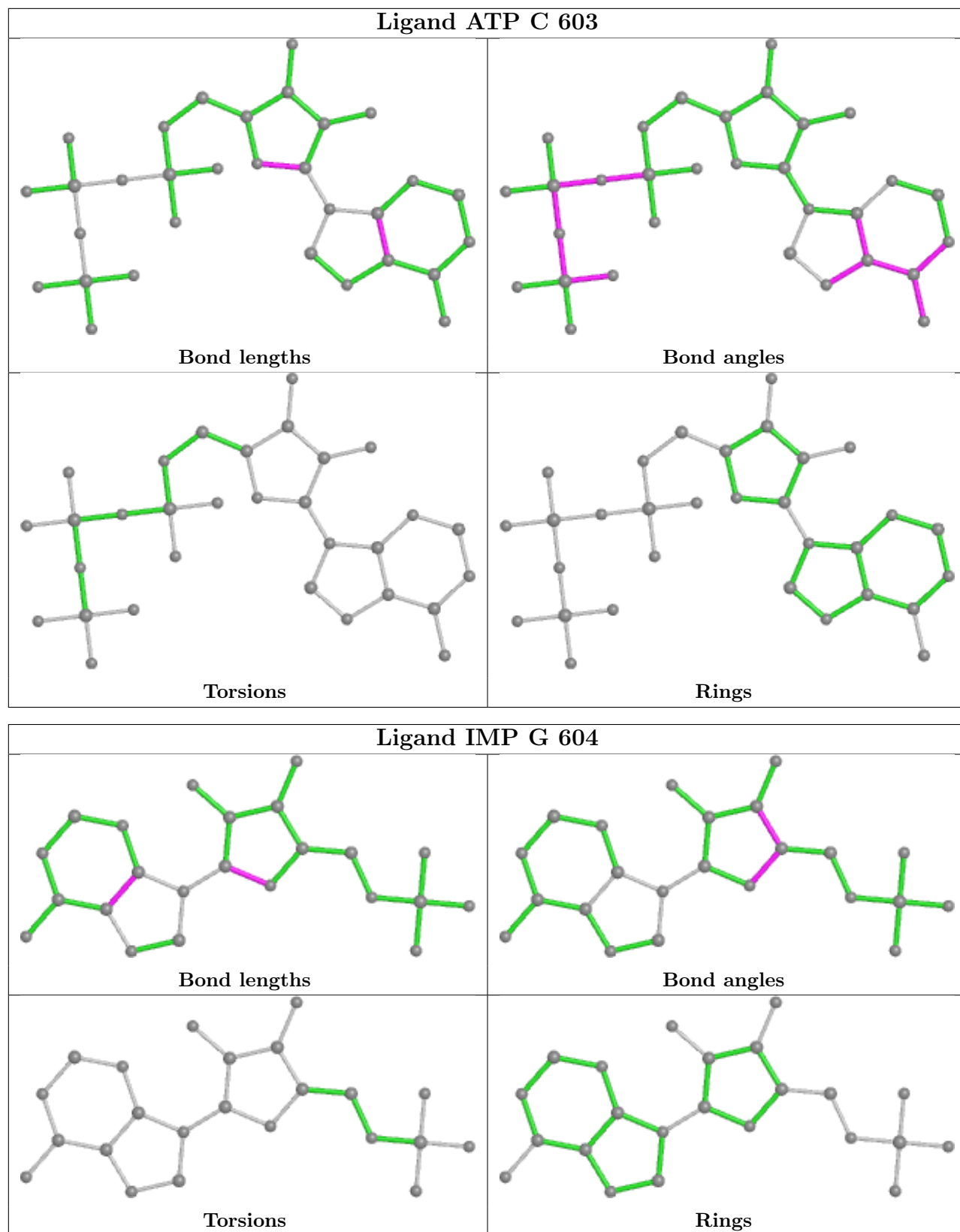
There are no ring outliers.

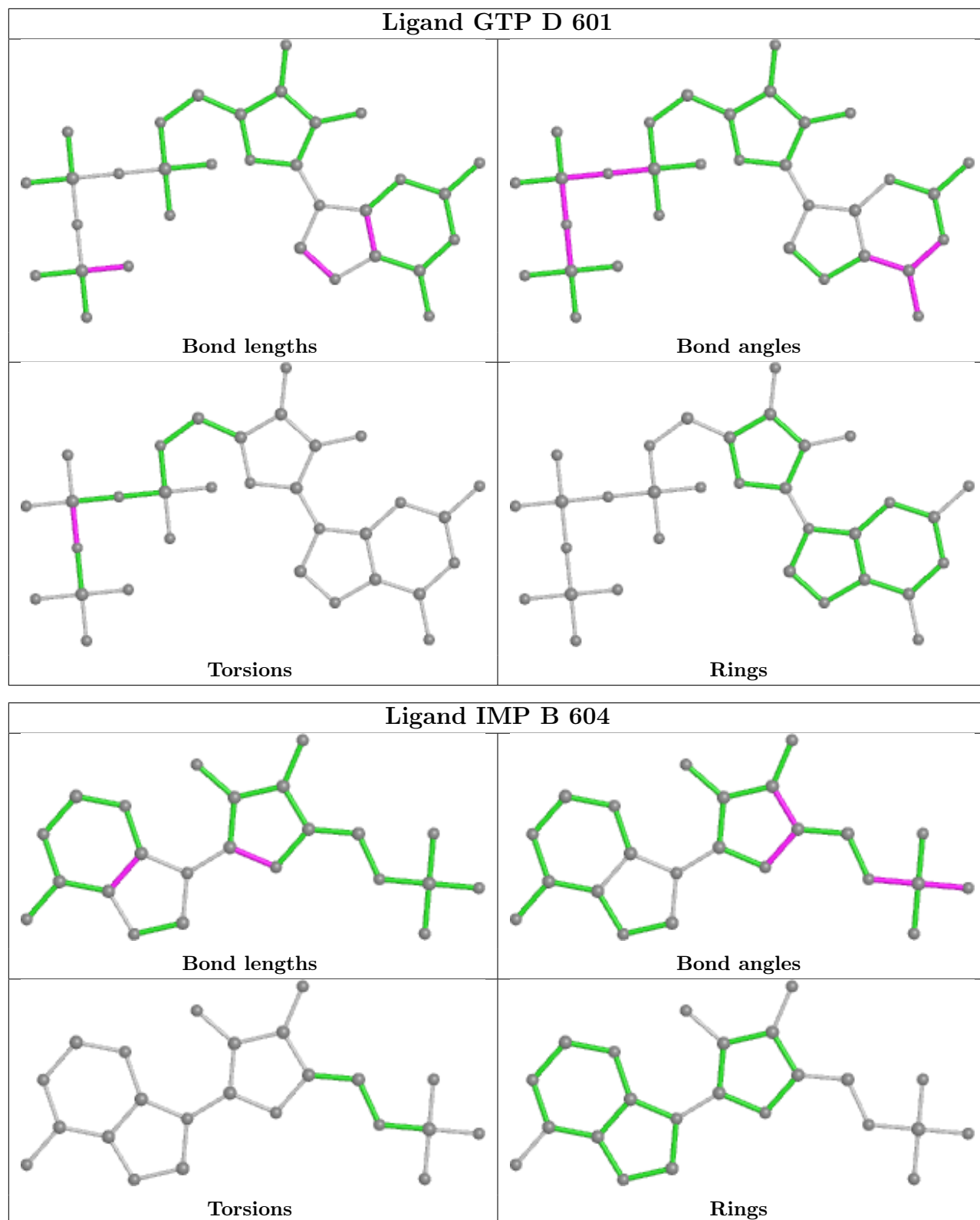
13 monomers are involved in 13 short contacts:

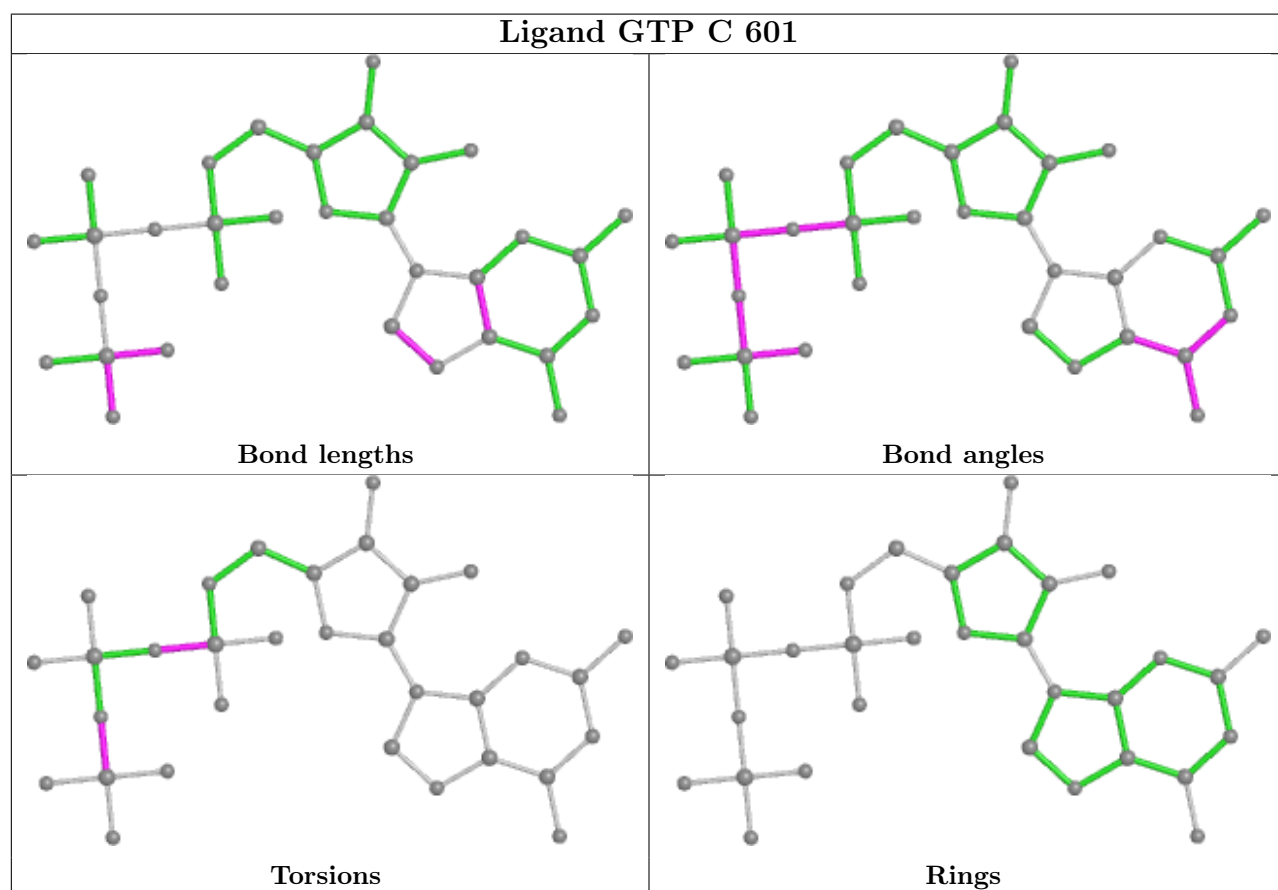
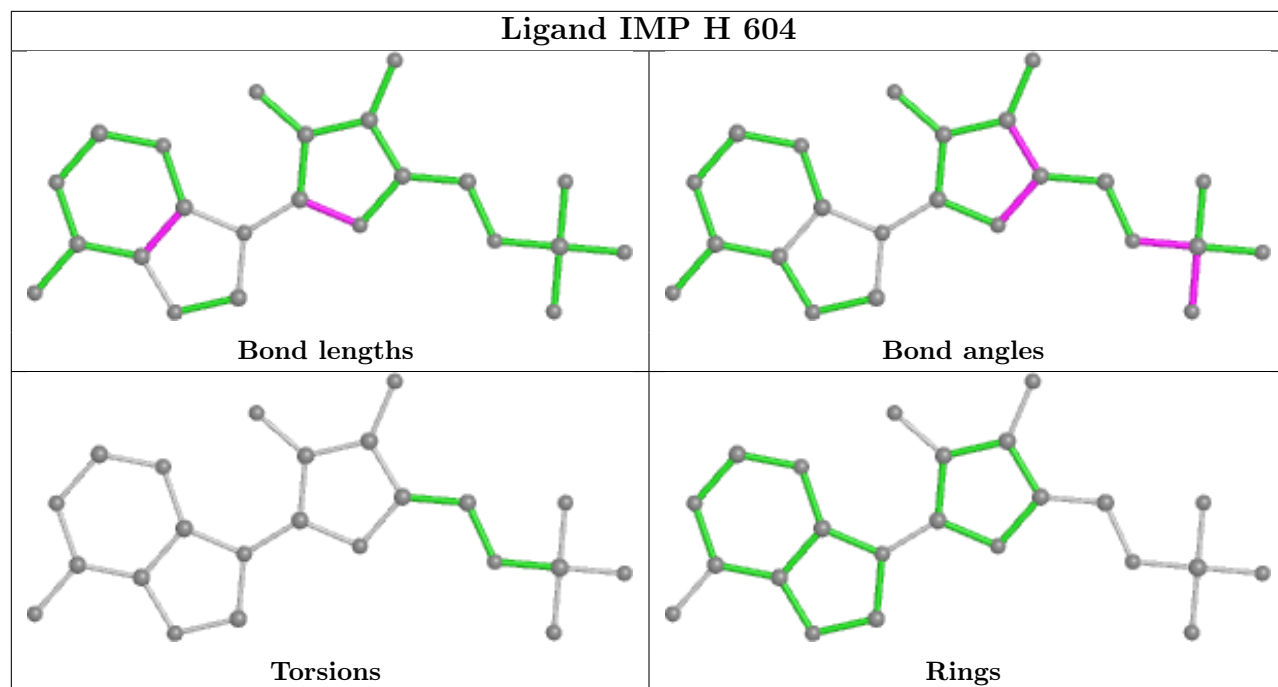
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	604	IMP	1	0
4	B	604	IMP	1	0
4	H	604	IMP	1	0
2	C	601	GTP	1	0
2	G	601	GTP	1	0
2	E	602	GTP	1	0
2	H	602	GTP	1	0
4	E	604	IMP	1	0
4	F	604	IMP	1	0
2	E	601	GTP	1	0
2	A	602	GTP	1	0
4	D	604	IMP	1	0
4	C	604	IMP	1	0

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.

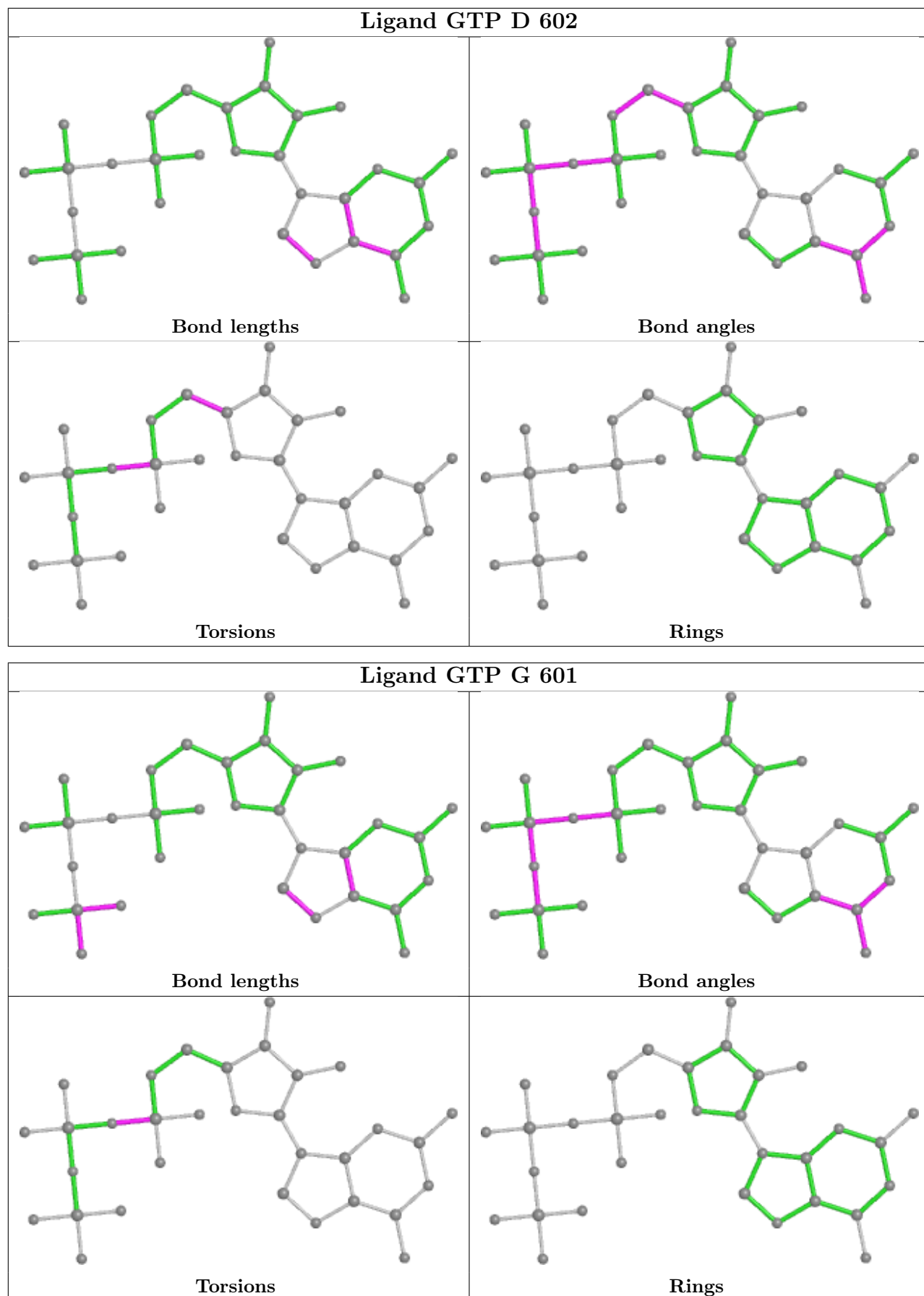


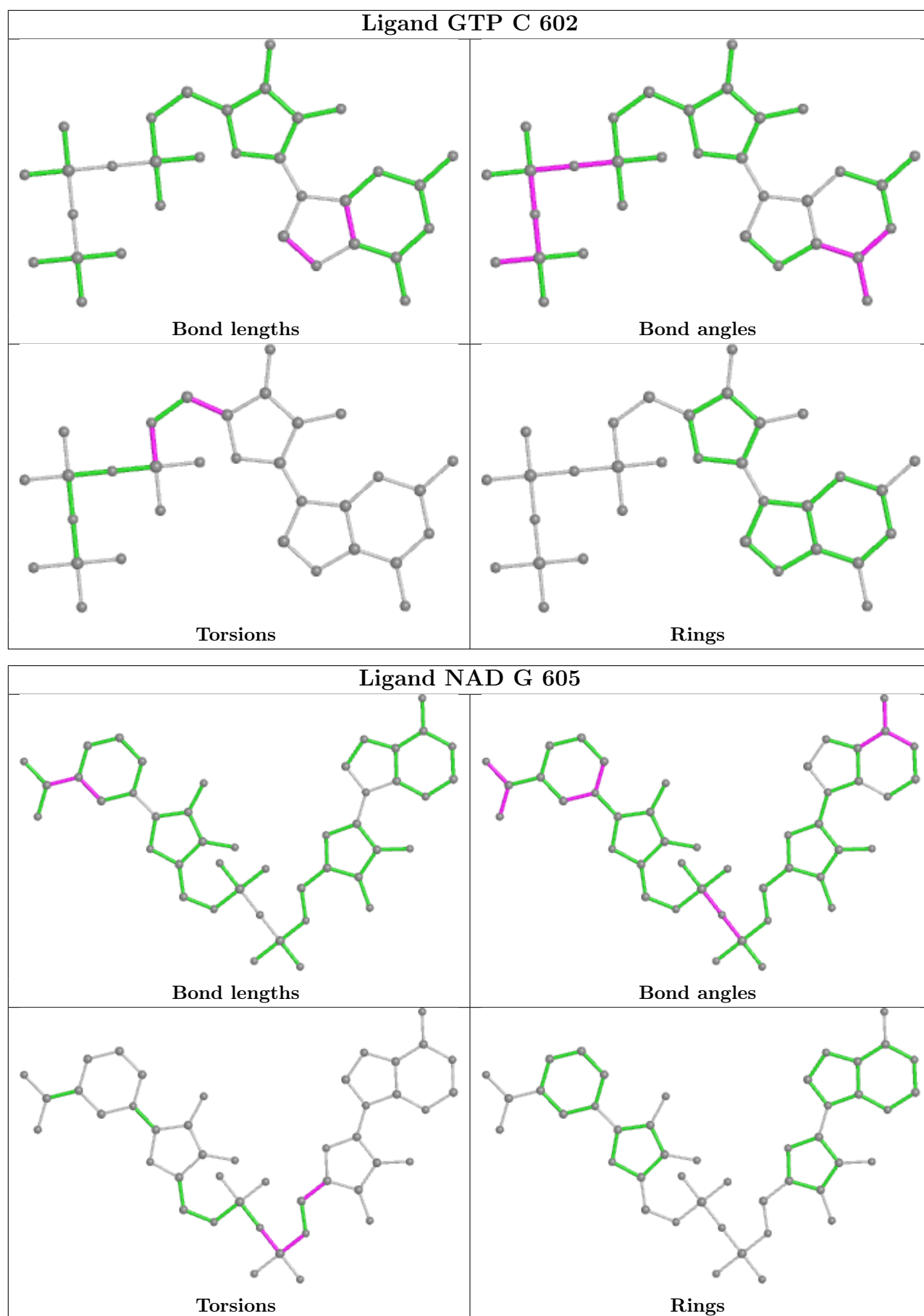


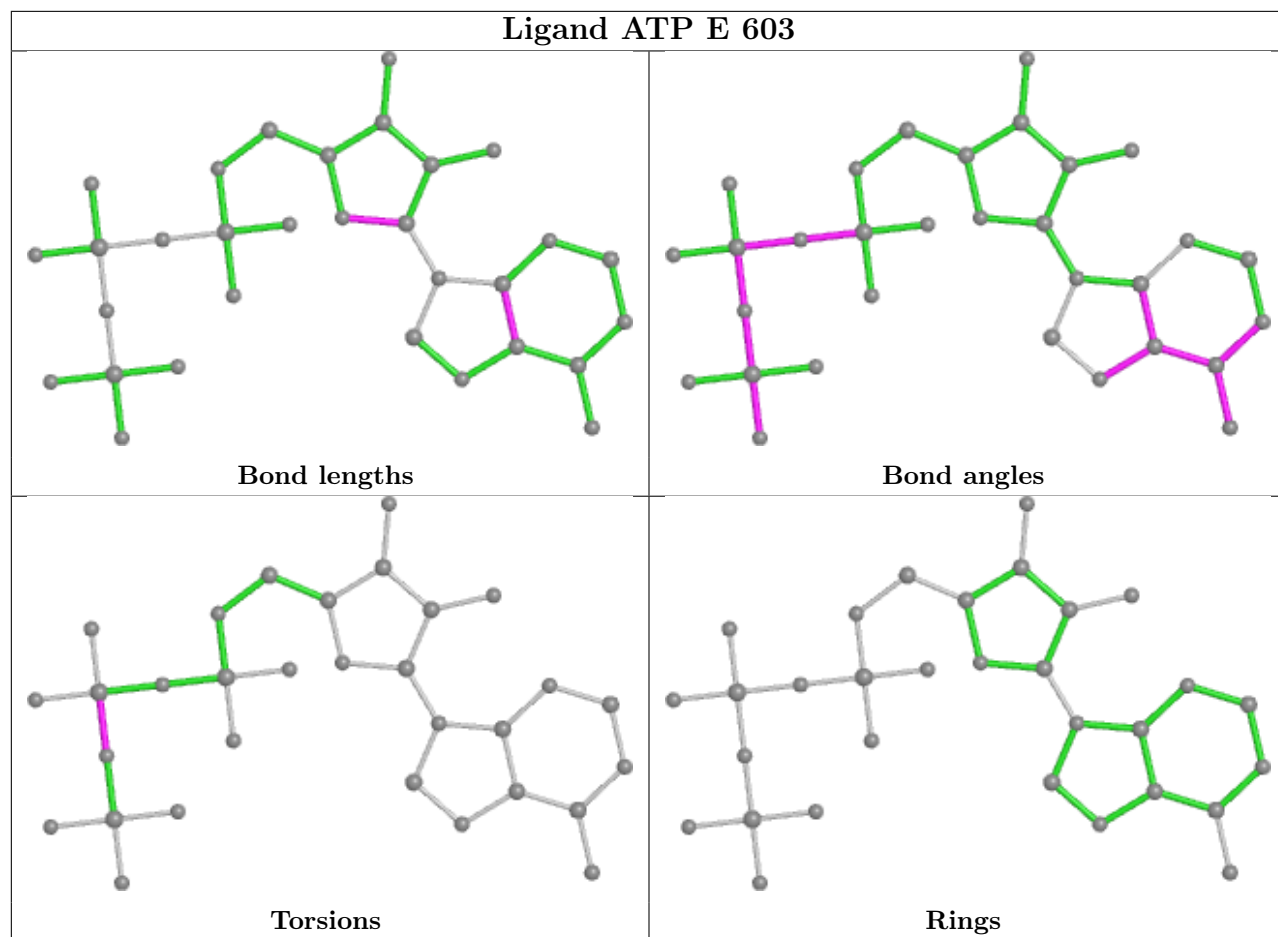


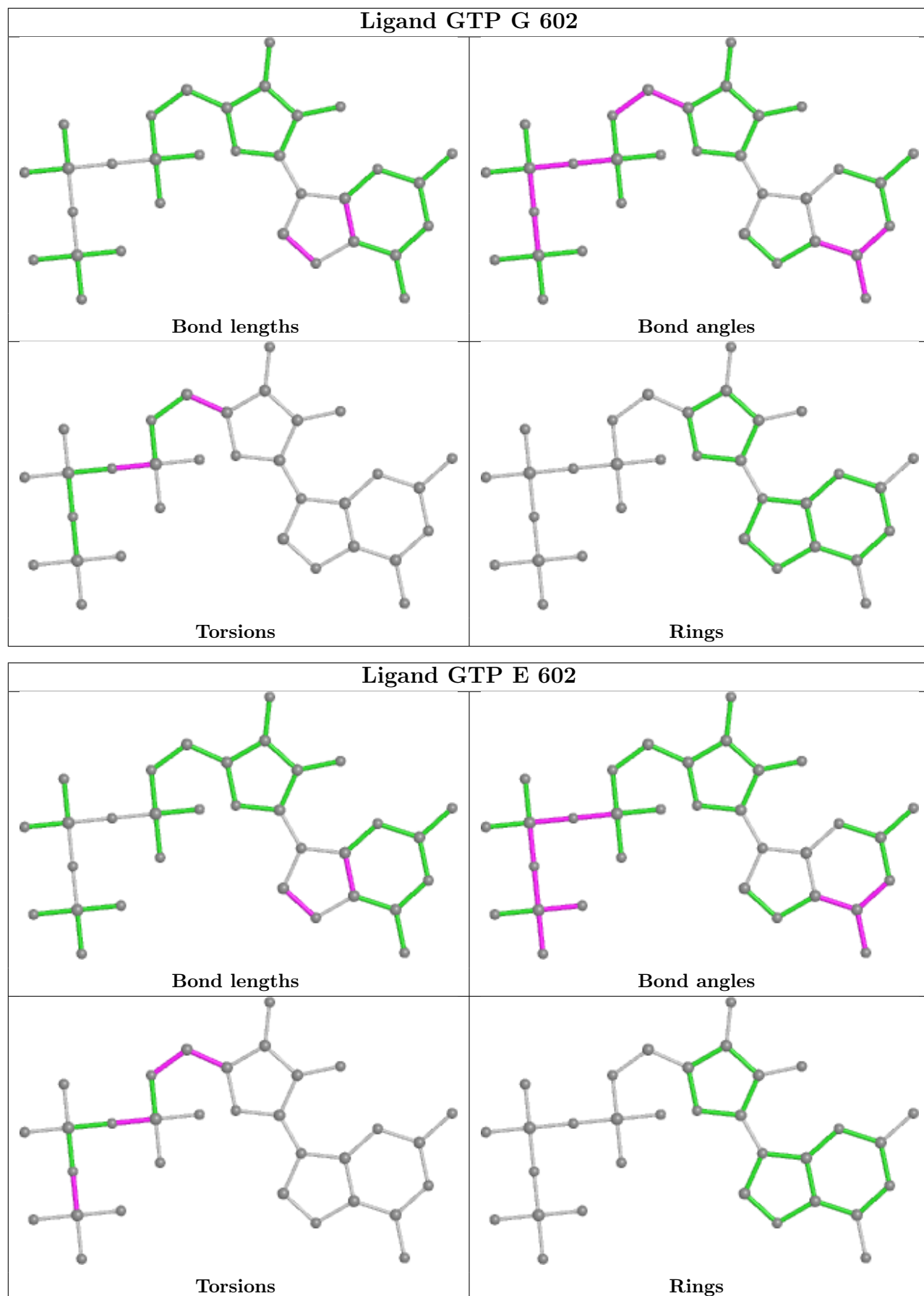


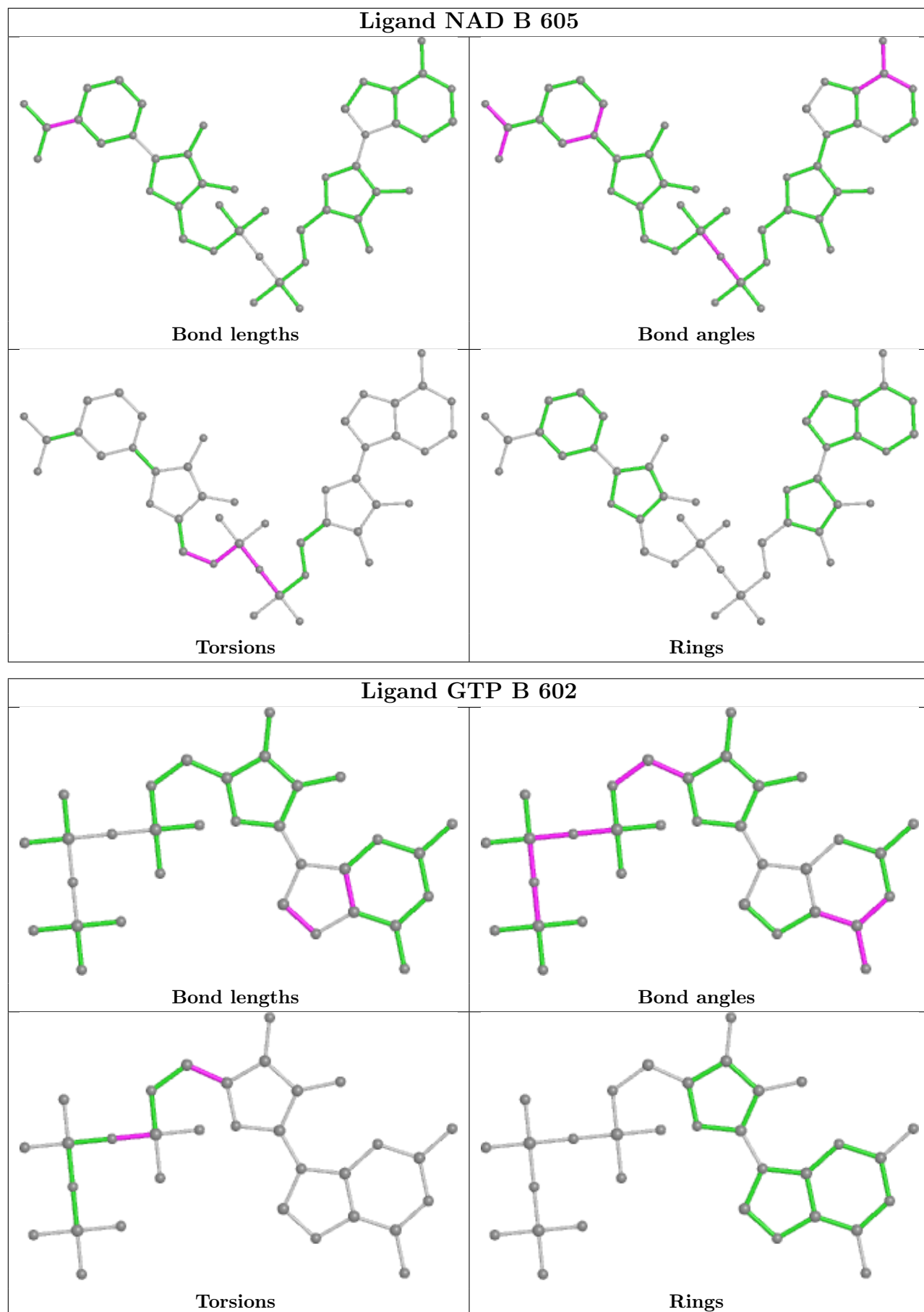


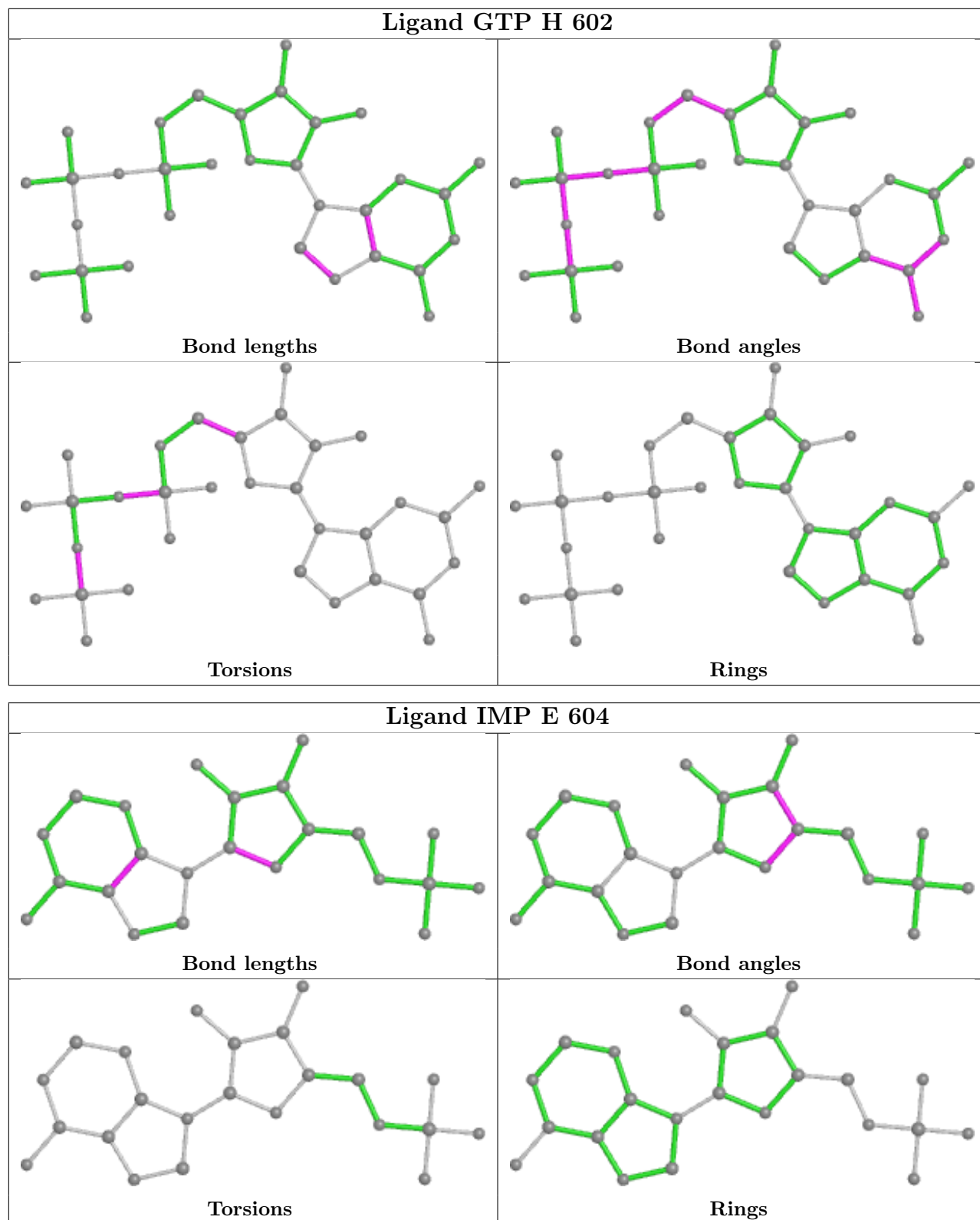


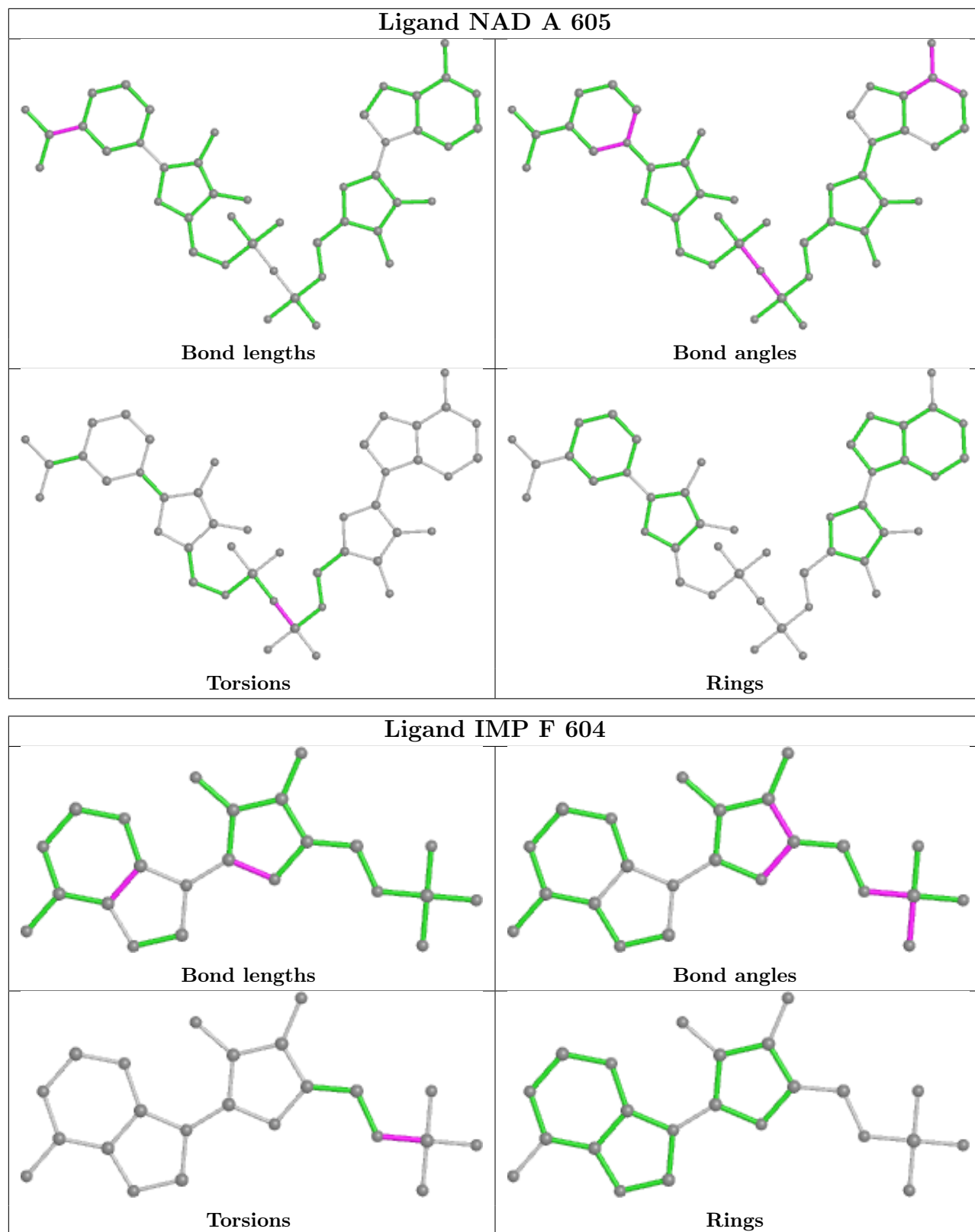


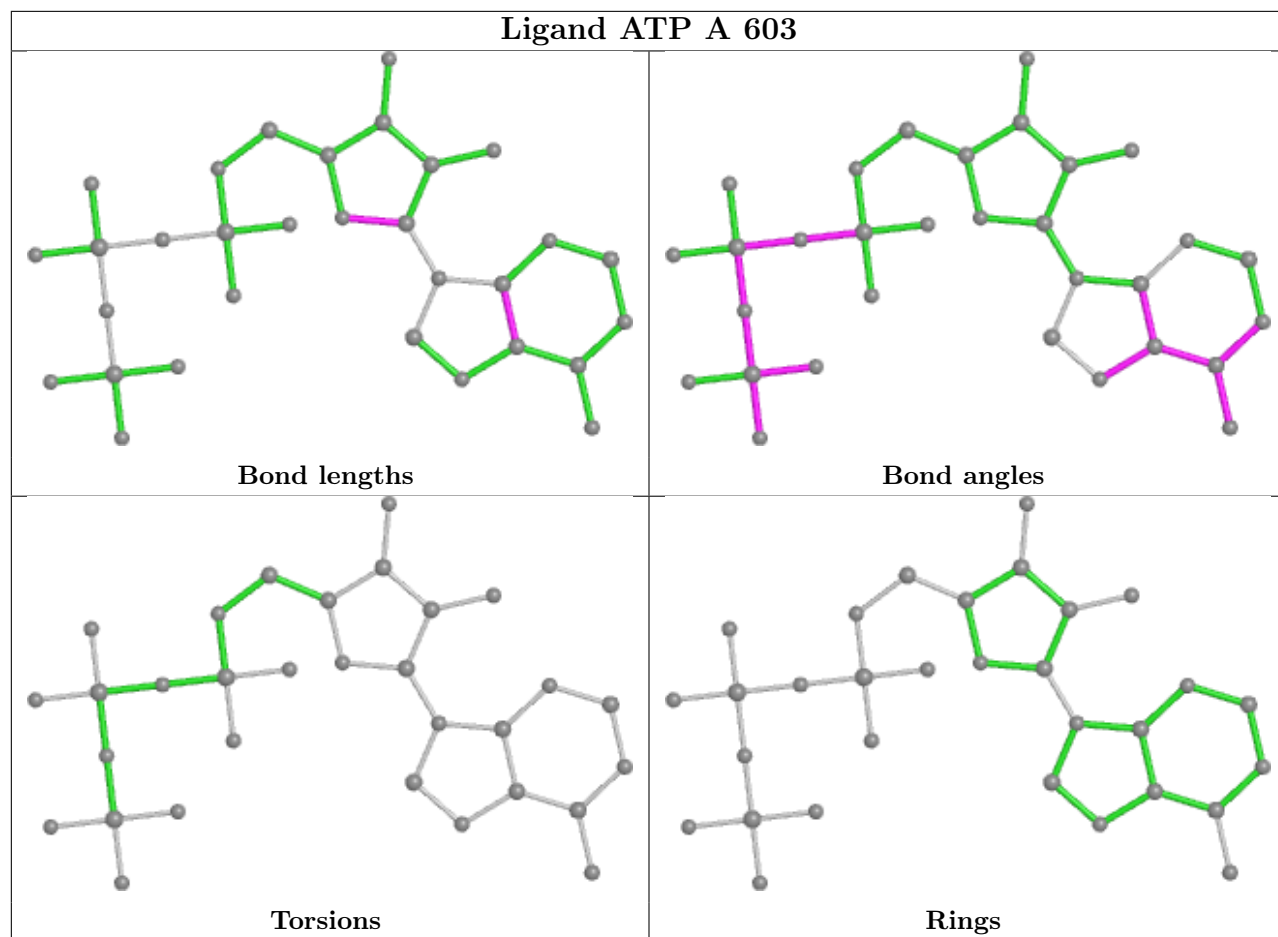




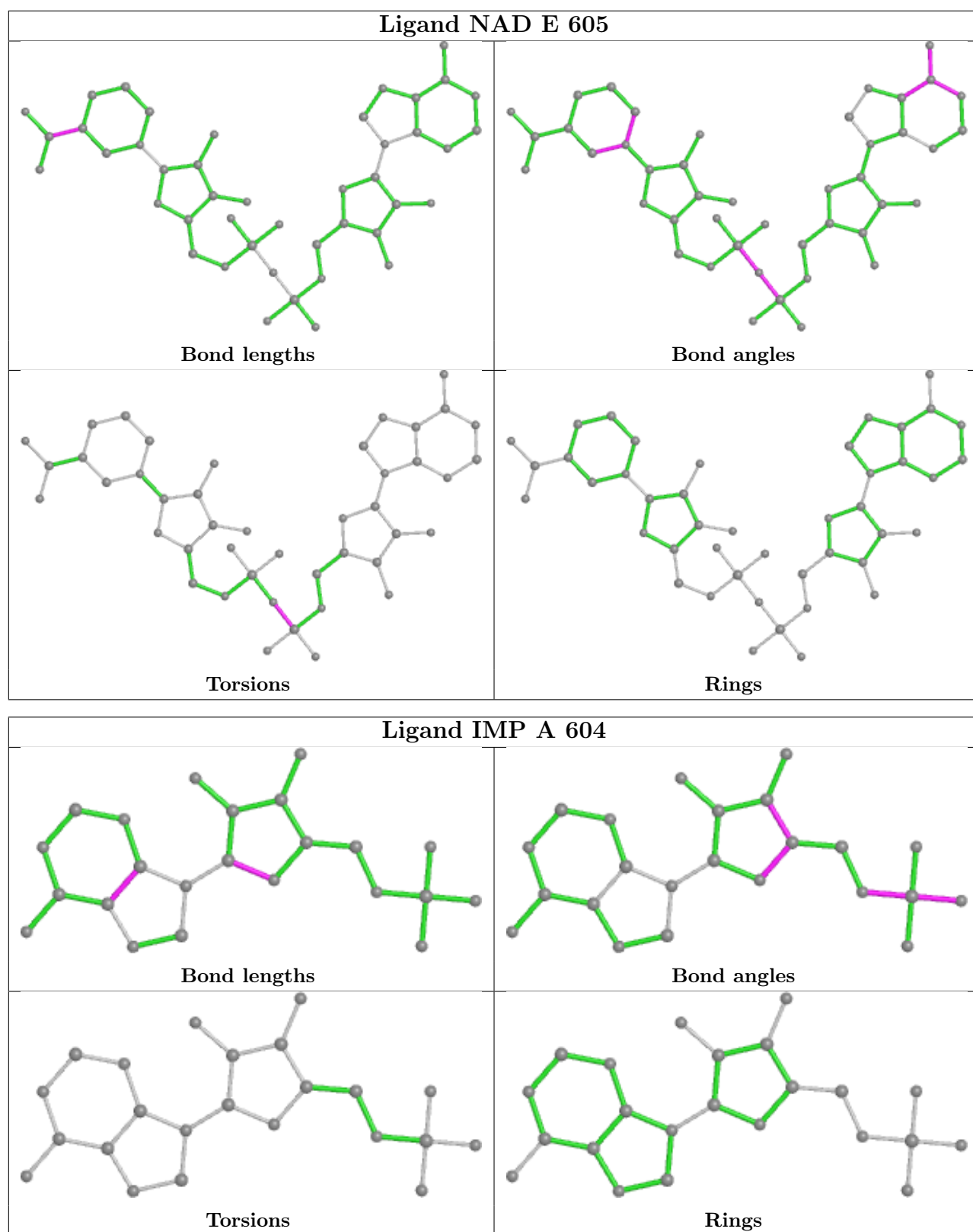


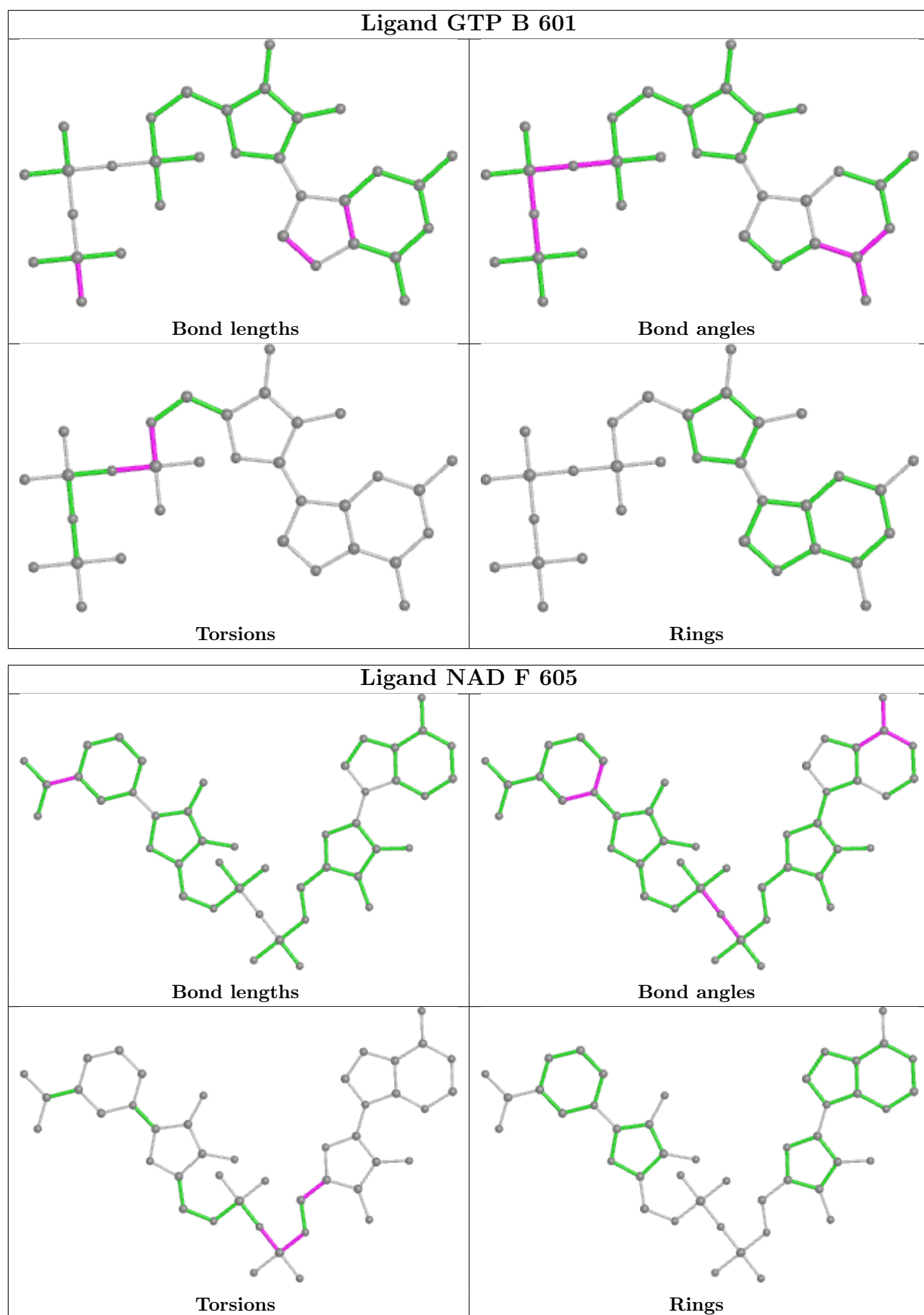


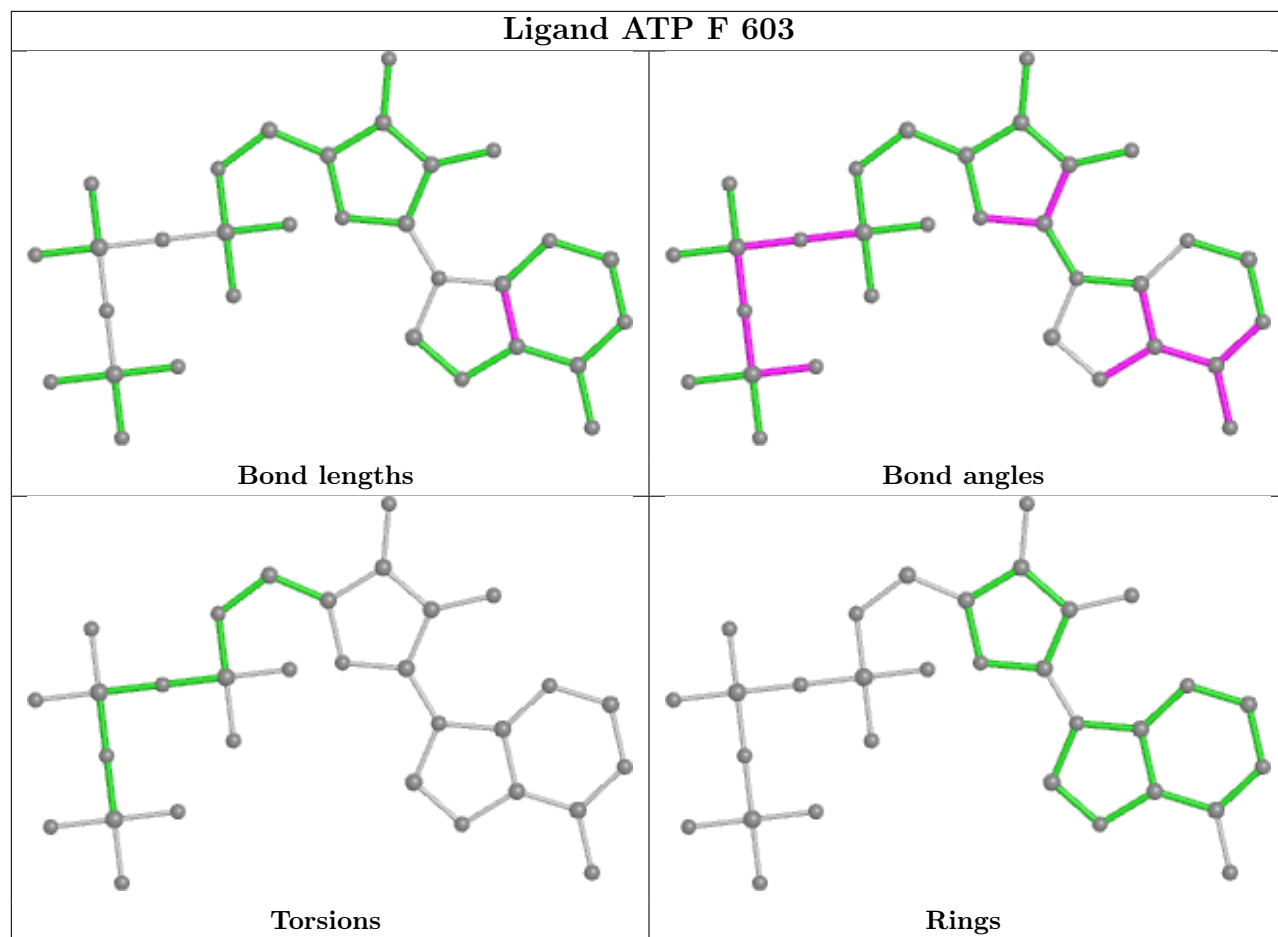


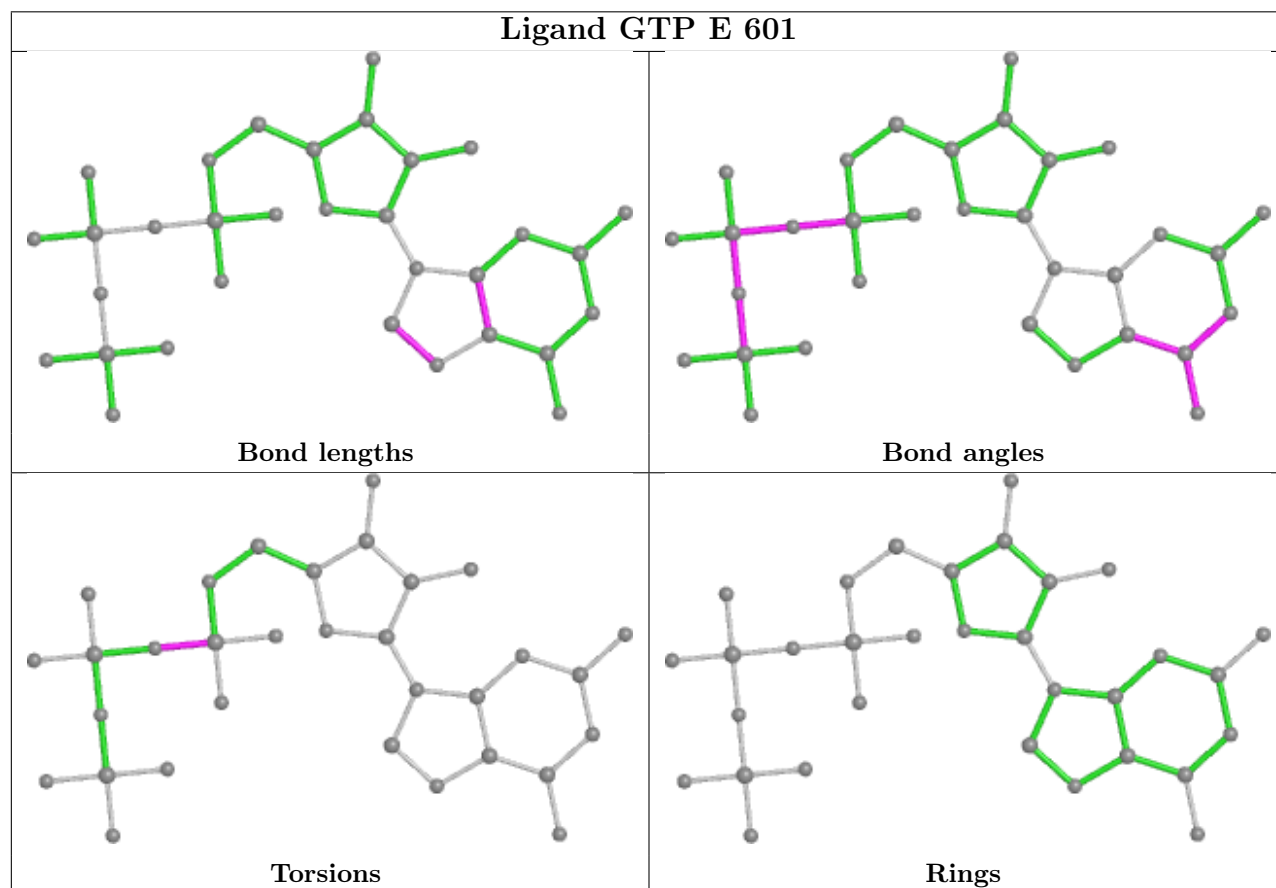
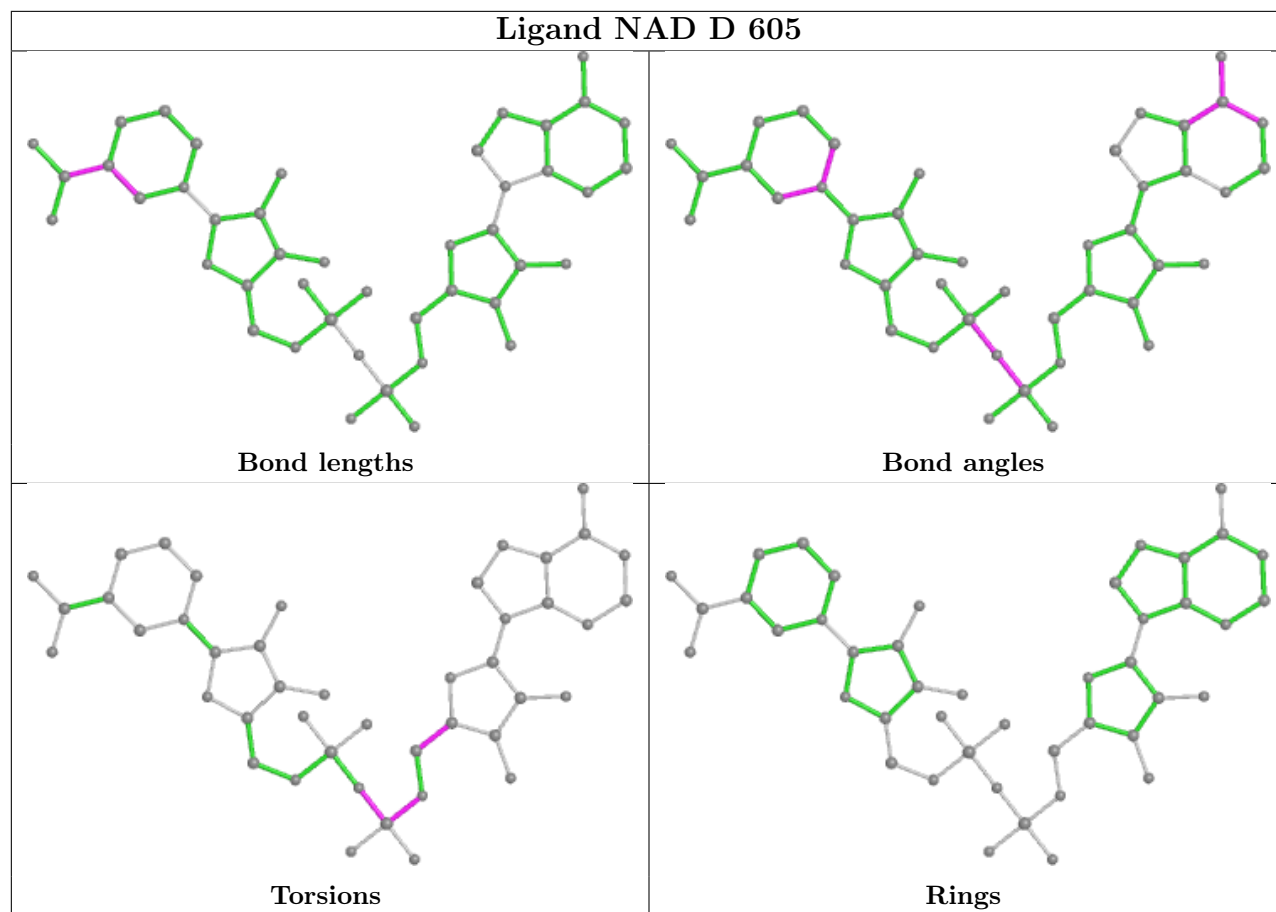


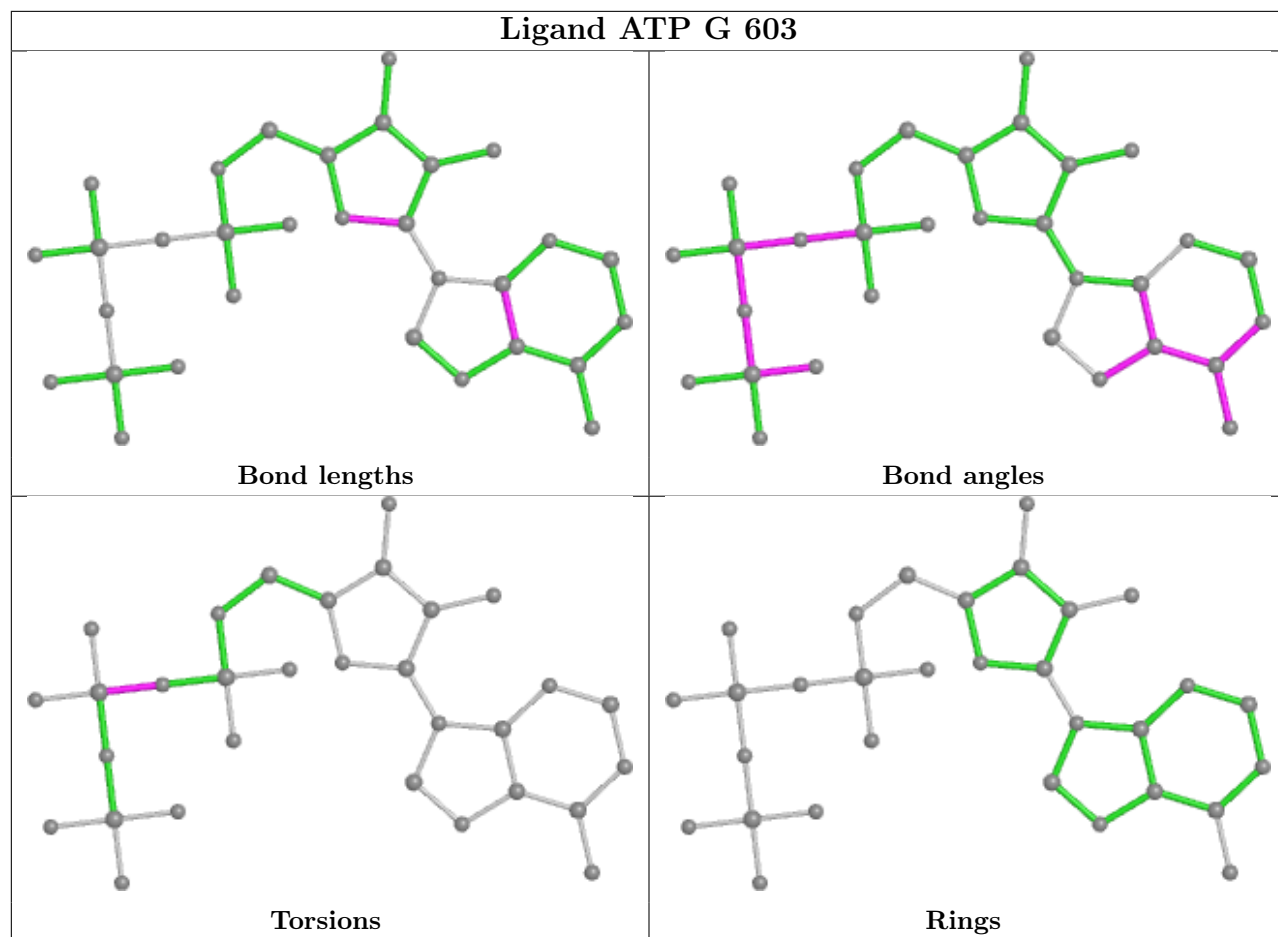


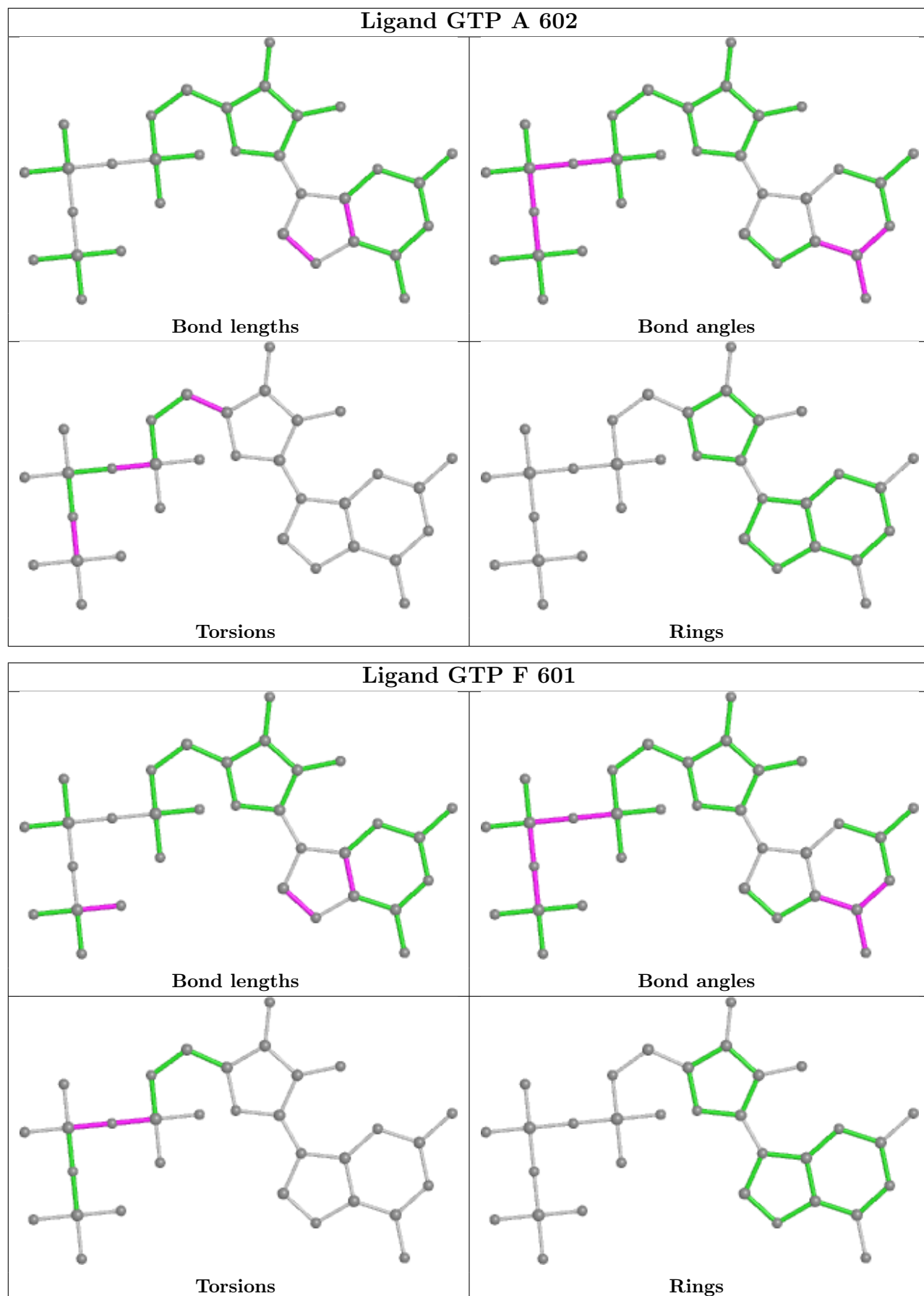


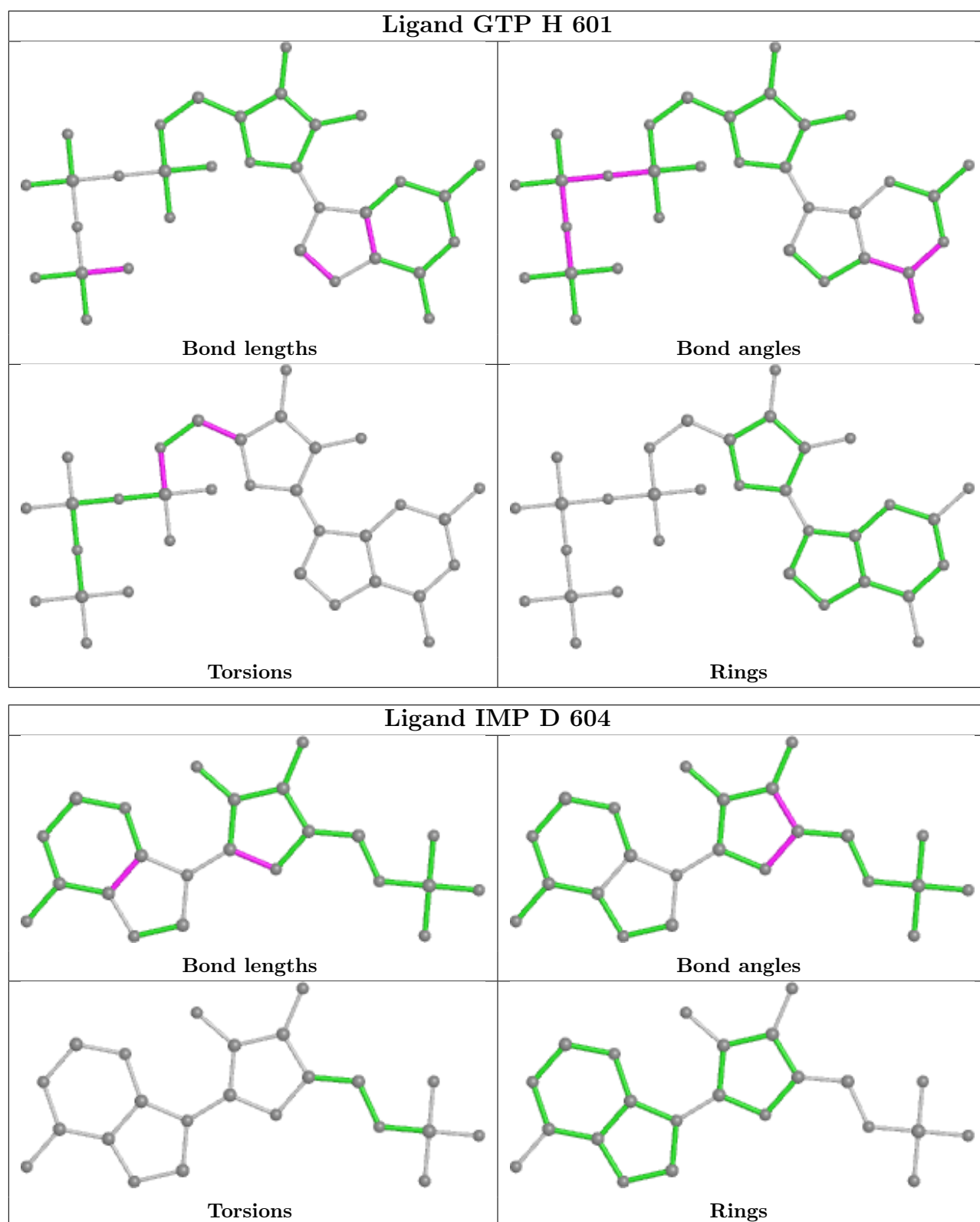


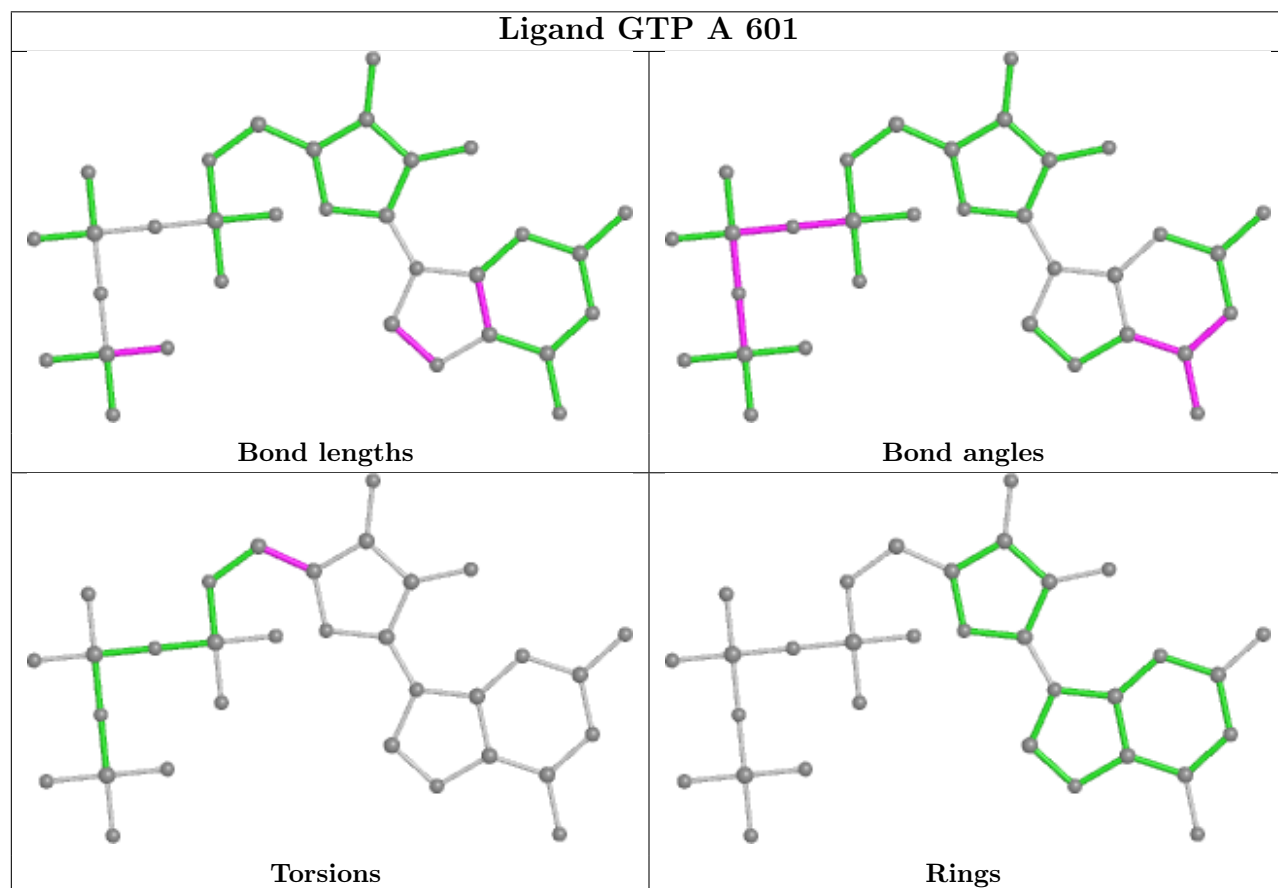
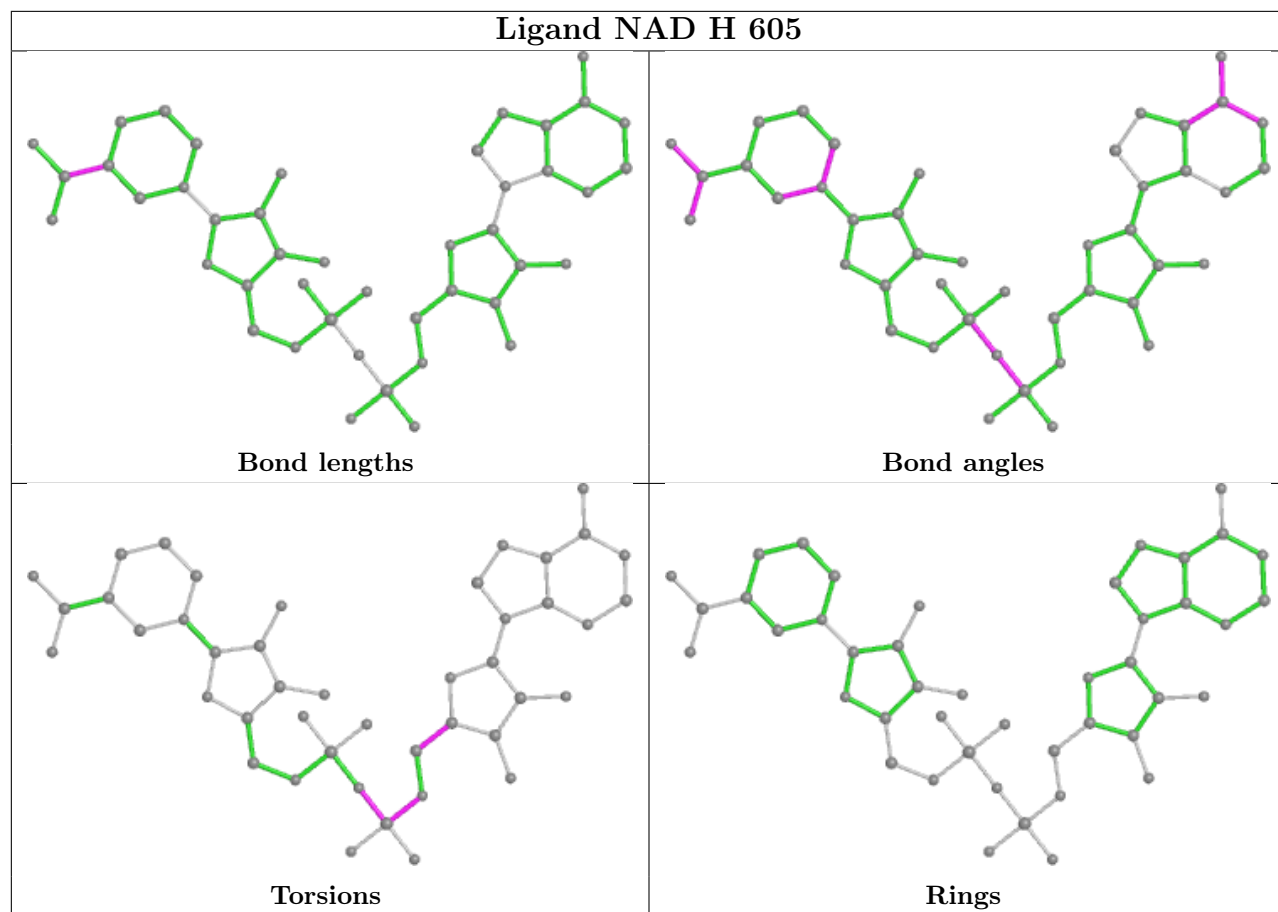




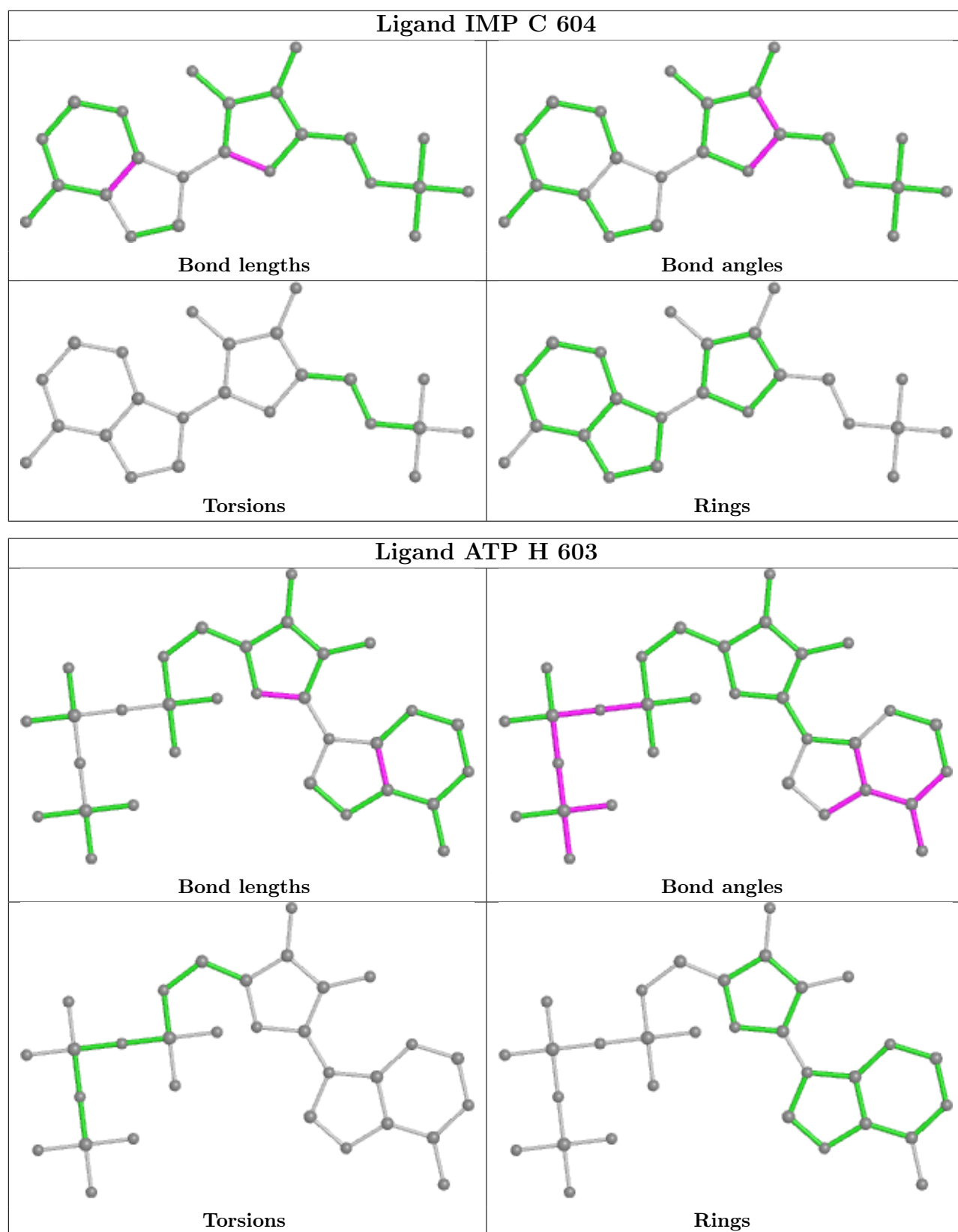


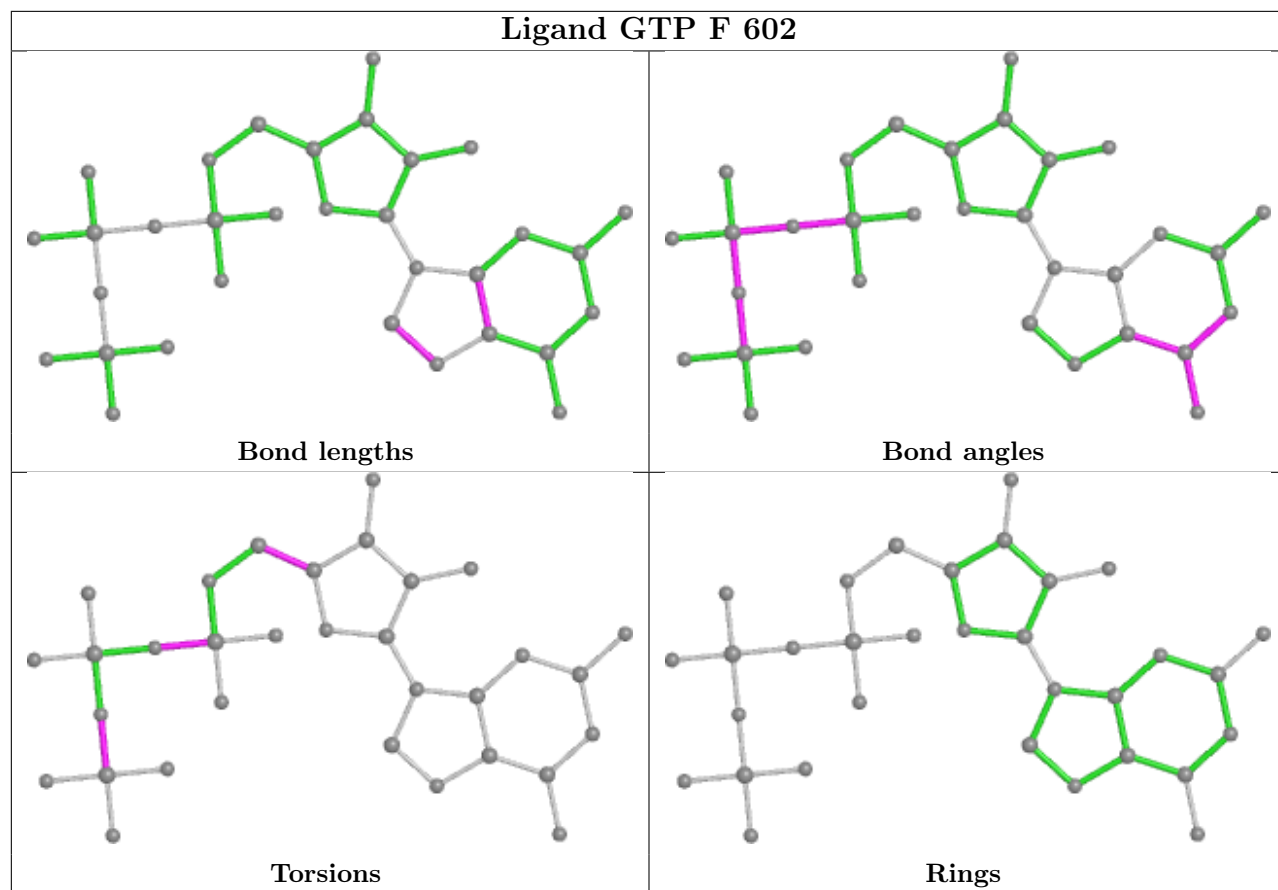


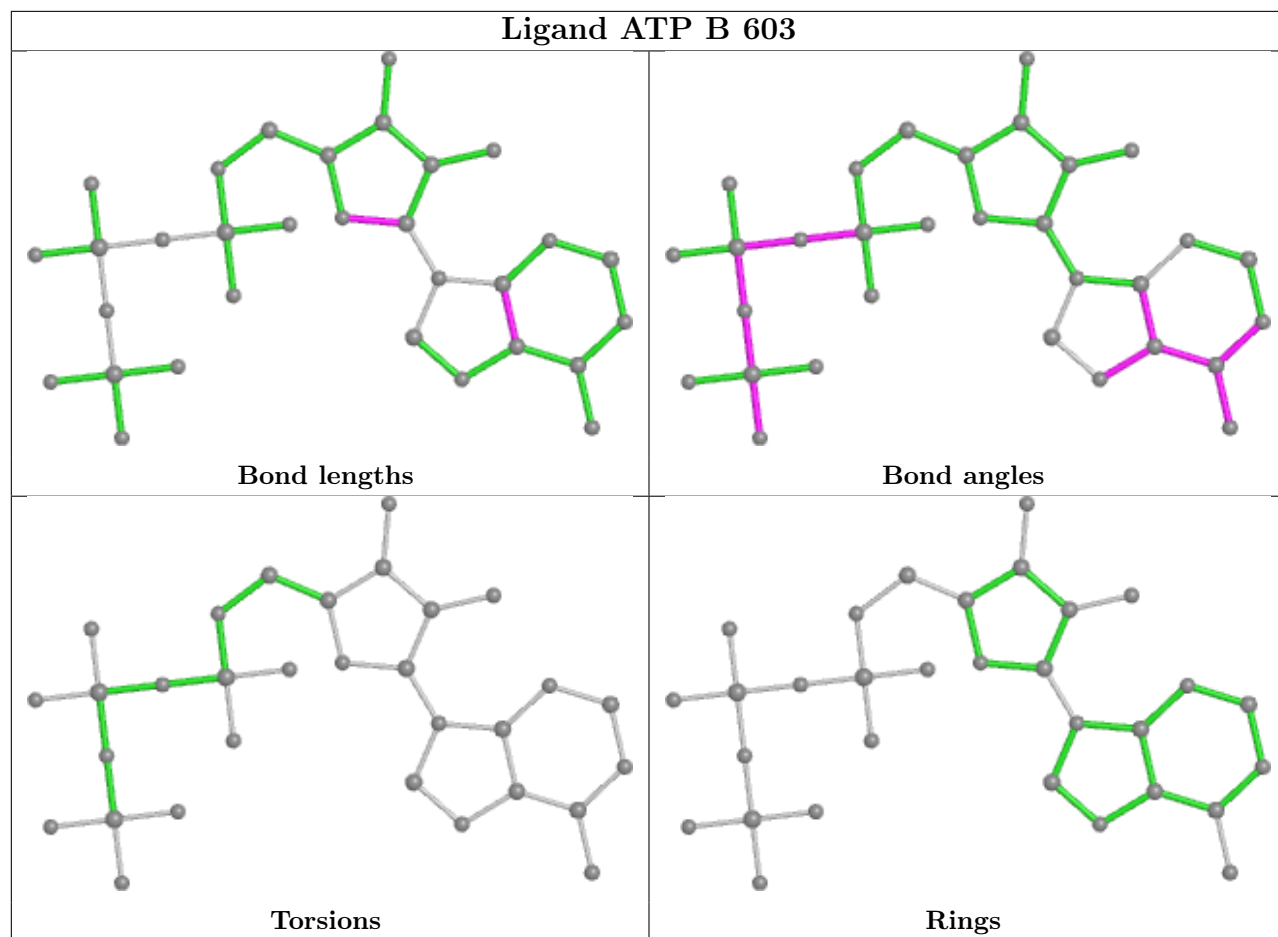


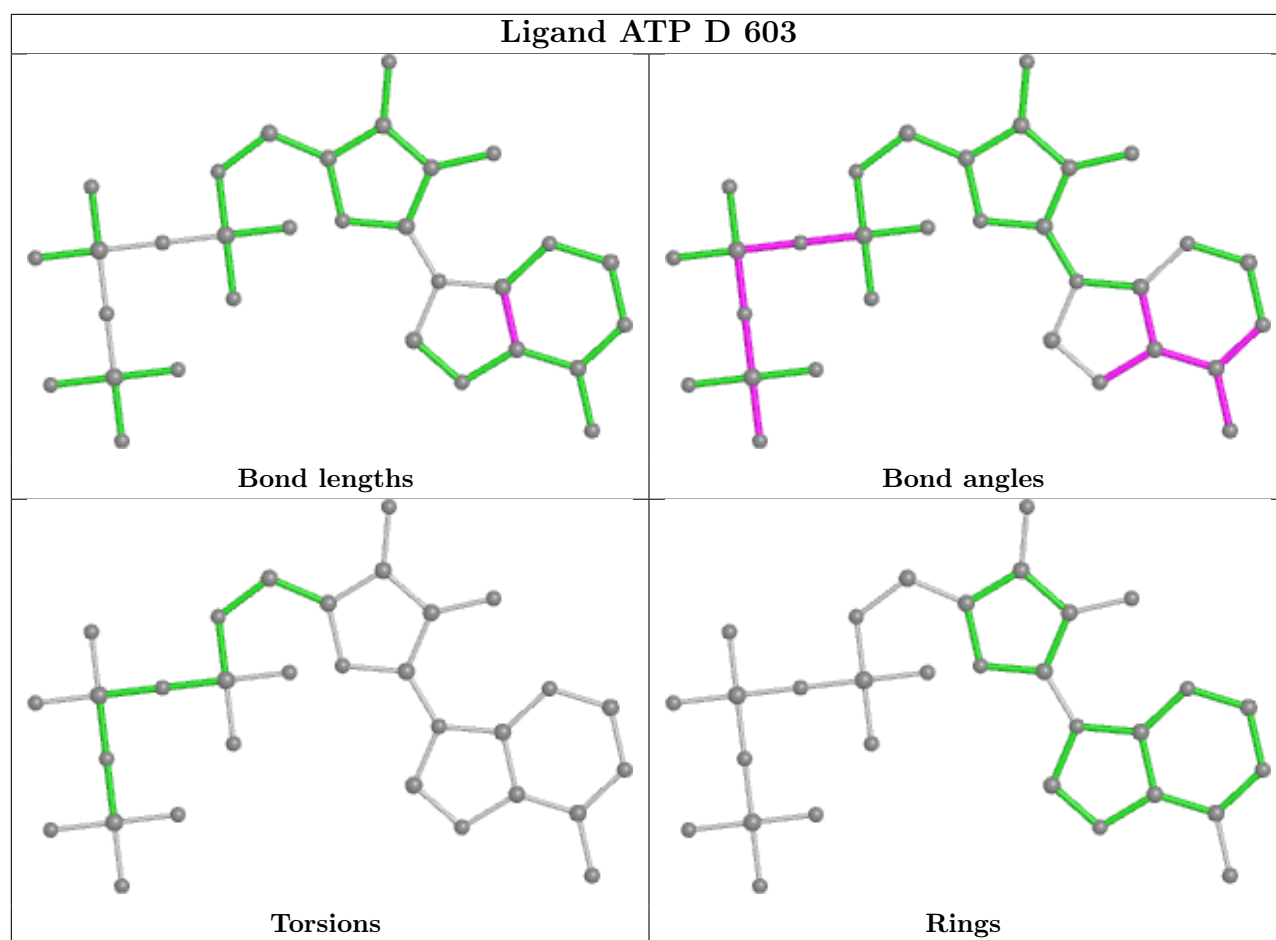












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

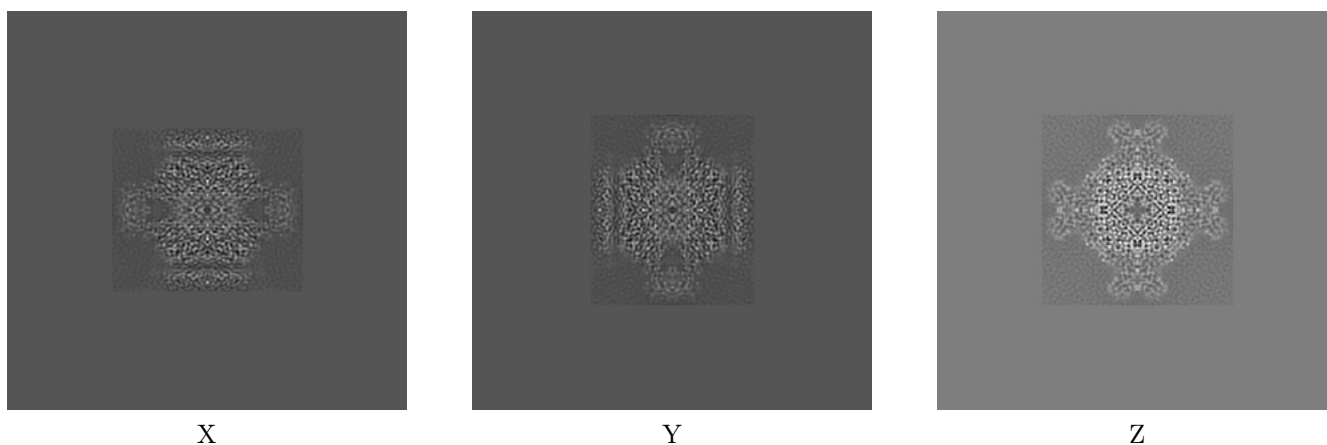
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24448. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

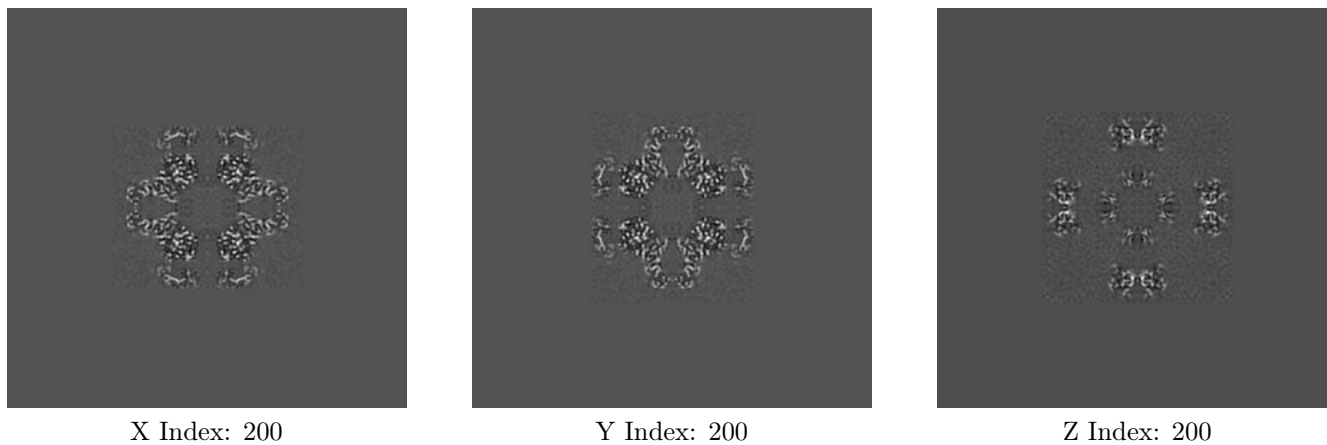
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

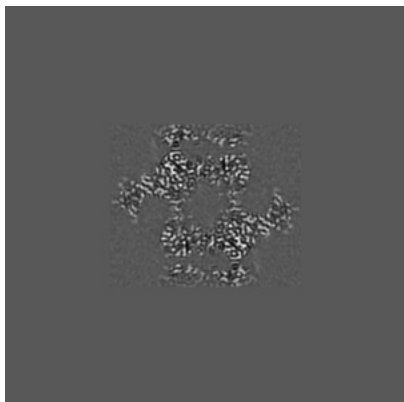
#### 6.2.1 Primary map



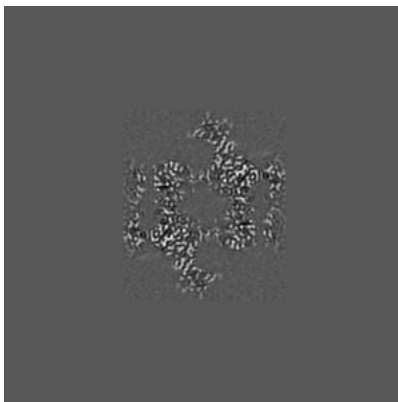
The images above show central slices of the map in three orthogonal directions.

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

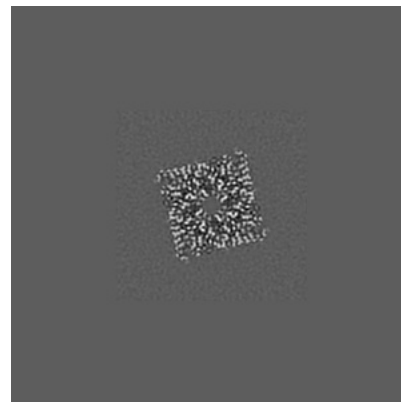
### 6.3.1 Primary map



X Index: 189



Y Index: 189

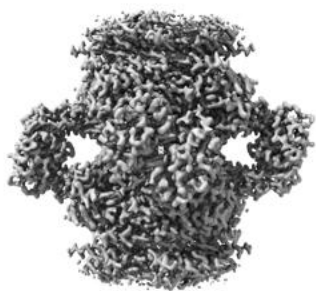


Z Index: 239

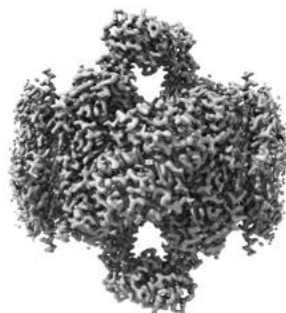
The images above show the largest variance slices of the map in three orthogonal directions.

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

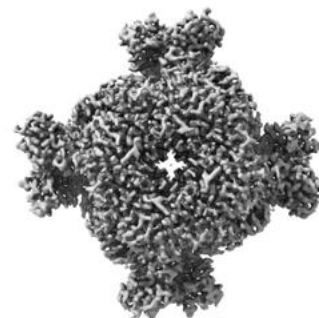
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

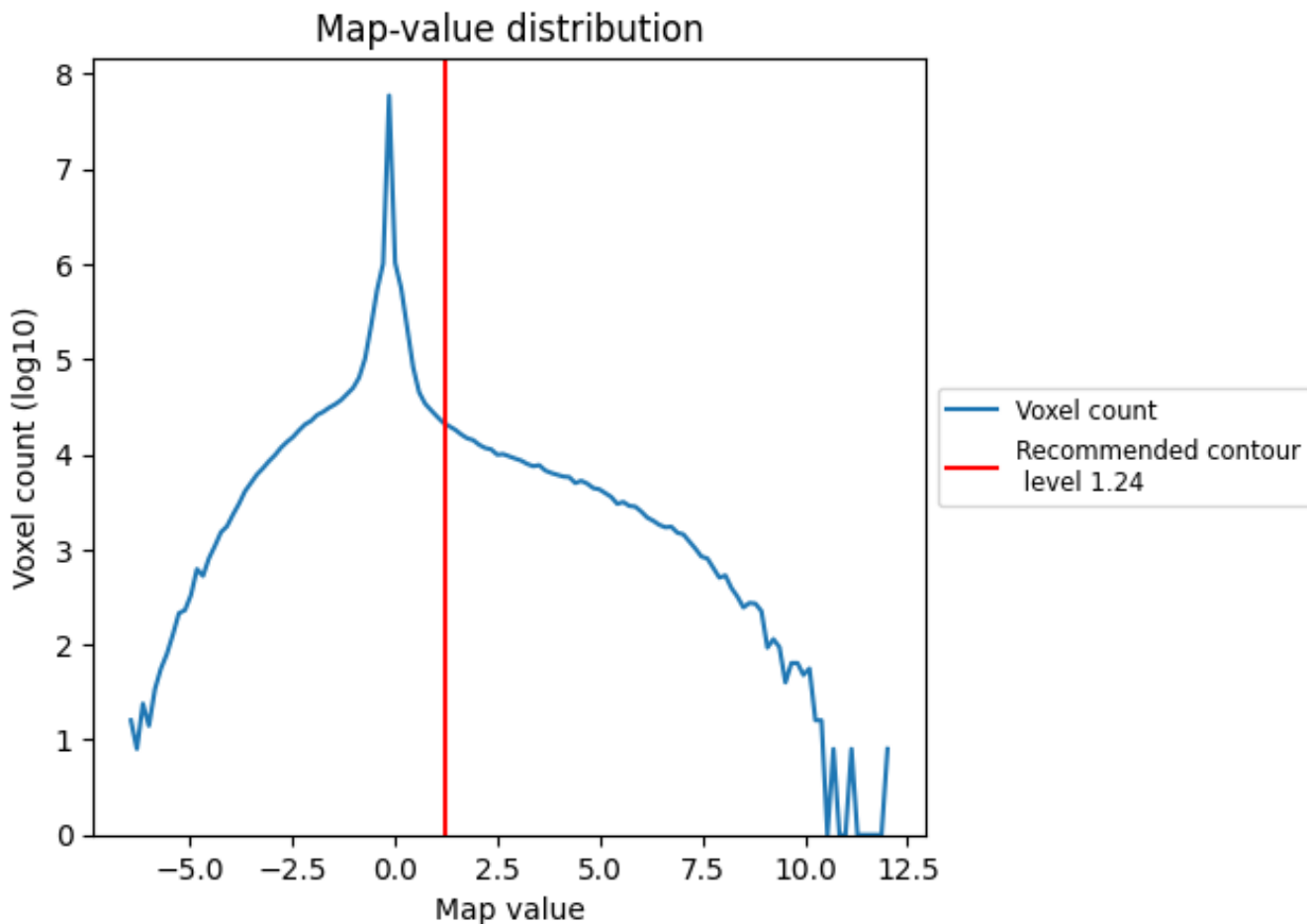
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

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

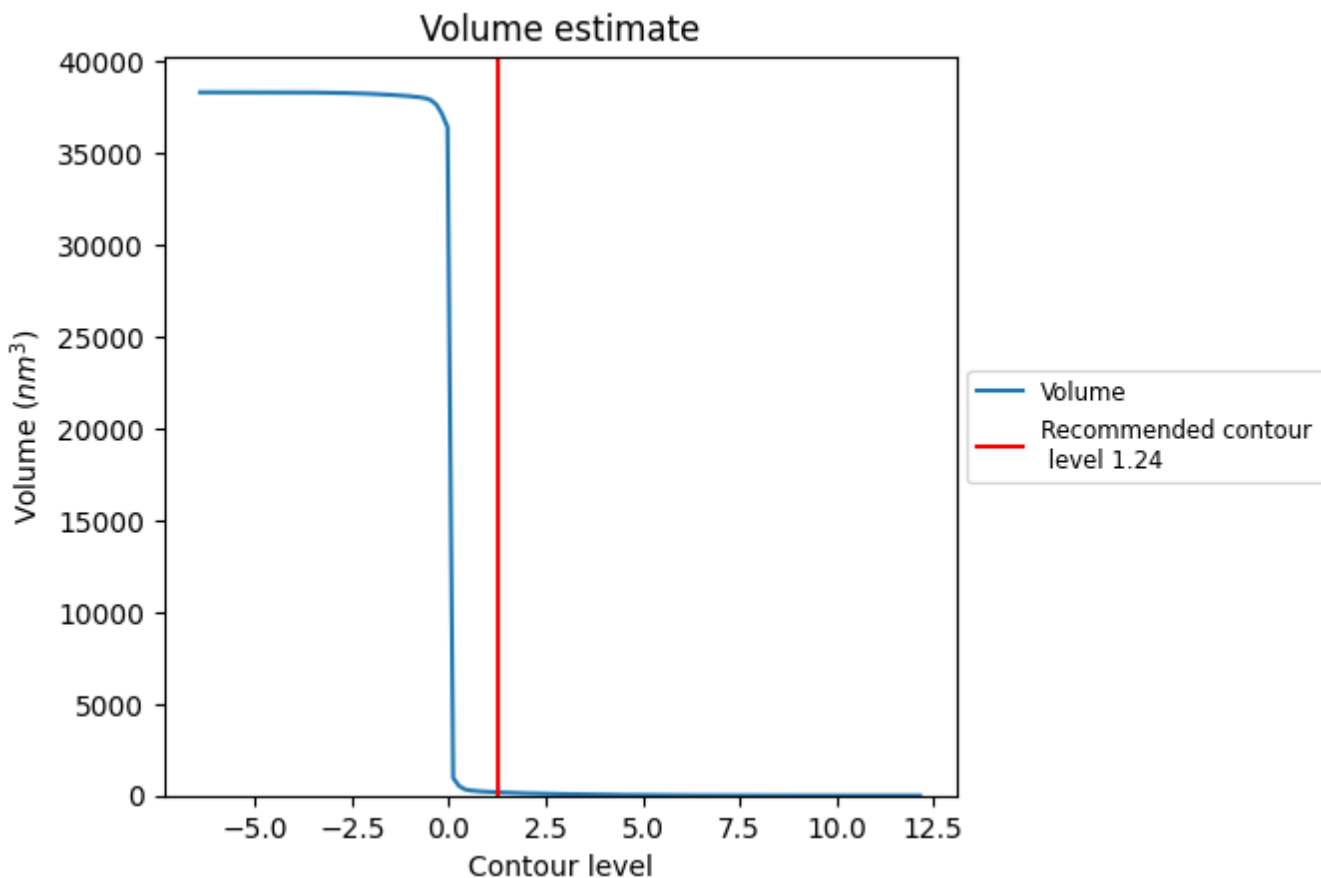
### 7.1 Map-value distribution [i](#)



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.



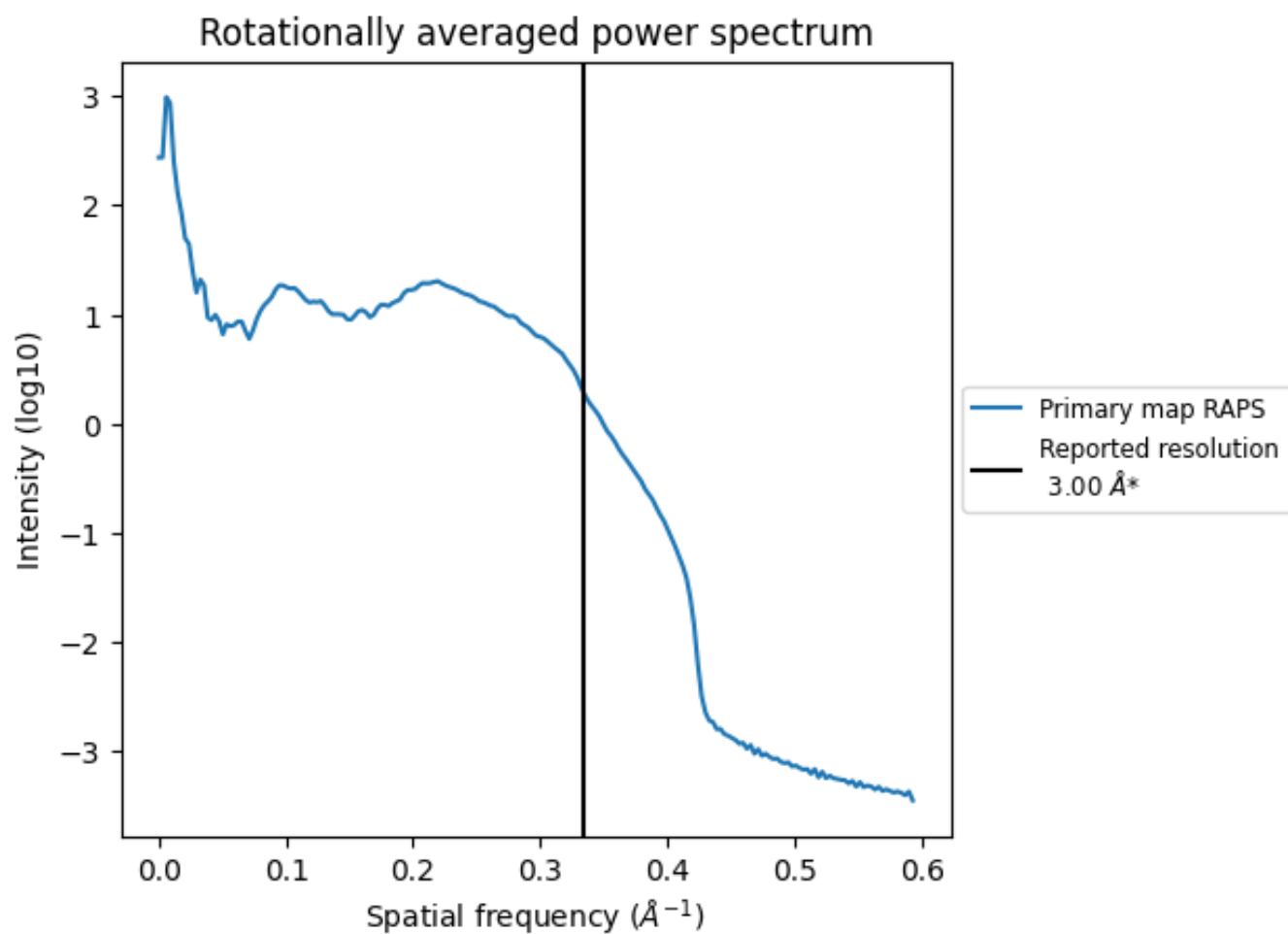
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm<sup>3</sup>; this corresponds to an approximate mass of 162 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  $0.333 \text{\AA}^{-1}$

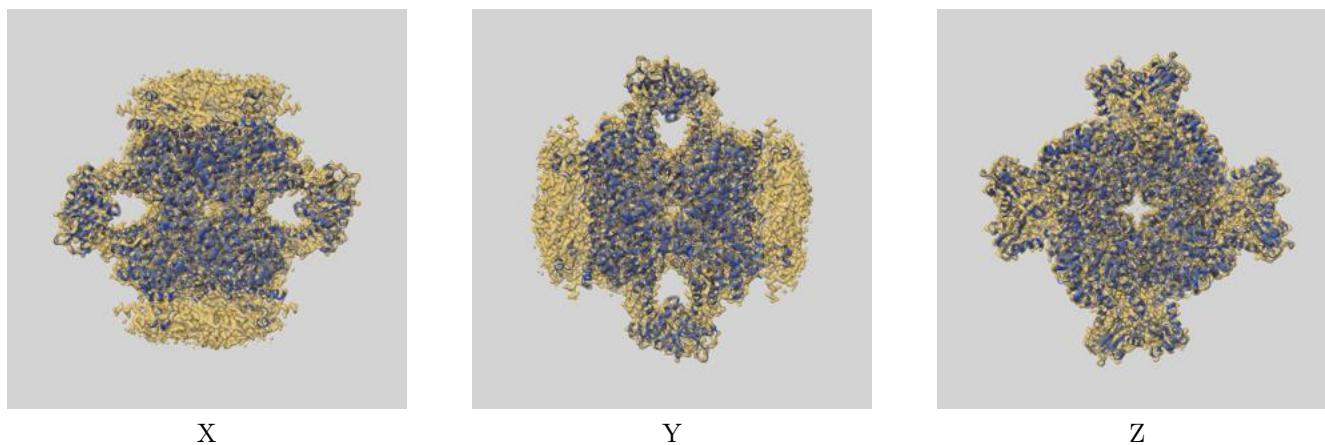
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

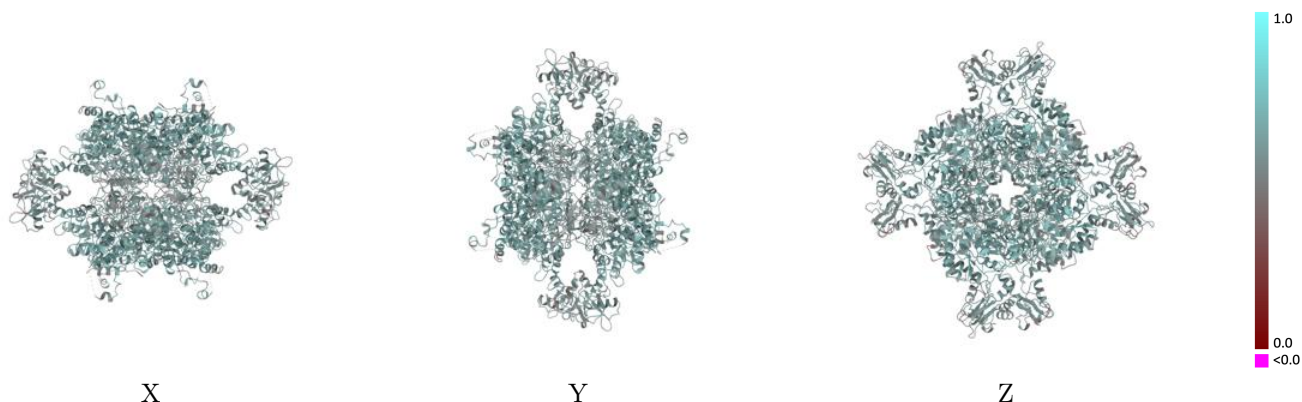
This section contains information regarding the fit between EMDB map EMD-24448 and PDB model 7RGD. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



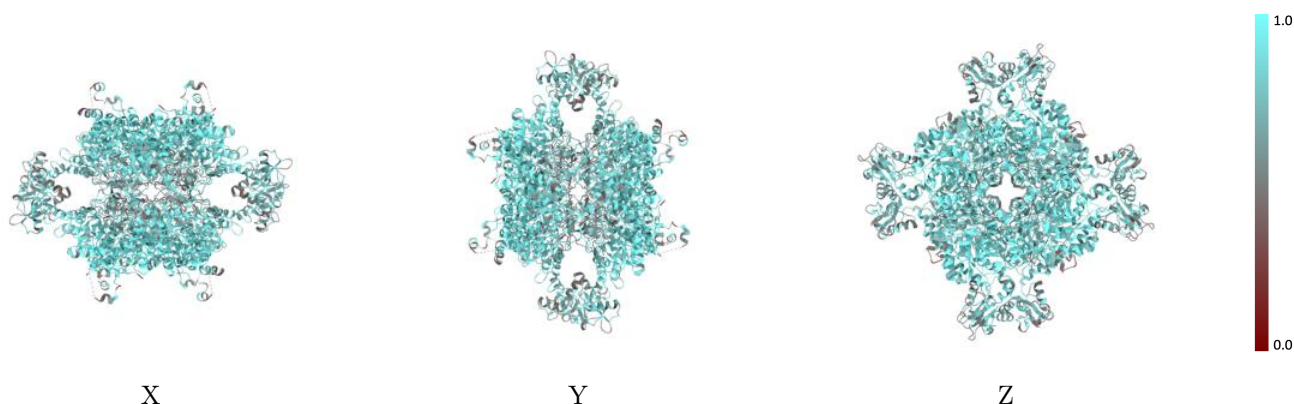
The images above show the 3D surface view of the map at the recommended contour level 1.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



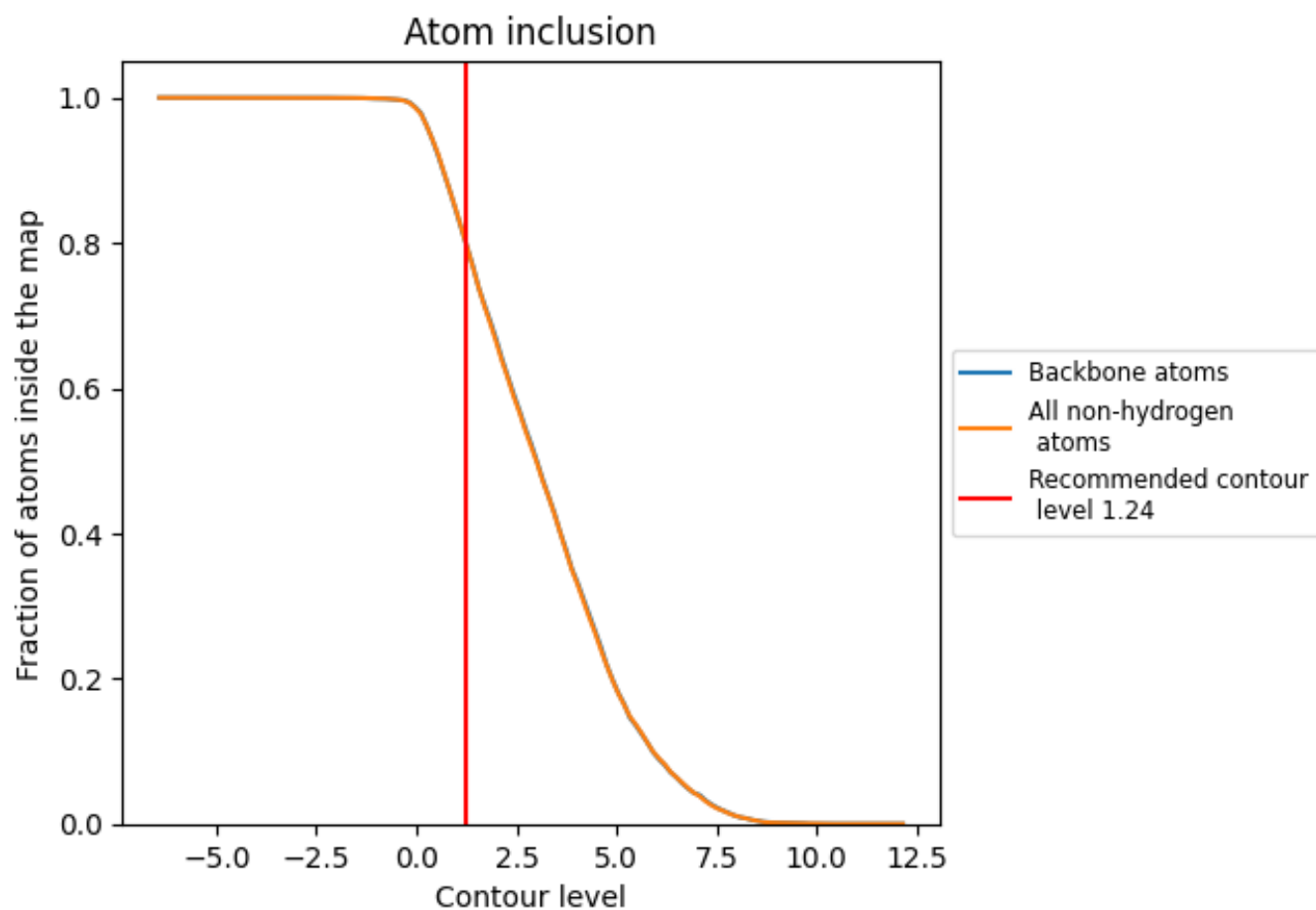
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.24).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (1.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8000	 0.5930
A	 0.8049	 0.5920
B	 0.8027	 0.5910
C	 0.8029	 0.5930
D	 0.8034	 0.5930
E	 0.8024	 0.5920
F	 0.8062	 0.5970
G	 0.8024	 0.5910
H	 0.8037	 0.5940

