



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:05 AM UTC

PDB ID : 6U8R / pdb_00006u8r
EMDB ID : EMD-20690
Title : Human IMPDH2 treated with ATP, IMP, and NAD⁺. Bent (1/4 compressed, 3/4 extended) segment reconstruction.
Authors : Johnson, M.C.; Kollman, J.M.
Deposited on : 2019-09-05
Resolution : 3.91 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

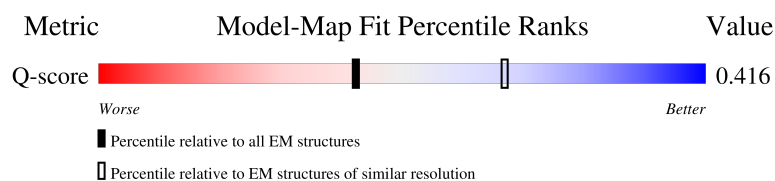
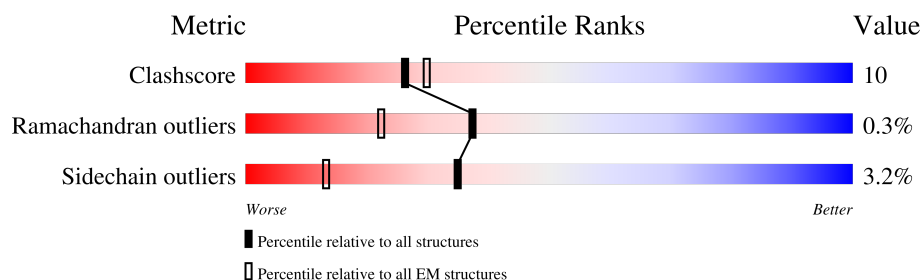
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 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.



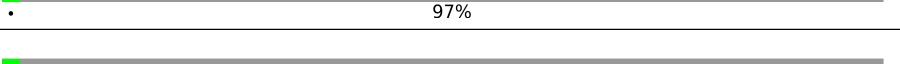
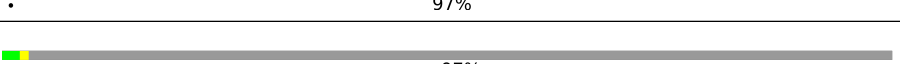
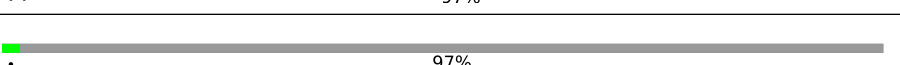
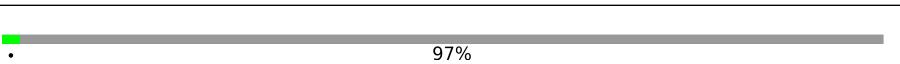
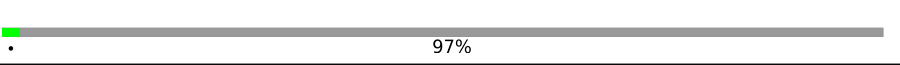
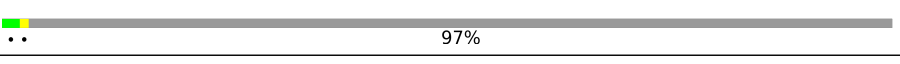
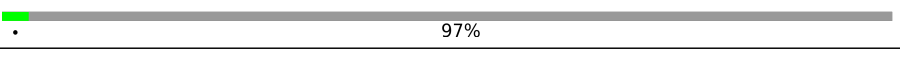
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7920 (3.41 - 4.41)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	
1	B	519	
1	C	519	
1	D	519	

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Mol	Chain	Length	Quality of chain
1	E	519	
1	F	519	
1	G	519	
1	H	519	
1	I	519	
1	J	519	
1	K	519	
1	L	519	
1	M	519	
1	N	519	
1	O	519	
1	P	519	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 31528 atoms, of which 0 are hydrogens and 0 are deuteriums.

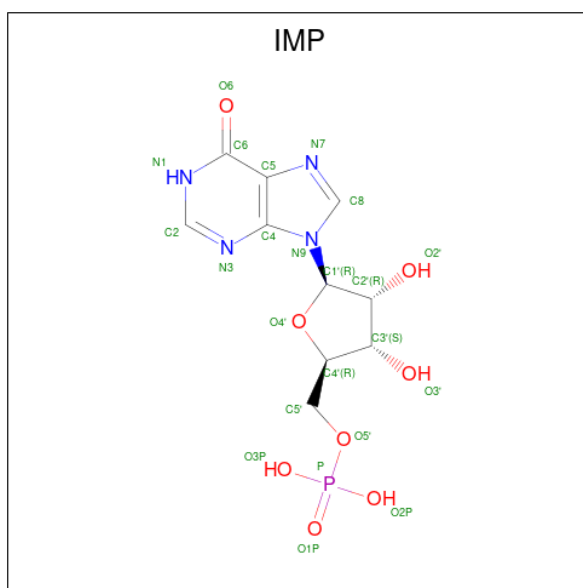
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

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

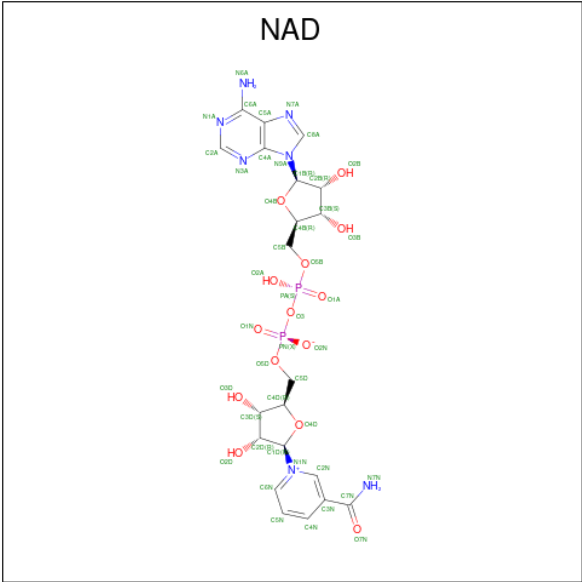
- Molecule 2 is INOSINIC ACID (CCD ID: IMP) (formula: C₁₀H₁₃N₄O₈P) (labeled as "Ligand

of Interest" by depositor).



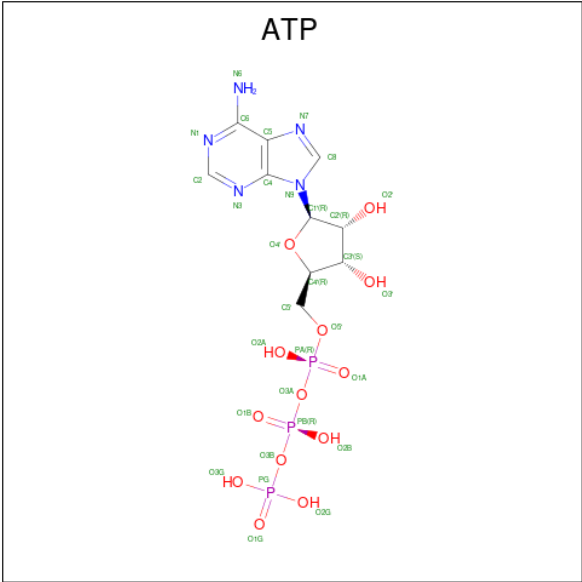
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	B	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	C	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	D	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	E	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	F	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	G	1	Total	C	N	O	P	0
			23	10	4	8	1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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (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	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	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	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	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	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	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	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

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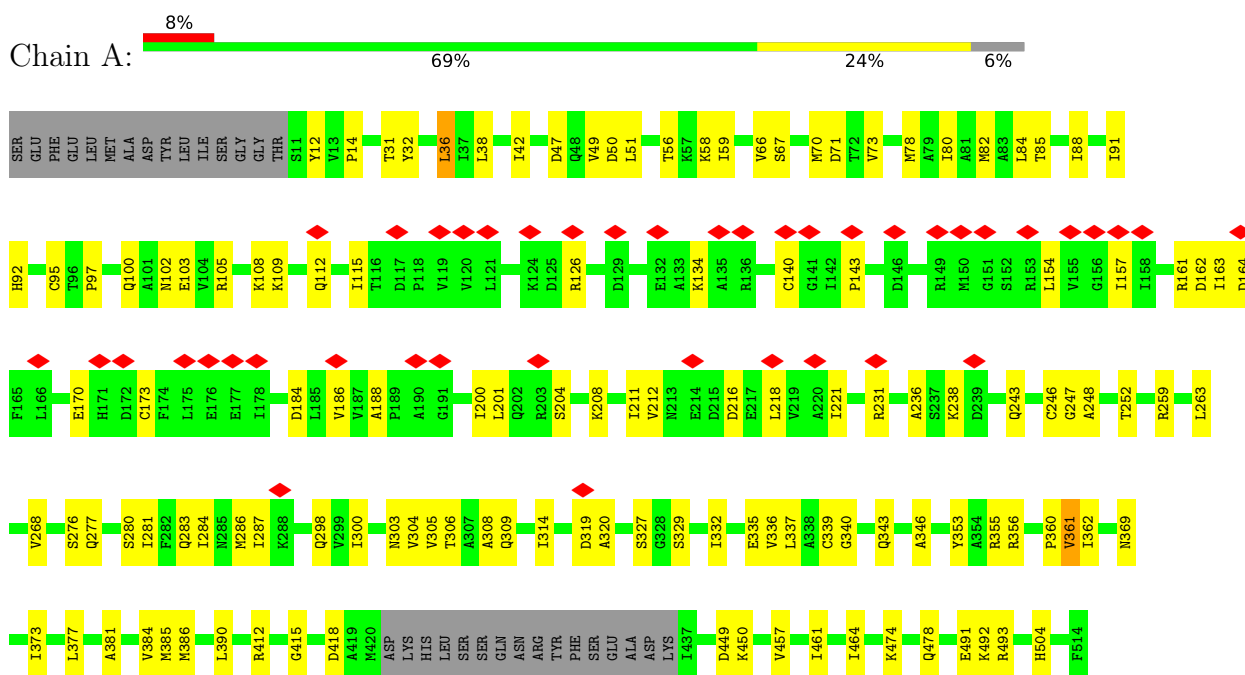
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Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

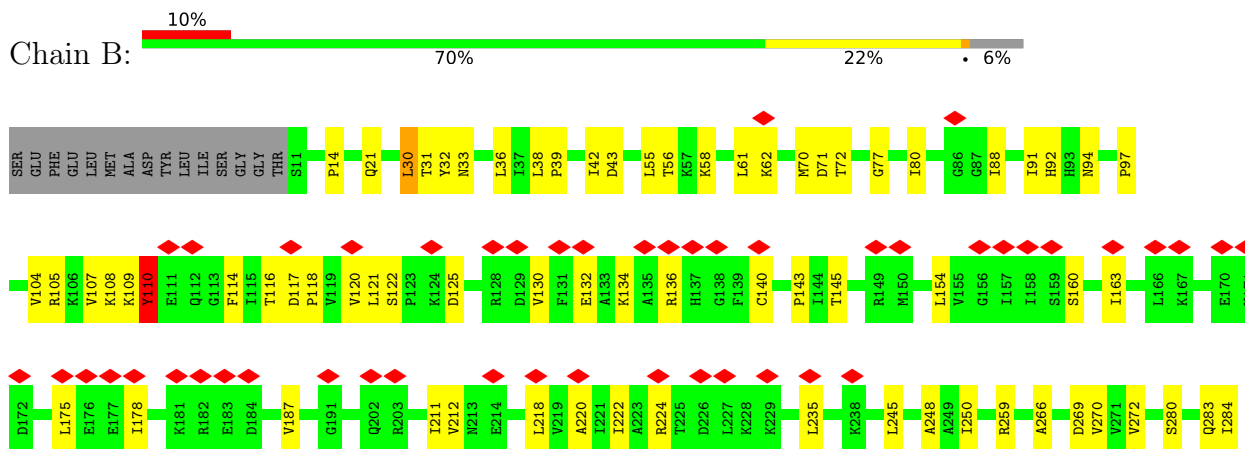
3 Residue-property plots

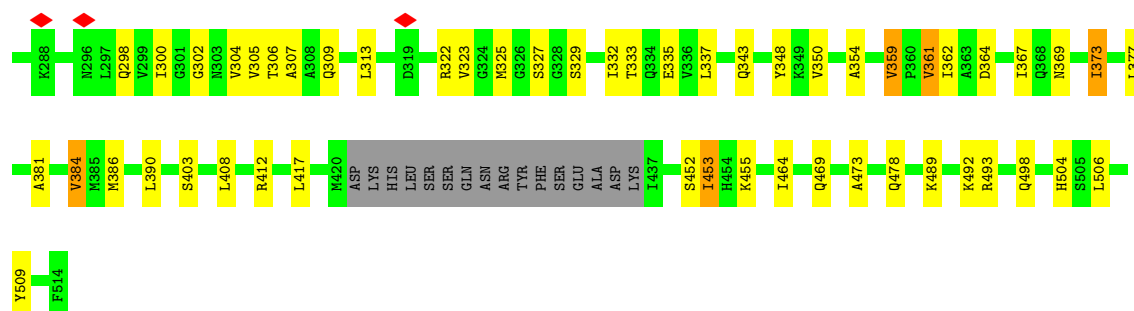
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

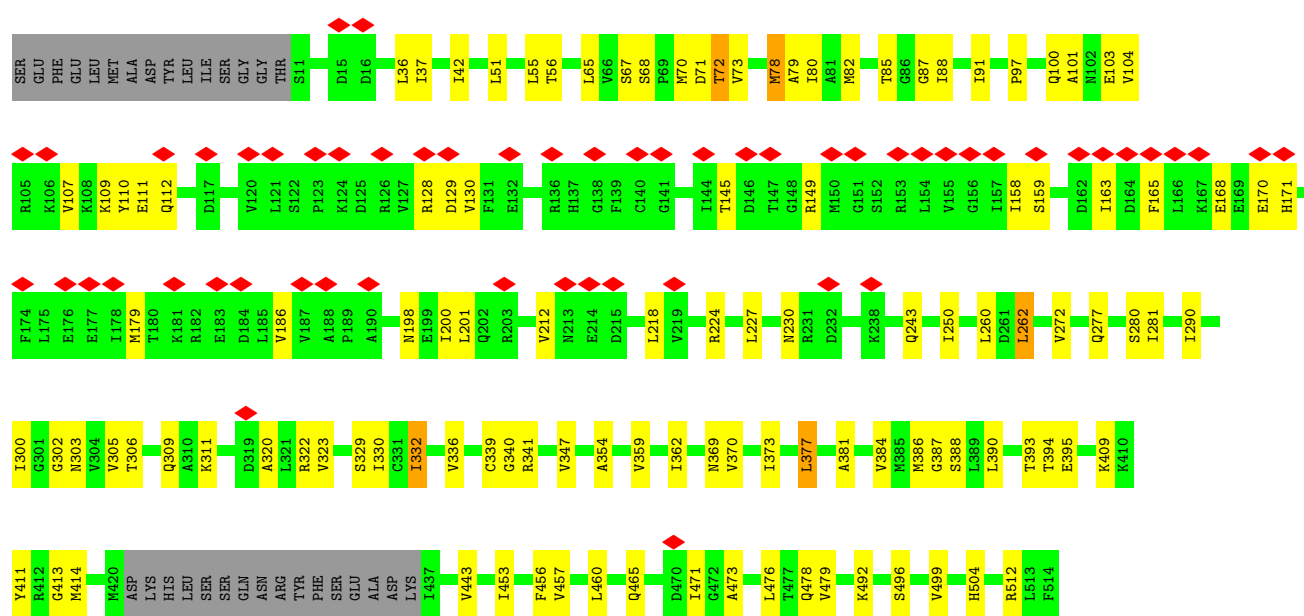


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

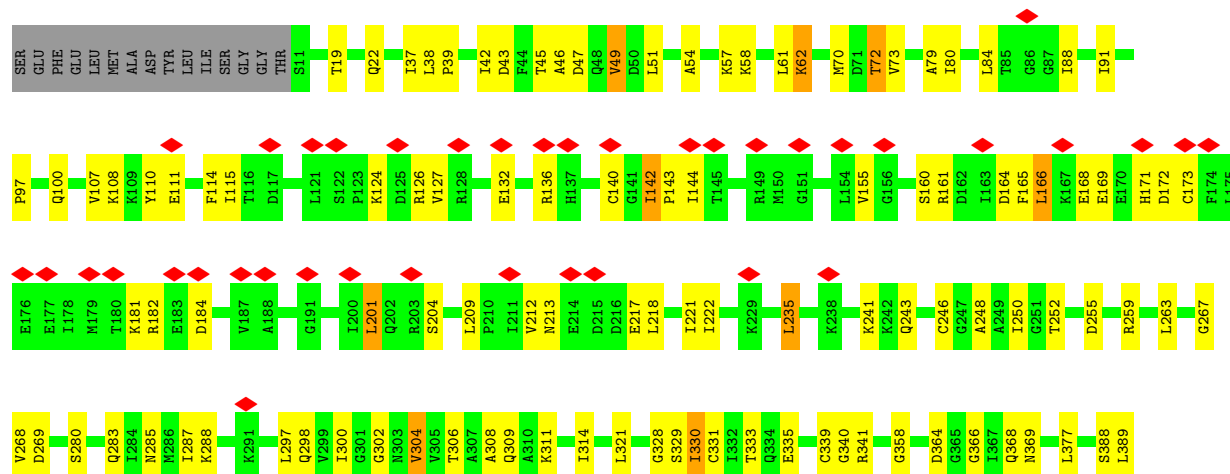


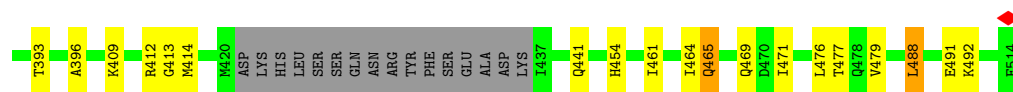


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

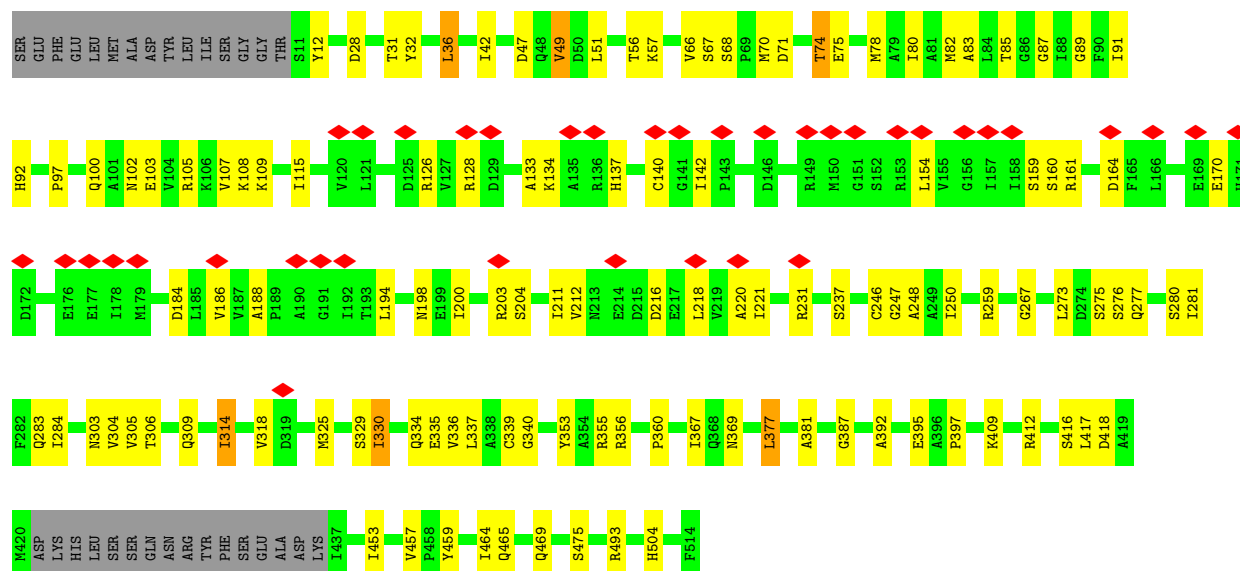


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

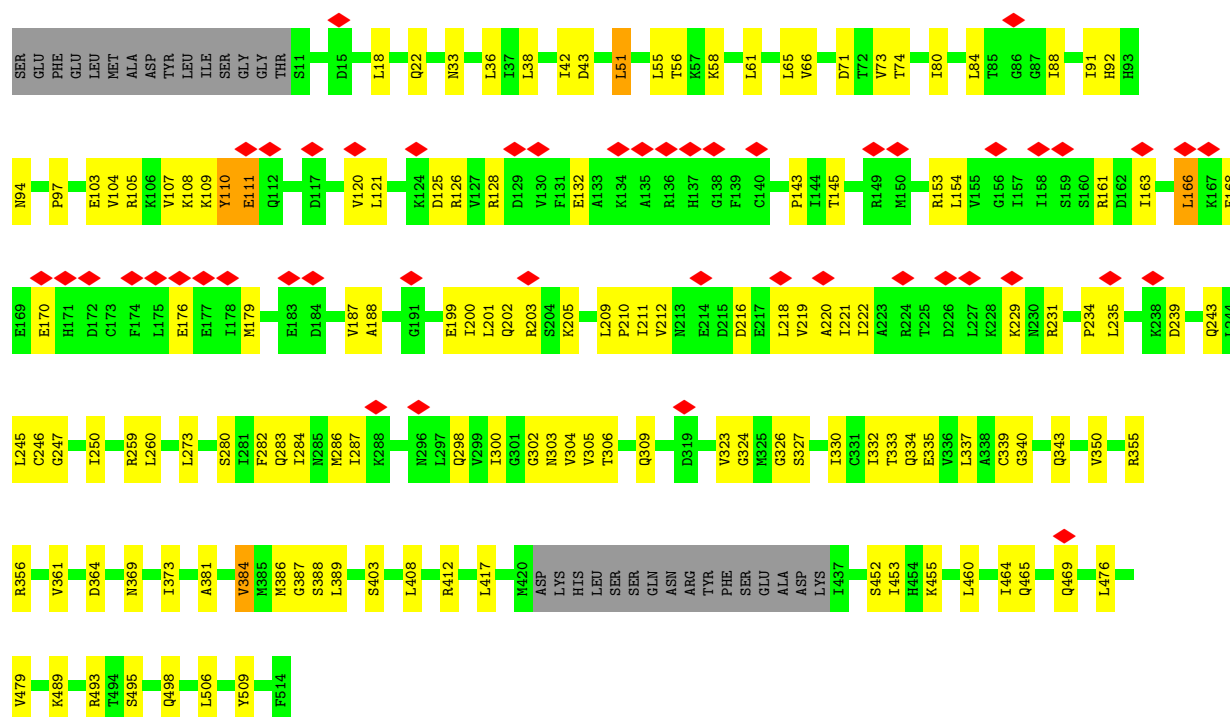




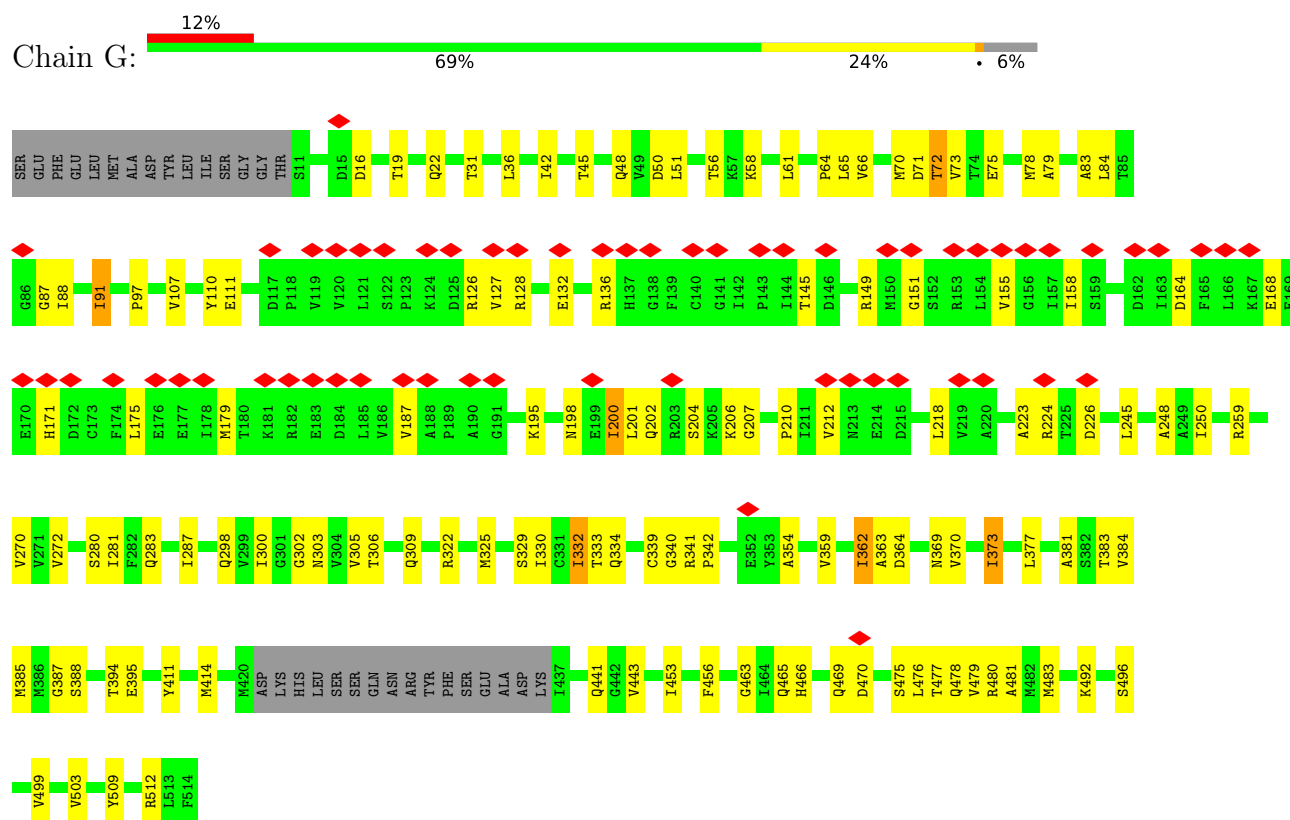
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



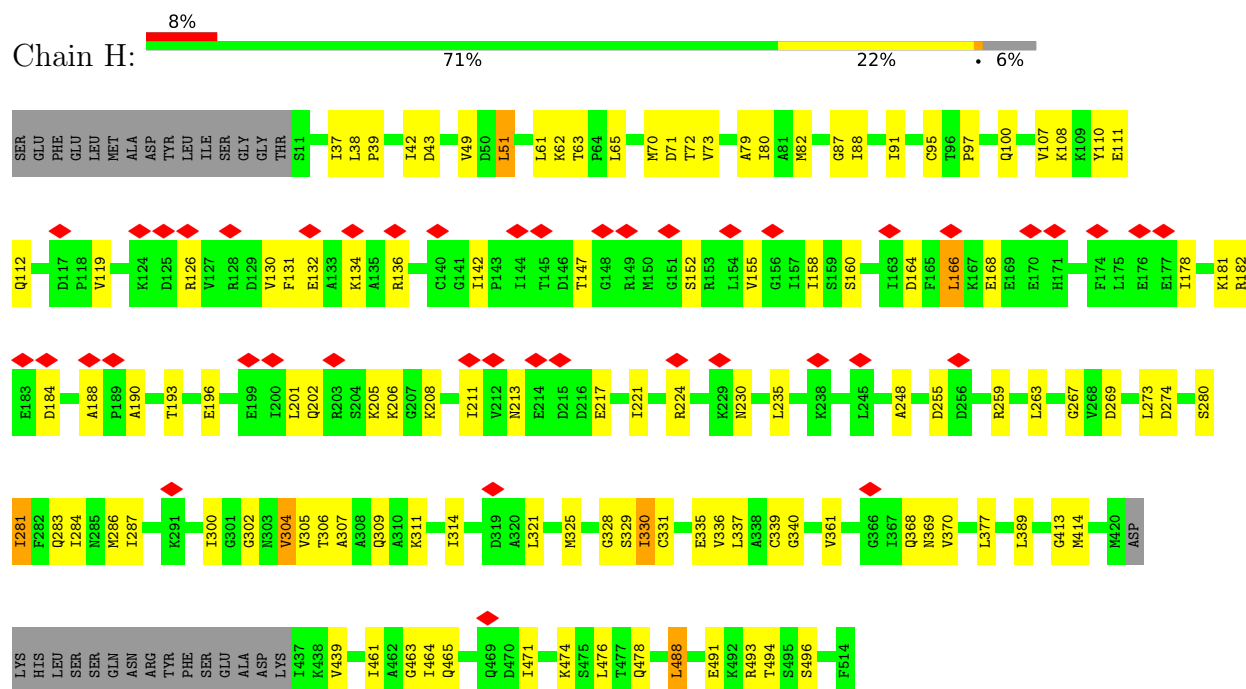
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



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



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



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



Chain 0: 97%

MET	LYS	ILE	GLY	LYS	ARG	SER	LYS	SER
MET	HIS	ALA	ASN	GLN	GLU	PRO	THR	ASP
TYR	LEU	ASP	VAL	ASN	GLU	LYS	PRO	GLY
SER	SER	GLY	VAL	LEU	LEU	ASP	LEU	PHE
GLU	GLN	ILE	ALA	GLY	VAL	VAL	SER	W1
LEU	ASN	GLN	ALA	ALA	ALA	ARG	SER	G9
LYS	ARG	ASN	GLN	ALA	PRO	ASP	PRO	T10
PHE	TYR	VAL	ALA	ILE	ALA	PHE	MET	S11
GLU	ALA	GLY	LYS	GLY	GLY	VAL	ASP	Y12
LYS	SER	HIS	ASN	HIS	ILE	GLU	THR	Y13
ARG	GLU	ILE	LEU	THR	THR	ALA	VAL	P14
THR	ALA	ALA	ILE	GLU	LEU	LYS	THR	P14
SER	ASP	LYS	ASP	ASP	GLY	ALA	GLU	ASP
SER	LYS	ALA	ALA	ASP	GLY	ALA	ALA	ASP
ALA	ILE	LEU	GLY	LYS	HIS	GLY	GLY	GLY
GLN	LYS	ALA	VAL	TYR	ASN	GLY	MET	LEU
VAL	VAL	LEU	ASP	ARG	GLU	PHE	ALA	THR
GLU	ALA	GLY	ALA	LEU	ILE	CYS	ILE	ALA
GLY	GLN	ALA	LEU	ASP	LEU	GLY	ALA	GLN
GLY	GLY	SER	ARG	LEU	GLN	ILE	MET	GLN
VAL	VAL	THR	VAL	LEU	ARG	PRO	ALA	LEU
HIS	SER	VAL	GLY	ALA	SER	ILE	LEU	PHE
SER	GLY	MET	MET	GLN	LYS	THR	THR	ASN
LEU	ALA	MET	GLY	ALA	LYS	ASP	GLY	CYS
HIS	VAL	GLY	SER	GLY	GLY	THR	ILE	GLY
SER	GLN	SER	GLY	VAL	LEU	GLY	ILE	ASP
TYR	ASP	LEU	SER	LYS	LEU	ARG	PHE	GLY
GLU	LYS	LEU	ILE	VAL	PRO	MET	THR	THR
LYS	GLY	ALA	CYS	VAL	ILE	GLY	ILE	LEU
ARG	SER	ALA	ILE	VAL	VAL	SER	HIS	TYR
LEU	ILE	THR	THR	LEU	ASN	ARG	ASN	ASN
PHE	LYS	THR	GLN	SER	GLU	LEU	ASN	ASP
	PHE	ALA	VAL	ASP	ASP	VAL	CYS	PHE
	VAL	ALA	VAL	SER	ASP	GLY	THR	LEU
	PRO	PRO	LEU	GLN	GLU	ILE	PRO	LEU
	TYR	GLY	ALA	GLY	LEU	ILE	GLJ	LEU
	LEU	GLY	CYS	ASN	VAL	SER	PHE	ASP
	TYR	TYR	GLY	SER	ALA	SER	GLN	PHE
	ILE	PHE	ARG	ILE	ILE	ARG	ASN	ILE
	ALA	SER	PRO	PHE	ILE	ASP	ASP	GLY
	GLY	SER	GLN	GLN	ALA	ILE	GLU	VAL
	ILE	ASP	ALA	ILE	ARG	ASP	VAL	THR
	GLN	GLY	THR	ASN	THR	PHE	ARG	THR
	HIS	ILE	ALA	MET	ASP	LEU	LYS	ALA
	SER	VAL	VAL	ILE	LEU	VAL	VAL	ASP
	CYS	LEU	TYR	LYS	LYS	GLJ	LYS	GLN
	GLN	LYS	VAL	TYR	LYS	GLU	VAL	VAL
	ASP	LYS	VAL	ILE	ASN	GLJ	TYR	VAL
	ILE	TYR	SER	LYS	ARG	HIS	GLU	ASP
	GLY	ARG	GLU	LYS	ASP	GLN	LEU	LEU
	ALA	GLY	TYR	LYS	TYR	CYS	THR	THR
	LYS	MET	ALA	TYR	PRO	PHE	PHI	LYS
	SER	GLY	ARG	PRO	LEU	ILE	ILE	LEU
	THR	LEU	PHE	ASN	ALA	GLJ	THR	THR
	GLN	ASP	GLY	LEU	SER	GLU	ASP	LYS
	VAL	ALA	VAL	VAL	VAL	ILE	PRO	LYS
	ARG	MET	VAL	ILE	LYS	THR	VAL	ILE
	ALA	ASP	VAL	GLY	LYS	LYS	LEU	THR

Chain P: 97%

[illegible]

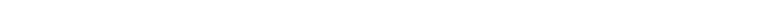
[illegible]

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

Chain K: 97%

ARG	ALA	ALA	MET	PRO	ILE	ALA	THR	VAL	THR	VAL	THR	SER
ALA	MET	GLY	ASP	VAL	GLY	LYS	LYS	LEU	LYS	LEU	LEU	GLU
MET	THR	ASN	HIS	ALA	ASN	LYS	ARG	ILE	ARG	SER	LYS	PHE
THR	LEU	VAL	LEU	ASP	VAL	VAL	LEU	THR	ASP	LEU	PRO	GLU
SER	SER	THR	SER	GLY	THR	CYS	VAL	VAL	ARG	ASP	LEU	LEU
GLY	GLN	ALA	GLN	ILE	ALA	GLY	VAL	VAL	VAL	SER	SER	D3
LEU	ASN	ALA	ASN	GLN	ALA	ALA	ALA	PRO	ASP	ASP	SER	M1
PHE	TYR	ALA	GLY	ALA	ILE	ILE	ALA	ALA	VAL	VAL	MET	A2
LYS	SER	THR	SER	HIS	ASN	THR	ILE	GLY	PHE	ASP	ASP	G9
ARG	GLU	ALA	GLU	ILE	LEU	HIS	THR	GLU	THR	THR	THR	T10
THR	ALA	ILE	ALA	ALA	ILE	GLU	LEU	LYS	ALA	THR	VAL	S11
SER	SER	ASP	ASP	LYS	ASP	ASP	LYS	ALA	ALA	THR	THR	Y12
SER	SER	LYS	LYS	ALA	ALA	ASP	GLU	ARG	GLU	GLU	ASP	V13
ALA	ALA	ILE	ILE	LEU	GLY	LYS	ALA	HIS	GLY	GLY	ASP	P14
GLN	LYS	VAL	VAL	ALA	VAL	TYR	ASN	GLY	GLY	GLY	GLY	ASP
VAL	VAL	VAL	GLY	LEU	VAL	ARG	ASN	GLY	MET	LEU	LEU	PHE
GLU	GLU	ALA	GLY	GLY	ALA	THR	GLU	GLY	ILE	THR	THR	THR
GLY	GLY	GLY	VAL	ALA	ALA	LEU	LEU	ILE	ALA	ALA	GLN	GLN
GLY	GLY	GLY	GLY	ALA	GLY	LEU	GLN	ILE	MET	ALA	LEU	LEU
GLY	GLY	GLY	VAL	THR	GLY	ALA	ARG	SER	ILE	ILE	PHE	PHE
HIS	HIS	SER	SER	VAL	GLY	GLN	LYS	THR	THR	THR	ASN	ASN
LEU	LEU	GLY	GLY	MET	GLY	GLN	LYS	LYS	THR	THR	ASN	ASN
LEU	ALA	GLY	GLY	MET	GLY	ALA	LYS	ASP	GLY	GLY	GLY	CYS
HIS	HIS	GLN	GLN	GLY	SER	VAL	LEU	GLY	THR	ILE	ILE	GLY
TYR	TYR	SER	ASP	LEU	SER	ASP	LYS	ARG	GLY	GLY	GLY	ASP
GLU	GLU	ASP	ASP	LEU	ILE	VAL	PRO	MET	GLY	PHE	LEU	LEU
LYS	LYS	ALA	GLY	ALA	ILE	VAL	ILE	GLY	ILE	ILE	THR	THR
ARG	ARG	ILE	ILE	THR	THR	LEU	ASN	ARG	SER	HIS	TYR	ASN
PHE	PHE	LYS	LYS	THR	GLN	ASP	GLU	LEU	ASN	ASN	ASP	ASP
						SER	VAL	VAL	CYS	THR	PHE	PHE
						SER	ASP	GLY	THR	THR	LEU	LEU
						SER	ASP	ARG	ASN	GLN	GLY	TYR
						ILE	ILE	ARG	ALA	ALA	ALA	ALA
						PRO	ILE	ILE	ASP	ASN	ASN	ASP
						GLN	ALA	ILE	ILE	VAL	VAL	VAL
						GLY	ALA	ILE	VAL	ARG	ARG	THR
						ASN	VAL	ILE	SER	PHE	LYS	ALA
						SER	ALA	SER	LEU	VAL	VAL	ASP
						ILE	LEU	LYS	LYS	LYS	LYS	GLN
						ILE	LYS	GLU	GLU	GLU	GLU	GLN
						TYR	ARG	HIS	HIS	GLU	LEU	LEU
						GLY	ASP	TYR	GLY	GLN	THR	THR
						VAL	TYR	GLY	CYS	GLY	THR	LYS
						THR	PRO	PHE	PHE	PHE	ALA	ALA
						ASN	LEU	LEU	LEU	LEU	LEU	LYS
						GLN	THR	THR	THR	THR	THR	THR
						VAL	ASN	VAL	VAL	VAL	VAL	VAL
						THR	THR	THR	THR	THR	THR	THR
						GLY	GLY	GLY	GLY	GLY	GLY	GLY
						ASP	ASP	ASP	ASP	ASP	ASP	ASP
						VAL	VAL	VAL	VAL	VAL		

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

Chain L:  97%

VAL	VAL	LEU	ASP	LYS	PRO	SER
VAL	THR	LEU	LEU	ASP	LEU	GLU
ALA	THR	CYS	VAL	ARG	VAL	PHE
ALA	ALA	GLY	VAL	VAL	SER	GLU
GLN	ALA	ALA	ALA	ARG	LEU	
ALA	ILE	ALA	PRO	ASP	PRO	M1
LYS	GLY	GLY	ALA	VAL	MET	
LEU	THR	ILE	ILE	PHE	ASP	T10
LEU	HIS	THR	THR	GLU	VAL	S11
ILE	GLU	LEU	LEU	LYS	THR	
ASP	ASP	LYS	LYS	ALA	THR	P14
ALA	ASP	GLU	GLU	ARG	ALA	ASP
GLY	GLY	LYS	ALA	HIS	GLY	GLY
VAL	TYR	ASN	ASN	VAL	MET	LEU
ASP	ASP	GLU	GLU	PHE	ALA	THR
ALA	ALA	ILE	ILE	CYS	ILE	ALA
LEU	ASP	LEU	LEU	GLY	ILE	GLN
ARG	ARG	GLN	GLN	ILE	MET	GLN
VAL	VAL	ARG	PRO	PRO	ALA	LEU
GLY	MET	GLY	ALA	ILE	THR	PHE
MET	GLN	LYS	LYS	THR	THR	ASN
GLY	ALA	LYS	ASP	ASP	GLY	CYS
SER	SER	GLY	LYS	THR	GLY	GLY
GLY	VAL	VAL	LYS	GLY	ILE	ASP
SER	ILE	VAL	LEU	ARG	GLY	GLY
ILE	VAL	VAL	PRO	MET	PHE	LEU
CYS	VAL	ILE	ILE	GLY	ILE	LEU
ILE	VAL	VAL	VAL	SER	HIS	TYR
THR	LEU	LEU	ASN	ARG	HIS	ASN
GLN	ASP	GLU	GLU	LEU	ASN	ASP
GLU	SER	ASP	ASP	VAL	CYS	PHE
VAL	VAL	SER	ASP	GLY	THR	LEU
LEU	LEU	GLN	GLU	ILE	PRO	ILE
ALA	ALA	GLY	LEU	ILE	GLU	LEU
CYS	ASN	ASN	VAL	SER	PHE	PRO
GLY	SER	ALA	ALA	LEU	GLN	GLY
ARG	ILE	ILE	ILE	ARG	ALA	TYR
PRO	PRO	PHE	ILE	ARG	ASN	ILE
GLN	GLN	GLN	ALA	ILE	GLU	ASP
ALA	ALA	ILE	ARG	ASP	VAL	PHE
THR	ASN	THR	THR	PHE	ARG	THR
ALA	MET	ASP	ASP	LEU	LYS	ASP
VAL	ILE	LEU	LEU	LYS	VAL	ASP
TYR	LYS	LYS	LYS	GLU	VAL	GLN
LYS	TYR	TYR	LYS	GLU	LYS	VAL
VAL	VAL	ILE	ASN	GLU	TYR	ASP
SER	LYS	LYS	ARG	HIS	GLU	LEU
GLU	GLU	ASP	ASP	ASP	GLN	THR
TYR	LYS	TYR	PRO	CYS	GLY	SER
ALA	ALA	TYR	TYR	PHE	PHE	ALA
ARG	ARG	ASN	LEU	GLU	ILE	THR
PHE	PHE	LEU	SER	GLU	ASP	LYS
GLY	GLY	GLN	LYS	ILE	PRO	LYS
VAL	VAL	ILE	ASP	MET	VAL	ILE
PRO	PRO	ILE	ALA	THR	VAL	THR
VAL	ILE	GLY	LYS	LYS	LEU	THR
ILE	ASN	GLN	LYS	ARG	SER	LYS
ALA	ASN	CTR	CTR	CTR	PRO	THR

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

TYR
SER
GLY
GLY
LEU
LYS
PHE
GLU
LYS
ARG
THR
SER
SER
ALA
GLN
VAL
GLY
GLY
VAL
HIS
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	16819	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	115.597	Depositor
Minimum map value	-89.660	Depositor
Average map value	0.084	Depositor
Map value standard deviation	3.293	Depositor
Recommended contour level	17	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.62	0/3766	0.85	0/5078
1	B	0.60	0/3766	0.86	3/5078 (0.1%)
1	C	0.60	0/3766	0.88	3/5078 (0.1%)
1	D	0.62	1/3766 (0.0%)	0.86	2/5078 (0.0%)
1	E	0.62	0/3766	0.86	0/5078
1	F	0.61	0/3766	0.87	1/5078 (0.0%)
1	G	0.62	0/3766	0.91	6/5078 (0.1%)
1	H	0.62	0/3766	0.89	3/5078 (0.1%)
1	I	0.47	0/104	1.08	0/141
1	J	0.51	0/104	1.02	0/141
1	K	0.45	0/104	1.08	0/141
1	L	0.51	0/104	1.16	0/141
1	M	0.52	0/104	1.12	1/141 (0.7%)
1	N	0.53	0/104	1.14	0/141
1	O	0.51	0/104	1.10	1/141 (0.7%)
1	P	0.52	0/104	1.07	0/141
All	All	0.61	1/30960 (0.0%)	0.88	20/41752 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	E	0	1
1	G	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	454	HIS	CA-C	-5.40	1.45	1.52

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	THR	CA-C-N	-6.23	116.62	122.66
1	D	72	THR	C-N-CA	-6.23	116.62	122.66
1	B	453	ILE	N-CA-C	-5.94	106.47	113.42
1	F	330	ILE	N-CA-C	-5.79	107.86	113.53
1	C	332	ILE	CG1-CB-CG2	-5.72	93.54	110.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	164	ASP	Peptide
1	D	62	LYS	Peptide
1	E	74	THR	Peptide
1	G	342	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3710	0	3766	96	0
1	B	3710	0	3766	84	0
1	C	3710	0	3766	75	0
1	D	3710	0	3766	90	0
1	E	3710	0	3766	86	0
1	F	3710	0	3766	89	0
1	G	3710	0	3766	80	0
1	H	3710	0	3766	80	0
1	I	102	0	99	1	0
1	J	102	0	99	3	0
1	K	102	0	99	5	0
1	L	102	0	99	1	0
1	M	102	0	99	1	0
1	N	102	0	99	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	102	0	99	1	0
1	P	102	0	99	0	0
2	A	23	0	11	3	0
2	B	23	0	11	0	0
2	C	23	0	11	2	0
2	D	23	0	11	3	0
2	E	23	0	11	3	0
2	F	23	0	11	2	0
2	G	23	0	11	4	0
2	H	23	0	11	1	0
3	A	44	0	24	2	0
3	B	44	0	24	0	0
3	C	44	0	24	1	0
3	D	44	0	24	0	0
3	E	44	0	22	1	0
3	F	44	0	24	1	0
3	G	44	0	24	1	0
3	H	44	0	24	3	0
4	A	62	0	24	1	0
4	B	62	0	24	1	0
4	C	62	0	24	2	0
4	D	62	0	23	3	0
4	E	62	0	24	2	0
4	F	62	0	24	1	0
4	G	62	0	24	0	0
4	H	62	0	24	2	0
All	All	31528	0	31389	637	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 10.

The worst 5 of 637 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:474:LYS:H	1:H:478:GLN:HE21	1.27	0.82
1:E:200:ILE:O	1:E:204:SER:HB3	1.82	0.80
1:E:36:LEU:HD13	1:E:493:ARG:HD2	1.65	0.78
1:A:36:LEU:HD13	1:A:493:ARG:HD2	1.71	0.72
1:F:283:GLN:HE22	1:F:302:GLY:H	1.37	0.71

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	484/519 (93%)	447 (92%)	37 (8%)	0	100	100
1	B	484/519 (93%)	446 (92%)	37 (8%)	1 (0%)	43	75
1	C	484/519 (93%)	438 (90%)	44 (9%)	2 (0%)	30	65
1	D	484/519 (93%)	450 (93%)	32 (7%)	2 (0%)	30	65
1	E	484/519 (93%)	446 (92%)	38 (8%)	0	100	100
1	F	484/519 (93%)	442 (91%)	40 (8%)	2 (0%)	30	65
1	G	484/519 (93%)	439 (91%)	43 (9%)	2 (0%)	30	65
1	H	484/519 (93%)	448 (93%)	34 (7%)	2 (0%)	30	65
1	I	12/519 (2%)	6 (50%)	6 (50%)	0	100	100
1	J	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	K	12/519 (2%)	8 (67%)	4 (33%)	0	100	100
1	L	12/519 (2%)	5 (42%)	7 (58%)	0	100	100
1	M	12/519 (2%)	8 (67%)	4 (33%)	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%)	6 (50%)	6 (50%)	0	100	100
All	All	3968/8304 (48%)	3610 (91%)	347 (9%)	11 (0%)	37	70

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	111	GLU
1	B	110	TYR
1	D	111	GLU
1	D	110	TYR
1	F	110	TYR

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/425 (94%)	387 (97%)	11 (3%)	38	59
1	B	398/425 (94%)	387 (97%)	11 (3%)	38	59
1	C	398/425 (94%)	386 (97%)	12 (3%)	36	57
1	D	398/425 (94%)	381 (96%)	17 (4%)	26	49
1	E	398/425 (94%)	389 (98%)	9 (2%)	44	63
1	F	398/425 (94%)	383 (96%)	15 (4%)	29	51
1	G	398/425 (94%)	381 (96%)	17 (4%)	26	49
1	H	398/425 (94%)	385 (97%)	13 (3%)	33	55
1	I	11/425 (3%)	11 (100%)	0	100	100
1	J	11/425 (3%)	11 (100%)	0	100	100
1	K	11/425 (3%)	11 (100%)	0	100	100
1	L	11/425 (3%)	11 (100%)	0	100	100
1	M	11/425 (3%)	11 (100%)	0	100	100
1	N	11/425 (3%)	11 (100%)	0	100	100
1	O	11/425 (3%)	11 (100%)	0	100	100
1	P	11/425 (3%)	11 (100%)	0	100	100
All	All	3272/6800 (48%)	3167 (97%)	105 (3%)	35	56

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	367	ILE
1	F	332	ILE
1	H	300	ILE
1	E	465	GLN
1	F	163	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	230	ASN
1	H	372	HIS
1	F	283	GLN
1	H	309	GLN
1	H	112	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	G	602	-	32,33,33	3.17	17 (53%)	48,52,52	2.87	12 (25%)
2	IMP	B	603	-	25,25,25	2.63	7 (28%)	37,38,38	2.17	12 (32%)
4	ATP	D	602	-	32,33,33	3.18	16 (50%)	48,52,52	2.89	12 (25%)
4	ATP	A	603	-	32,33,33	3.17	18 (56%)	48,52,52	2.97	14 (29%)
4	ATP	C	602	-	32,33,33	3.20	17 (53%)	48,52,52	2.86	12 (25%)
2	IMP	F	603	-	25,25,25	2.60	7 (28%)	37,38,38	2.08	10 (27%)
4	ATP	F	601	-	32,33,33	3.21	16 (50%)	48,52,52	2.89	13 (27%)
4	ATP	C	601	-	32,33,33	3.16	16 (50%)	48,52,52	2.91	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	B	604	-	46,48,48	3.45	21 (45%)	64,73,73	2.40	17 (26%)
4	ATP	E	603	-	32,33,33	3.19	18 (56%)	48,52,52	2.96	13 (27%)
2	IMP	A	601	-	25,25,25	2.54	6 (24%)	37,38,38	2.37	9 (24%)
4	ATP	D	601	-	32,33,33	3.21	18 (56%)	48,52,52	2.94	12 (25%)
4	ATP	H	602	-	32,33,33	3.15	16 (50%)	48,52,52	2.85	14 (29%)
2	IMP	D	603	-	25,25,25	2.62	7 (28%)	37,38,38	2.33	10 (27%)
3	NAD	H	604	-	46,48,48	3.47	21 (45%)	64,73,73	2.39	13 (20%)
4	ATP	H	601	-	32,33,33	3.21	18 (56%)	48,52,52	2.82	12 (25%)
3	NAD	G	604	-	46,48,48	3.46	21 (45%)	64,73,73	2.40	15 (23%)
4	ATP	B	602	-	32,33,33	3.21	17 (53%)	48,52,52	2.84	11 (22%)
4	ATP	F	602	-	32,33,33	3.33	16 (50%)	48,52,52	2.87	11 (22%)
3	NAD	A	602	-	46,48,48	3.47	21 (45%)	64,73,73	2.28	13 (20%)
4	ATP	G	601	-	32,33,33	3.18	17 (53%)	48,52,52	3.06	13 (27%)
3	NAD	C	604	-	46,48,48	3.52	21 (45%)	64,73,73	2.38	14 (21%)
4	ATP	A	604	-	32,33,33	3.21	18 (56%)	48,52,52	2.82	11 (22%)
4	ATP	E	604	-	32,33,33	3.21	16 (50%)	48,52,52	2.91	12 (25%)
4	ATP	B	601	-	32,33,33	3.10	16 (50%)	48,52,52	2.92	12 (25%)
2	IMP	G	603	-	25,25,25	2.64	7 (28%)	37,38,38	2.10	10 (27%)
3	NAD	E	602	-	46,48,48	3.51	22 (47%)	64,73,73	2.44	15 (23%)
2	IMP	C	603	-	25,25,25	2.63	7 (28%)	37,38,38	2.26	8 (21%)
2	IMP	E	601	-	25,25,25	2.64	6 (24%)	37,38,38	2.25	9 (24%)
3	NAD	D	604	-	46,48,48	3.48	21 (45%)	64,73,73	2.38	15 (23%)
3	NAD	F	604	-	46,48,48	3.50	21 (45%)	64,73,73	2.36	16 (25%)
2	IMP	H	603	-	25,25,25	2.62	7 (28%)	37,38,38	2.29	10 (27%)

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
4	ATP	G	602	-	-	5/22/38/38	0/3/3/3
2	IMP	B	603	-	-	5/10/26/26	0/3/3/3
4	ATP	D	602	-	-	9/22/38/38	0/3/3/3
4	ATP	A	603	-	-	9/22/38/38	0/3/3/3
4	ATP	C	602	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	F	603	-	-	2/10/26/26	0/3/3/3
4	ATP	F	601	-	-	8/22/38/38	0/3/3/3
4	ATP	C	601	-	-	8/22/38/38	0/3/3/3
3	NAD	B	604	-	-	9/30/62/62	0/5/5/5
4	ATP	E	603	-	-	7/22/38/38	0/3/3/3
2	IMP	A	601	-	-	0/10/26/26	0/3/3/3
4	ATP	D	601	-	-	2/22/38/38	0/3/3/3
4	ATP	H	602	-	-	2/22/38/38	0/3/3/3
2	IMP	D	603	-	-	2/10/26/26	0/3/3/3
3	NAD	H	604	-	-	13/30/62/62	0/5/5/5
4	ATP	H	601	-	-	5/22/38/38	0/3/3/3
3	NAD	G	604	-	-	10/30/62/62	0/5/5/5
4	ATP	B	602	-	-	5/22/38/38	0/3/3/3
4	ATP	F	602	-	-	7/22/38/38	0/3/3/3
3	NAD	A	602	-	-	15/30/62/62	0/5/5/5
4	ATP	G	601	-	-	4/22/38/38	0/3/3/3
3	NAD	C	604	-	-	9/30/62/62	0/5/5/5
4	ATP	A	604	-	-	7/22/38/38	0/3/3/3
4	ATP	E	604	-	-	6/22/38/38	0/3/3/3
4	ATP	B	601	-	-	4/22/38/38	0/3/3/3
2	IMP	G	603	-	-	5/10/26/26	0/3/3/3
3	NAD	E	602	-	-	13/30/62/62	0/5/5/5
2	IMP	C	603	-	-	5/10/26/26	0/3/3/3
2	IMP	E	601	-	-	5/10/26/26	0/3/3/3
3	NAD	D	604	-	-	13/30/62/62	0/5/5/5
3	NAD	F	604	-	-	16/30/62/62	0/5/5/5
2	IMP	H	603	-	-	0/10/26/26	0/3/3/3

The worst 5 of 493 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ATP	C2'-C3'	-10.51	1.24	1.53
4	H	602	ATP	C2'-C3'	-10.50	1.24	1.53
4	E	603	ATP	C2'-C3'	-10.49	1.25	1.53
4	A	604	ATP	C2'-C3'	-10.48	1.25	1.53
4	E	604	ATP	C2'-C3'	-10.45	1.25	1.53

The worst 5 of 395 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	604	ATP	N6-C6-N1	-9.40	97.44	118.38
4	C	601	ATP	N6-C6-N1	-9.35	97.55	118.38
4	A	603	ATP	N6-C6-N1	-9.34	97.57	118.38
4	B	601	ATP	N6-C6-N1	-9.29	97.70	118.38
4	D	601	ATP	N6-C6-N1	-9.22	97.84	118.38

There are no chirality outliers.

5 of 214 torsion outliers are listed below:

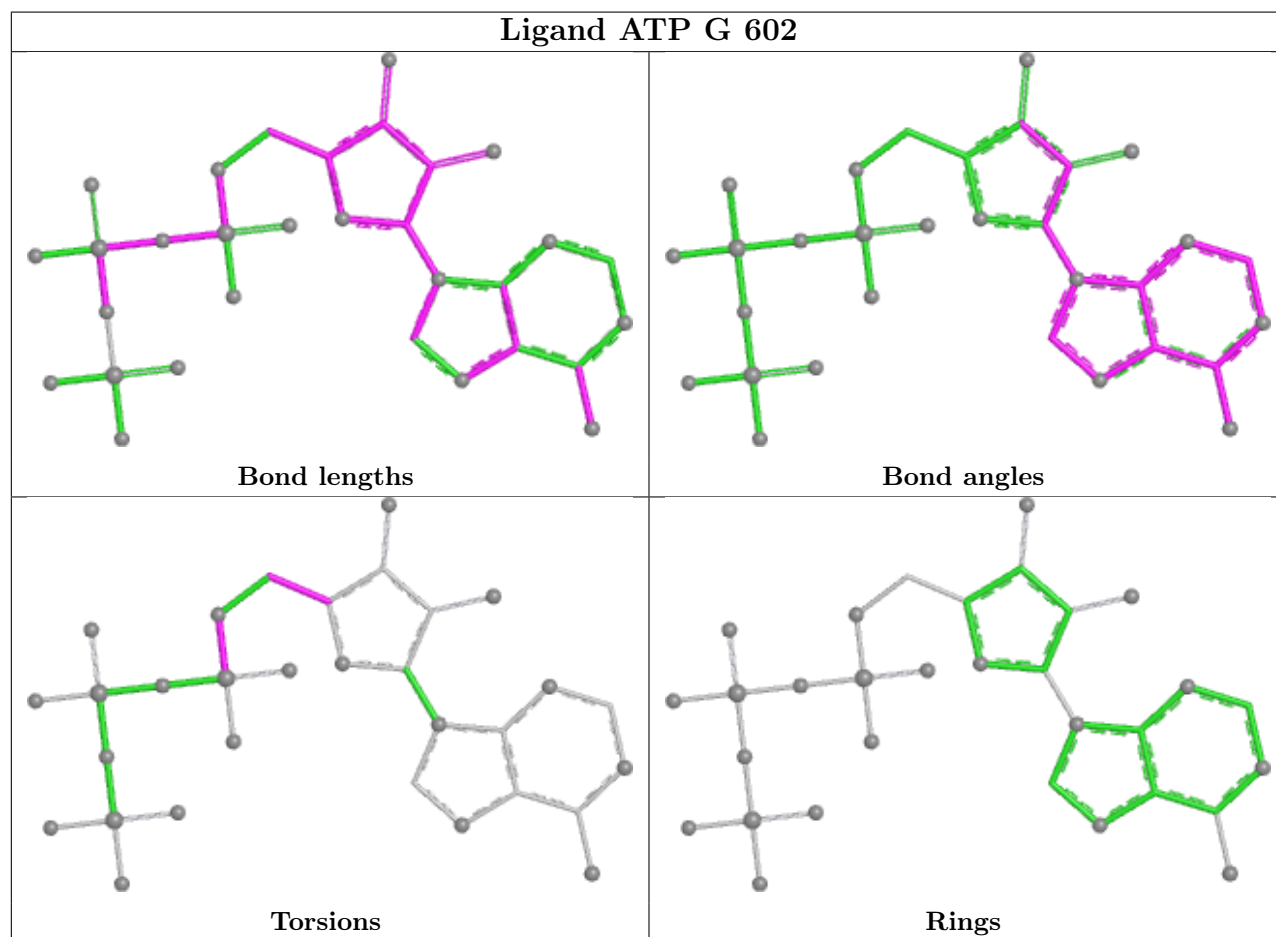
Mol	Chain	Res	Type	Atoms
2	B	603	IMP	C5'-O5'-P-O2P
2	B	603	IMP	C5'-O5'-P-O3P
2	B	603	IMP	O4'-C4'-C5'-O5'
2	C	603	IMP	C5'-O5'-P-O1P
2	C	603	IMP	C5'-O5'-P-O2P

There are no ring outliers.

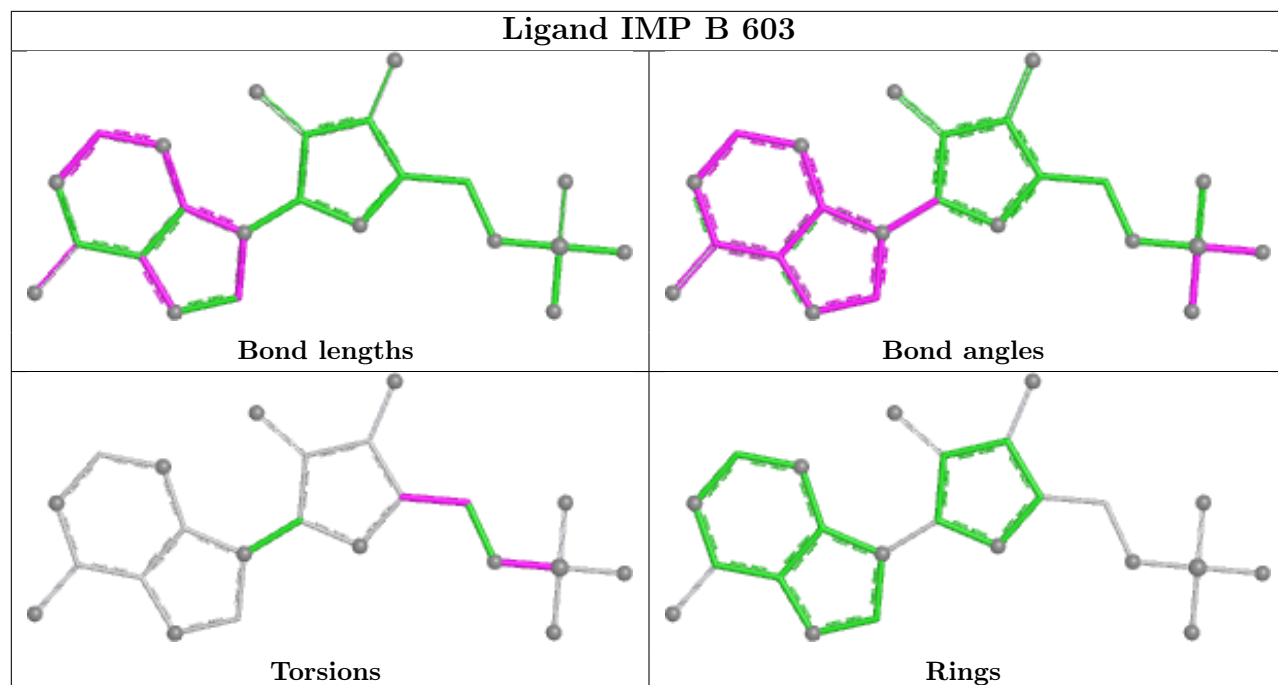
21 monomers are involved in 39 short contacts:

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

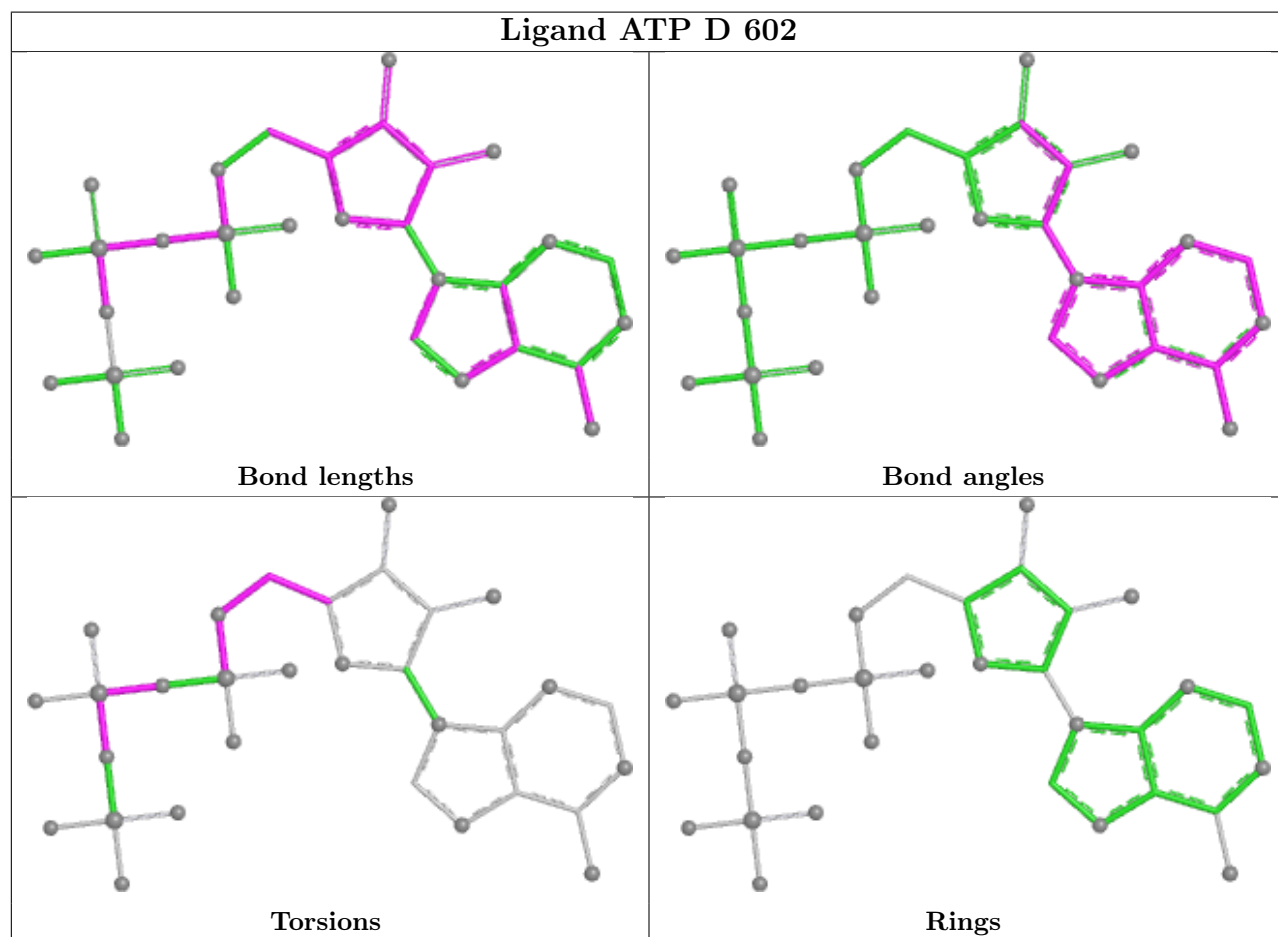
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

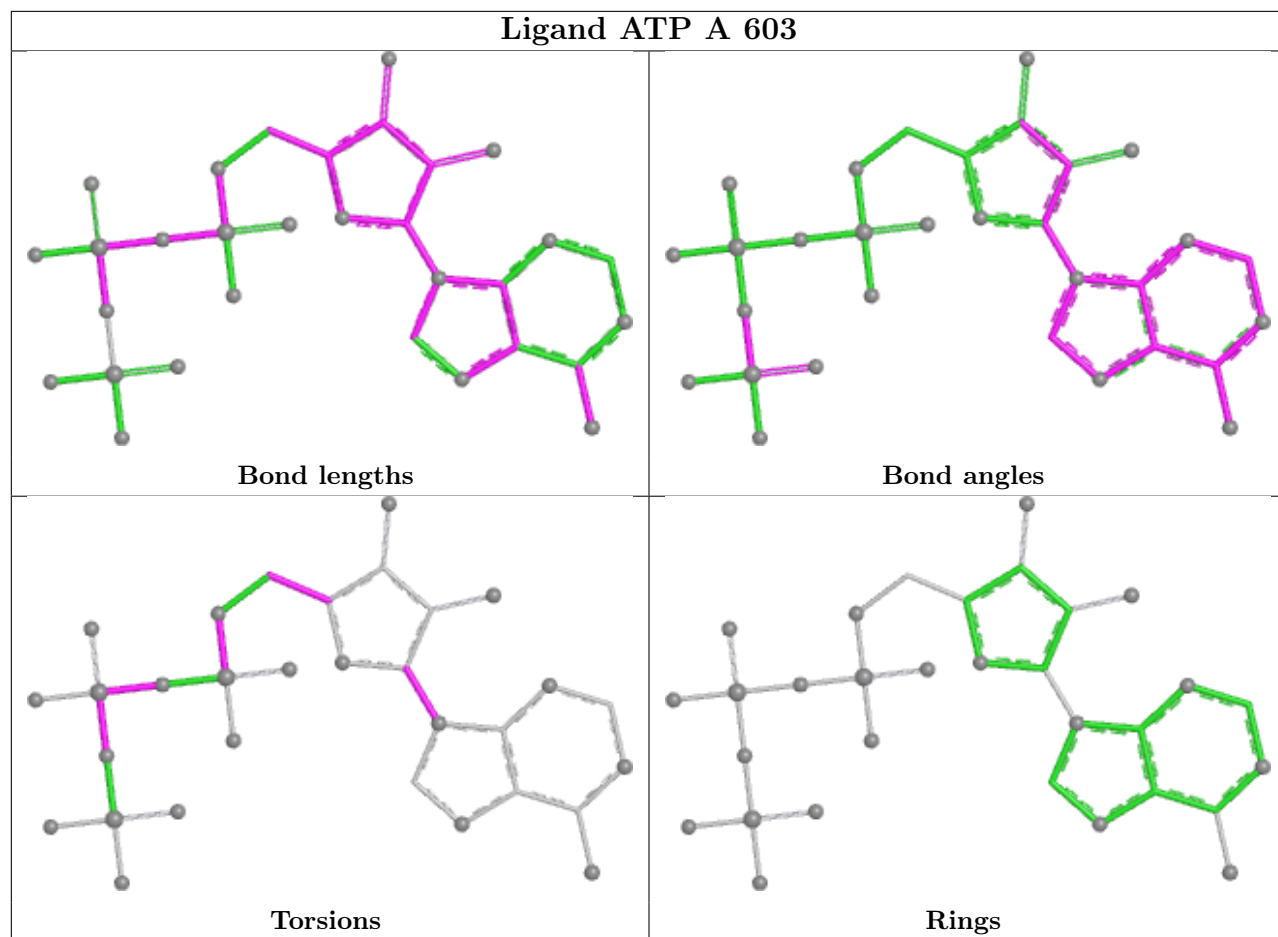


Ligand IMP B 603

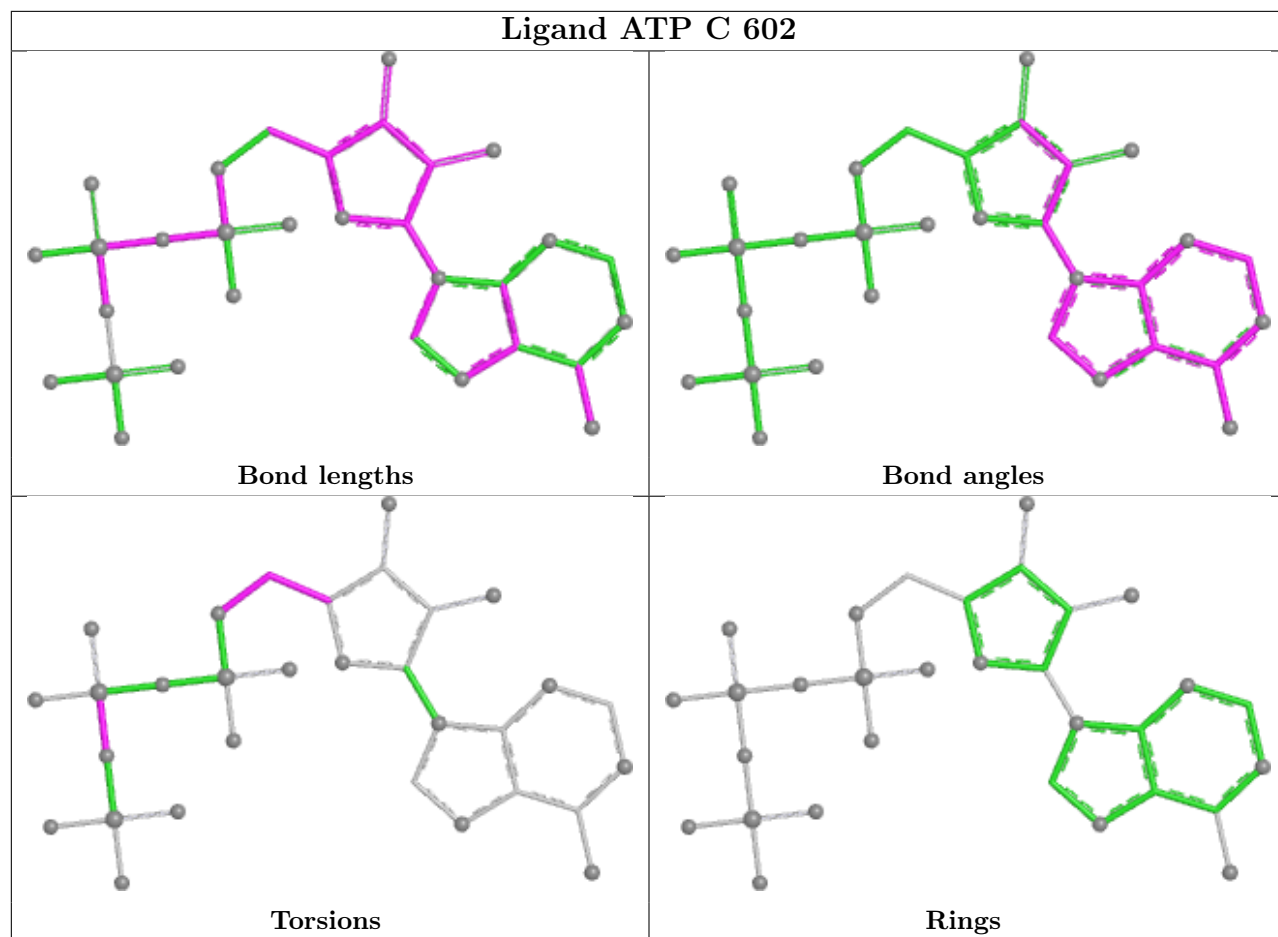


Ligand ATP D 602

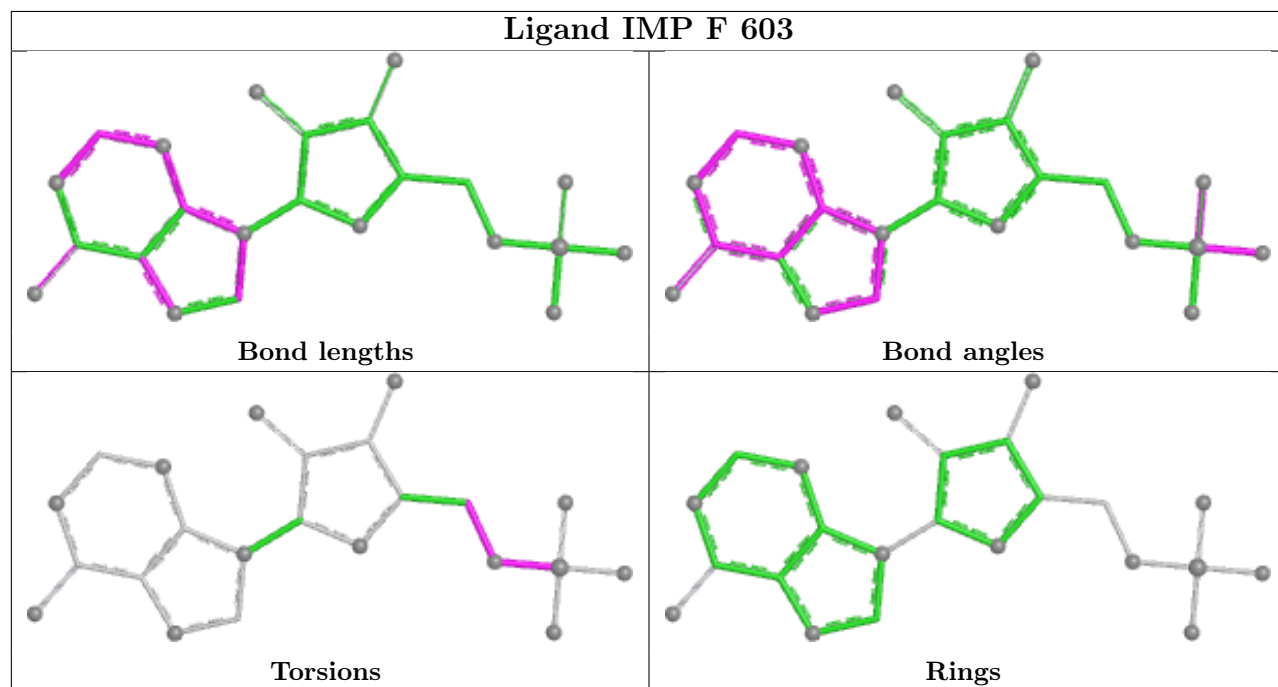




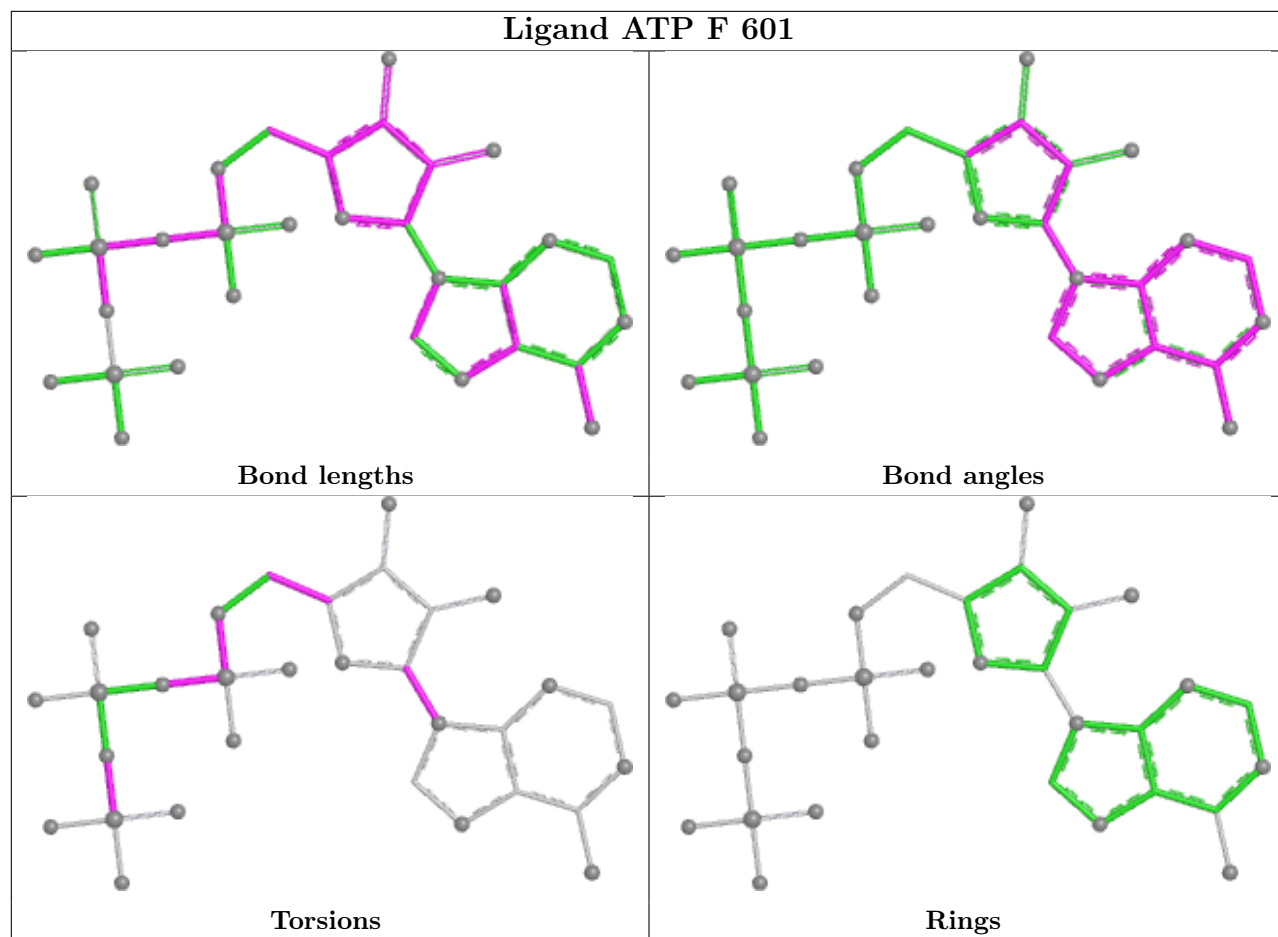
Ligand ATP C 602

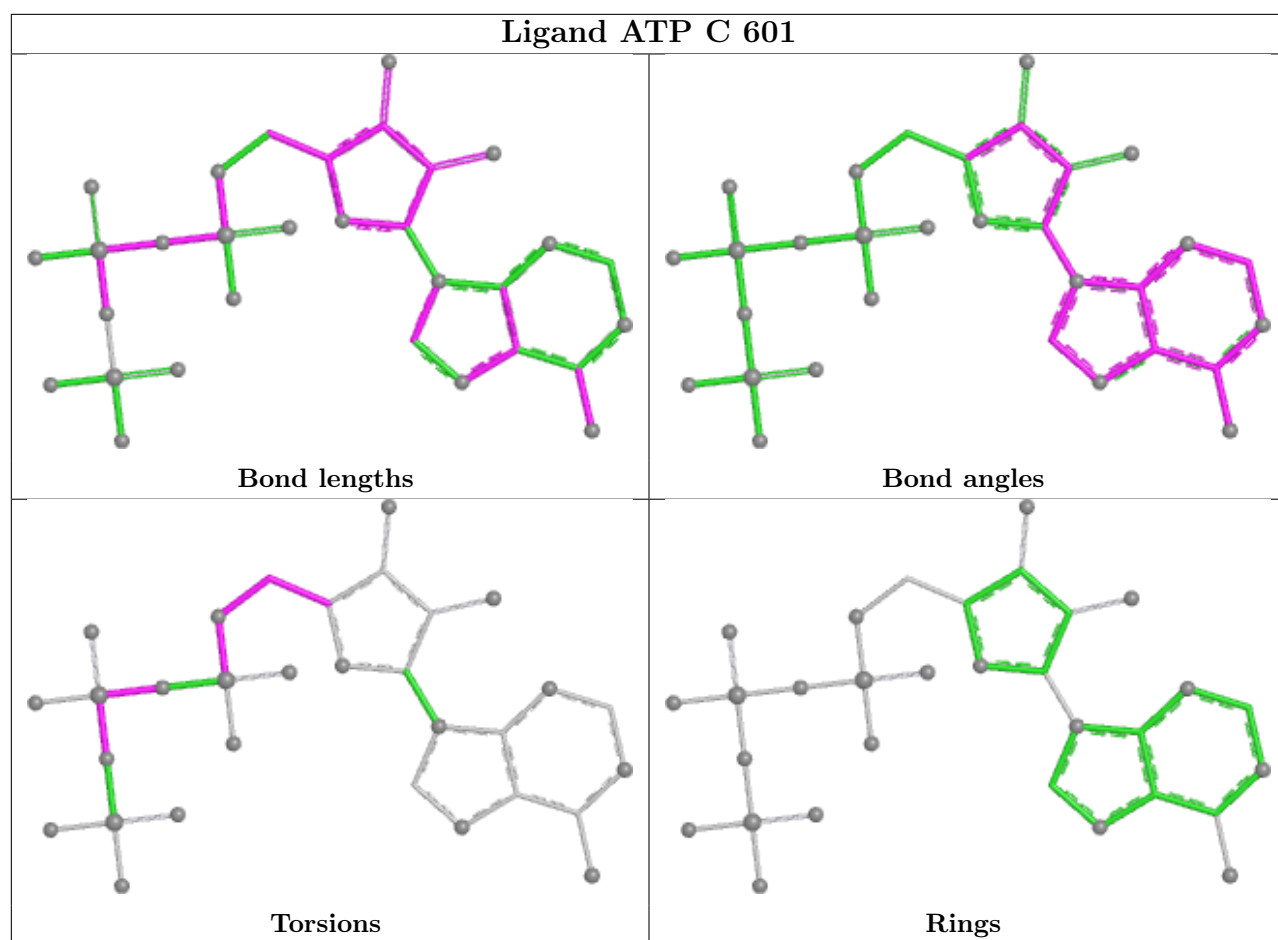


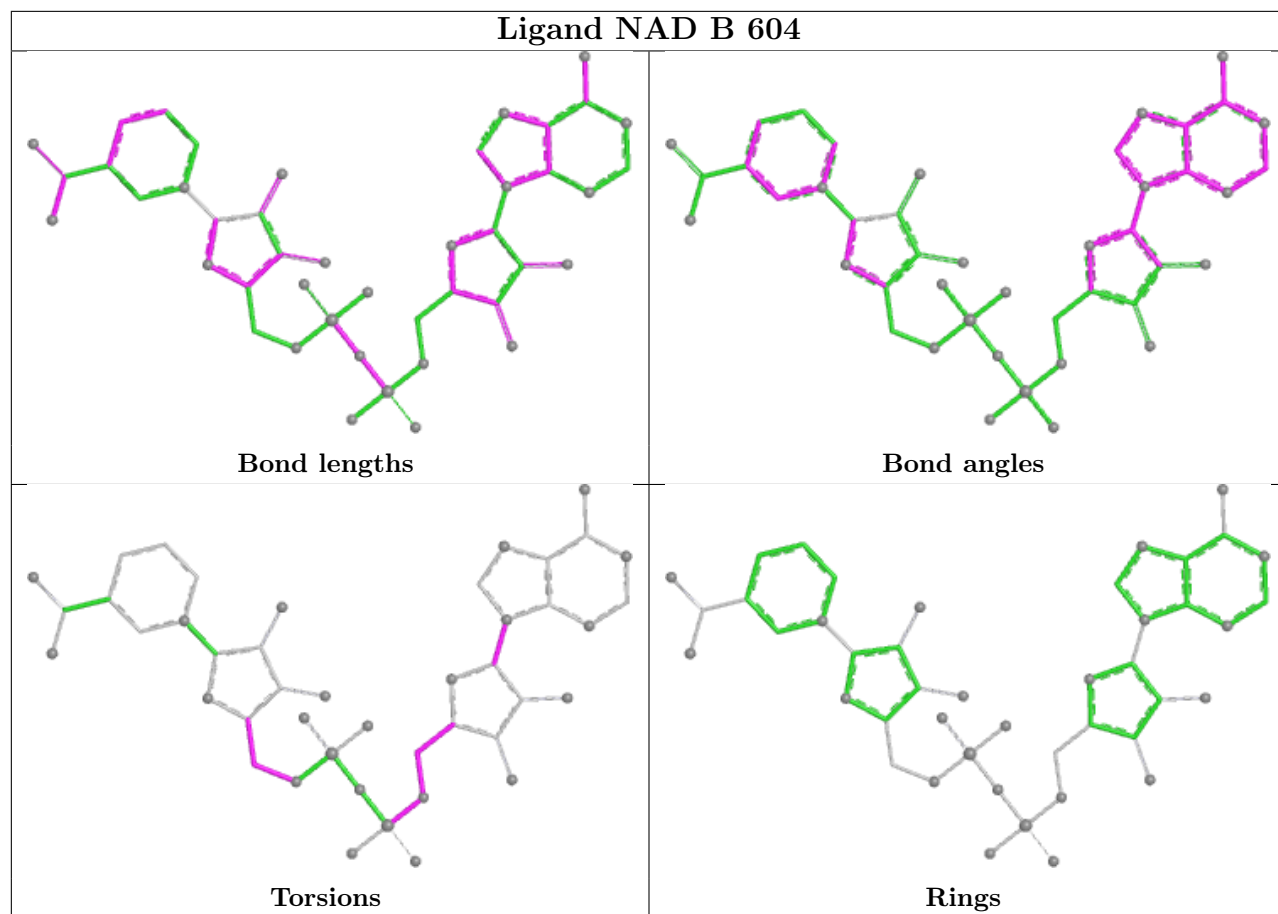
Ligand IMP F 603



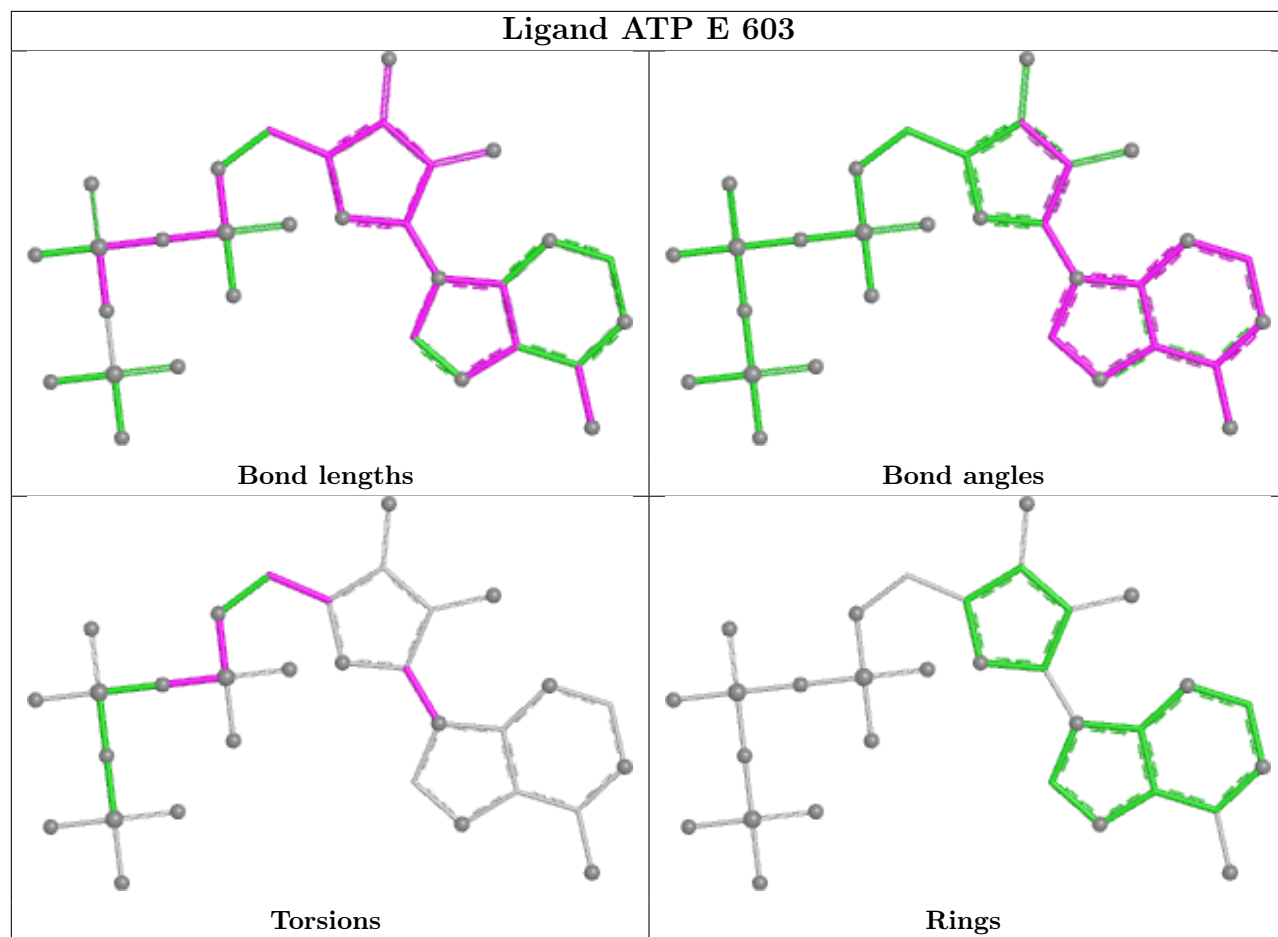
Ligand ATP F 601



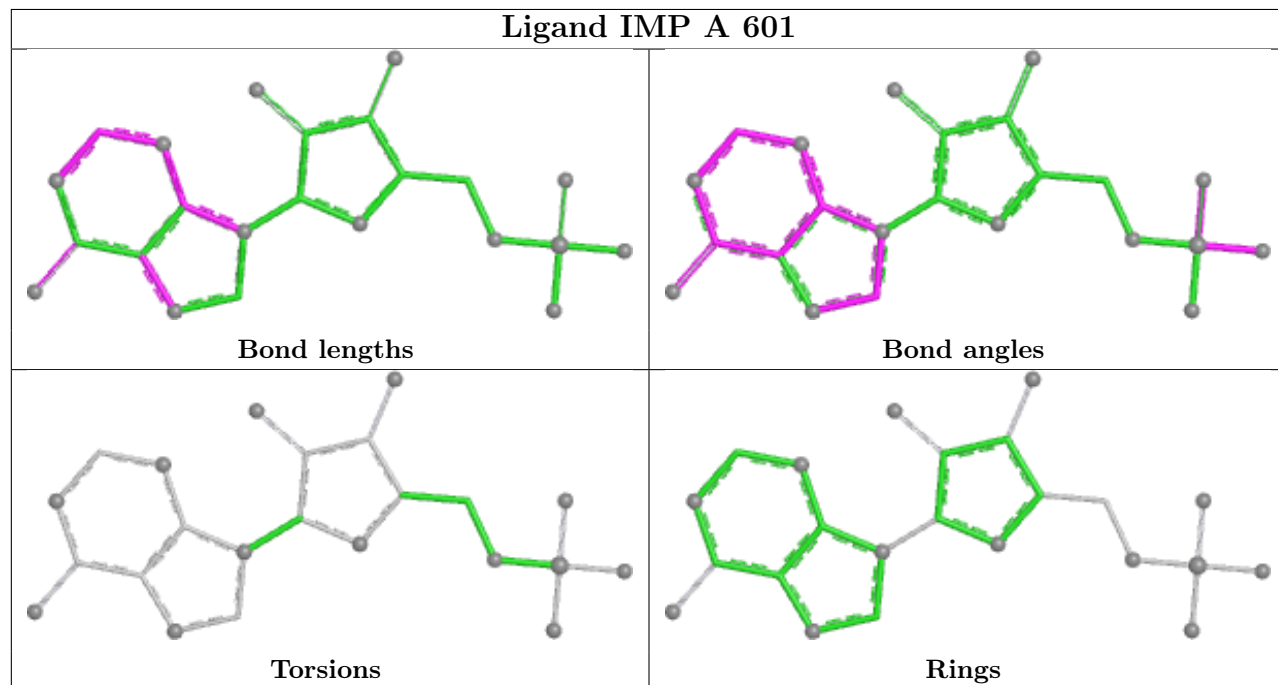


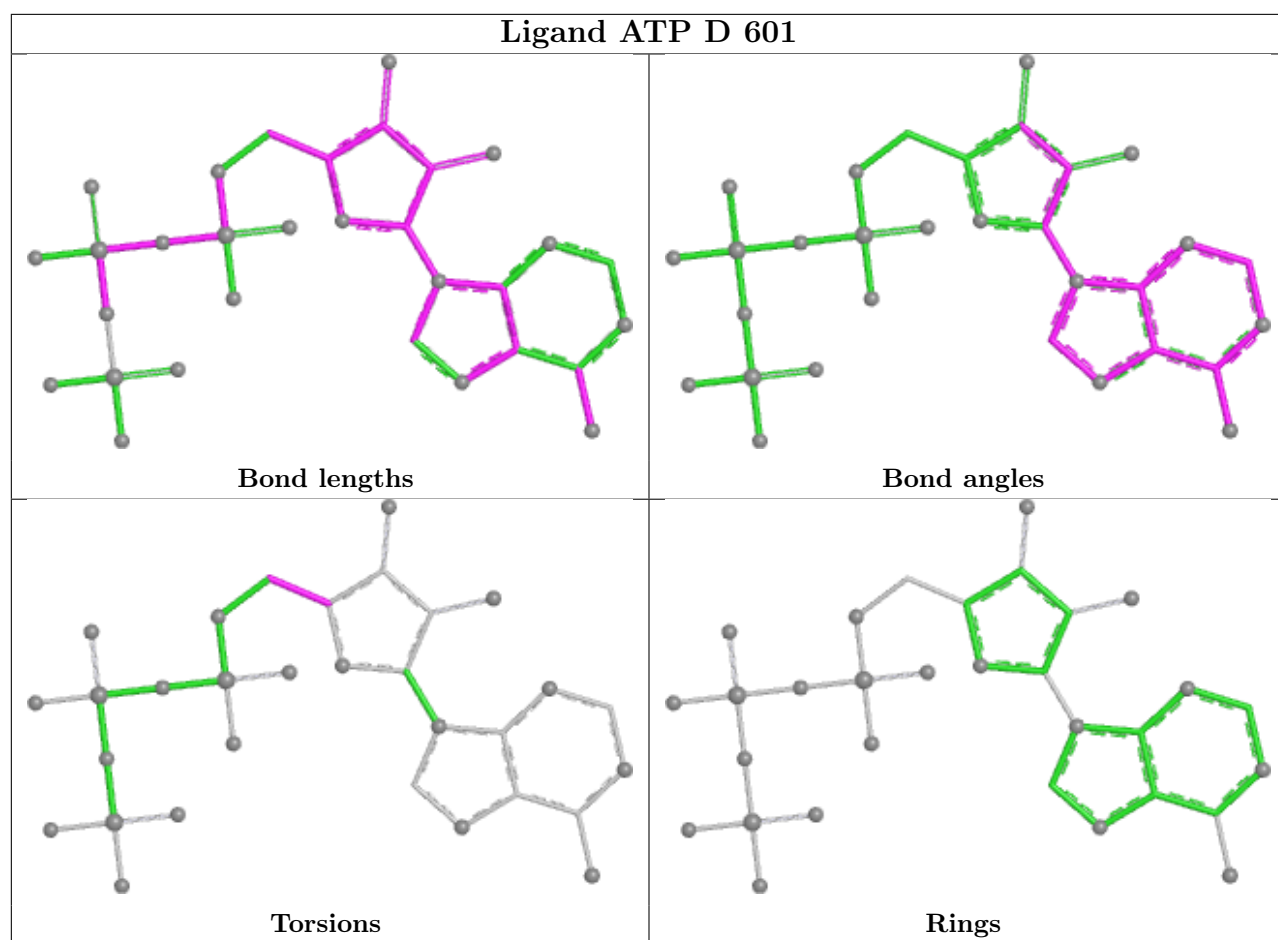


Ligand ATP E 603

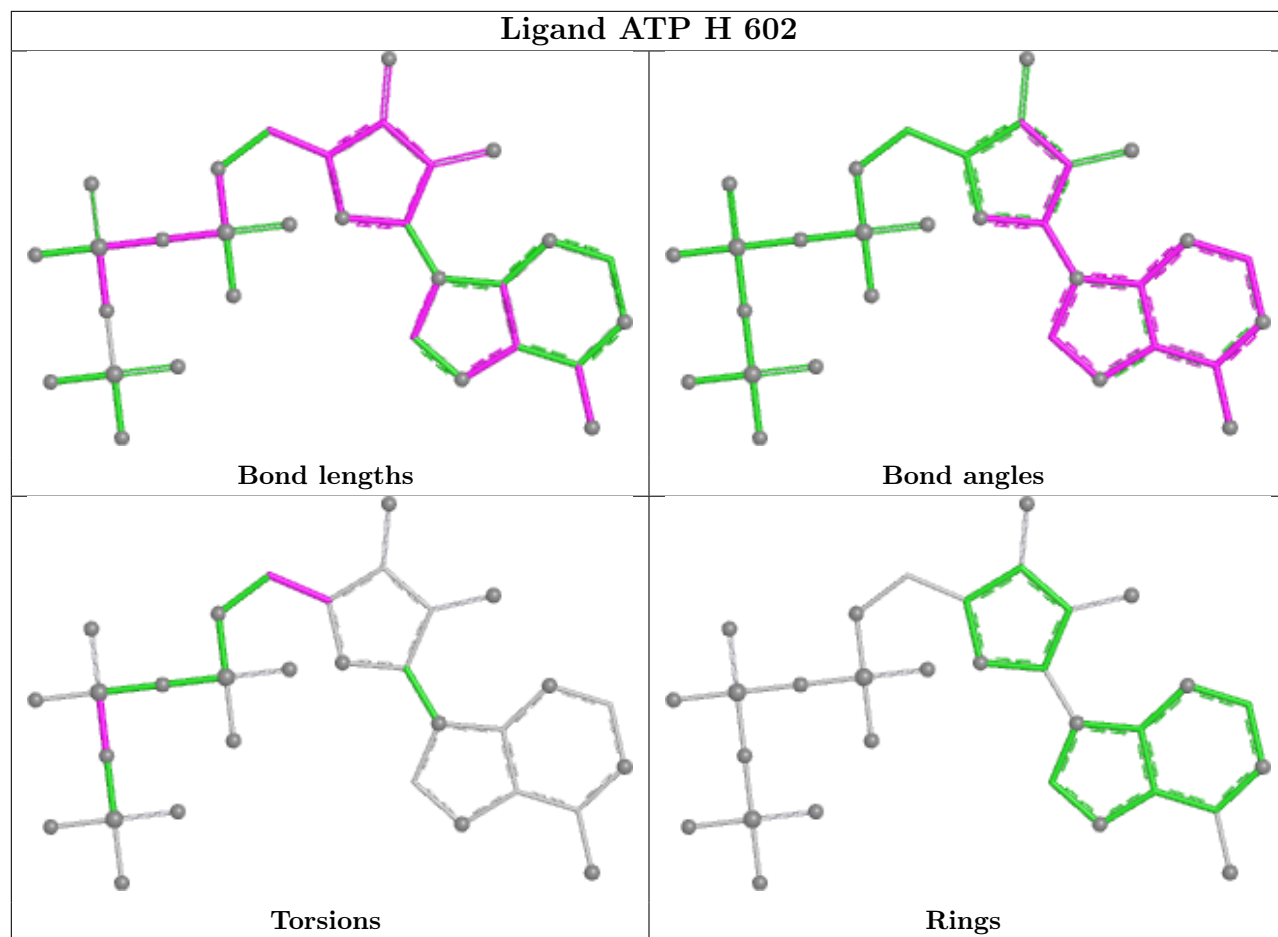


Ligand IMP A 601

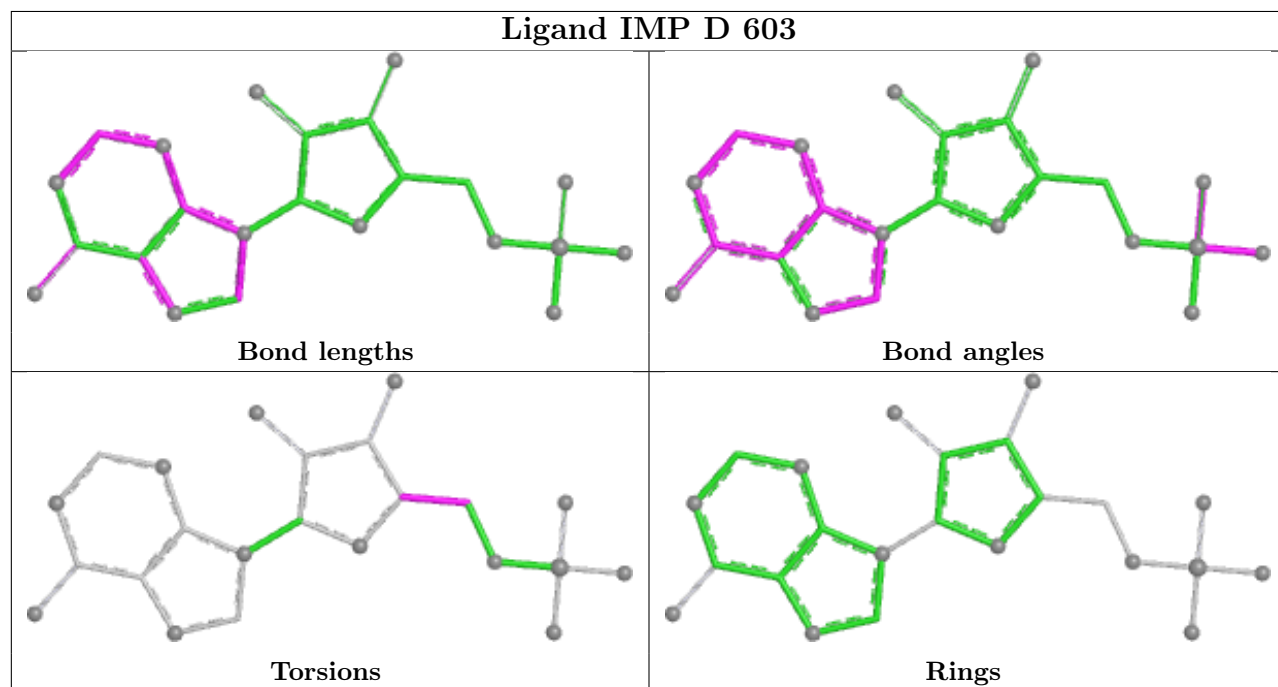


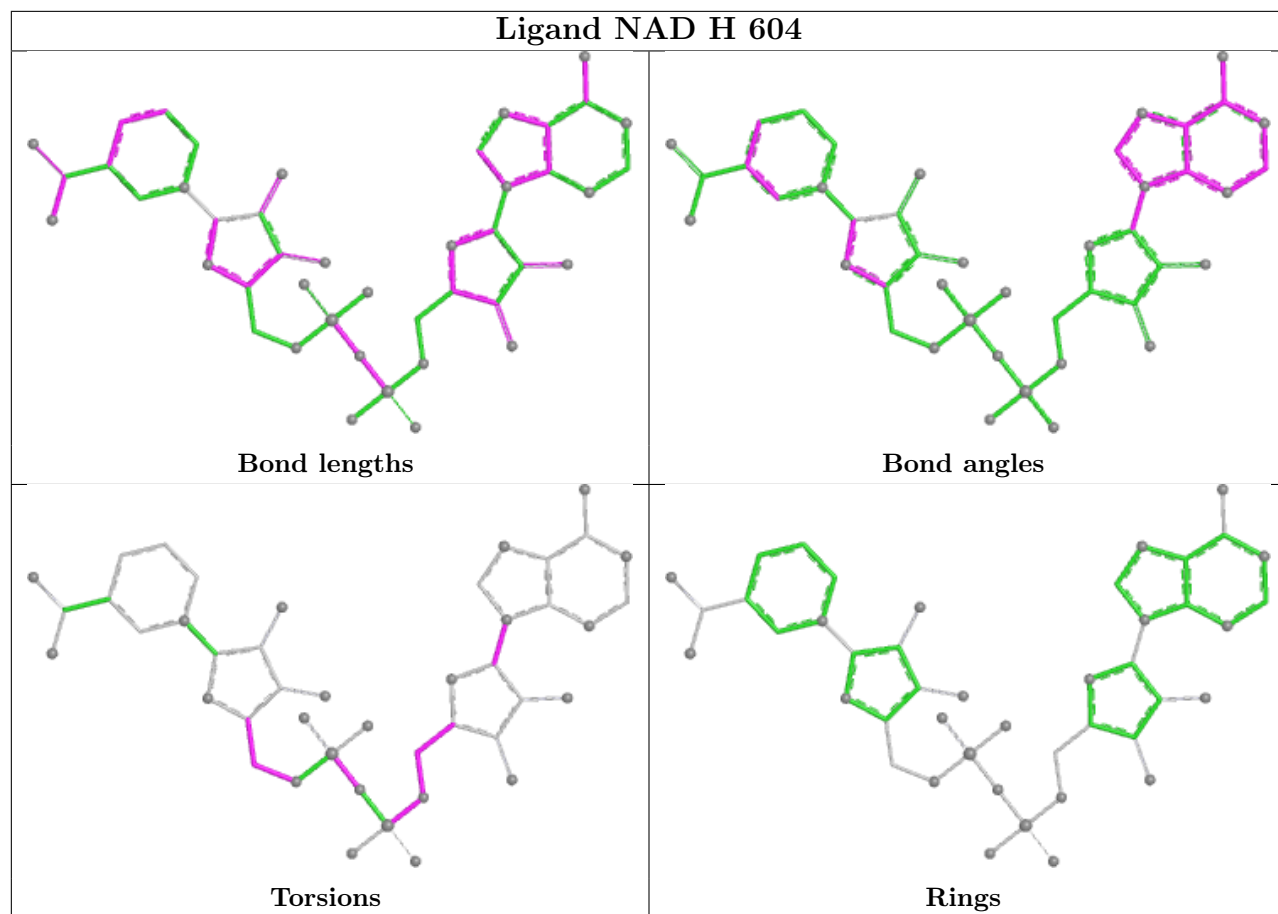


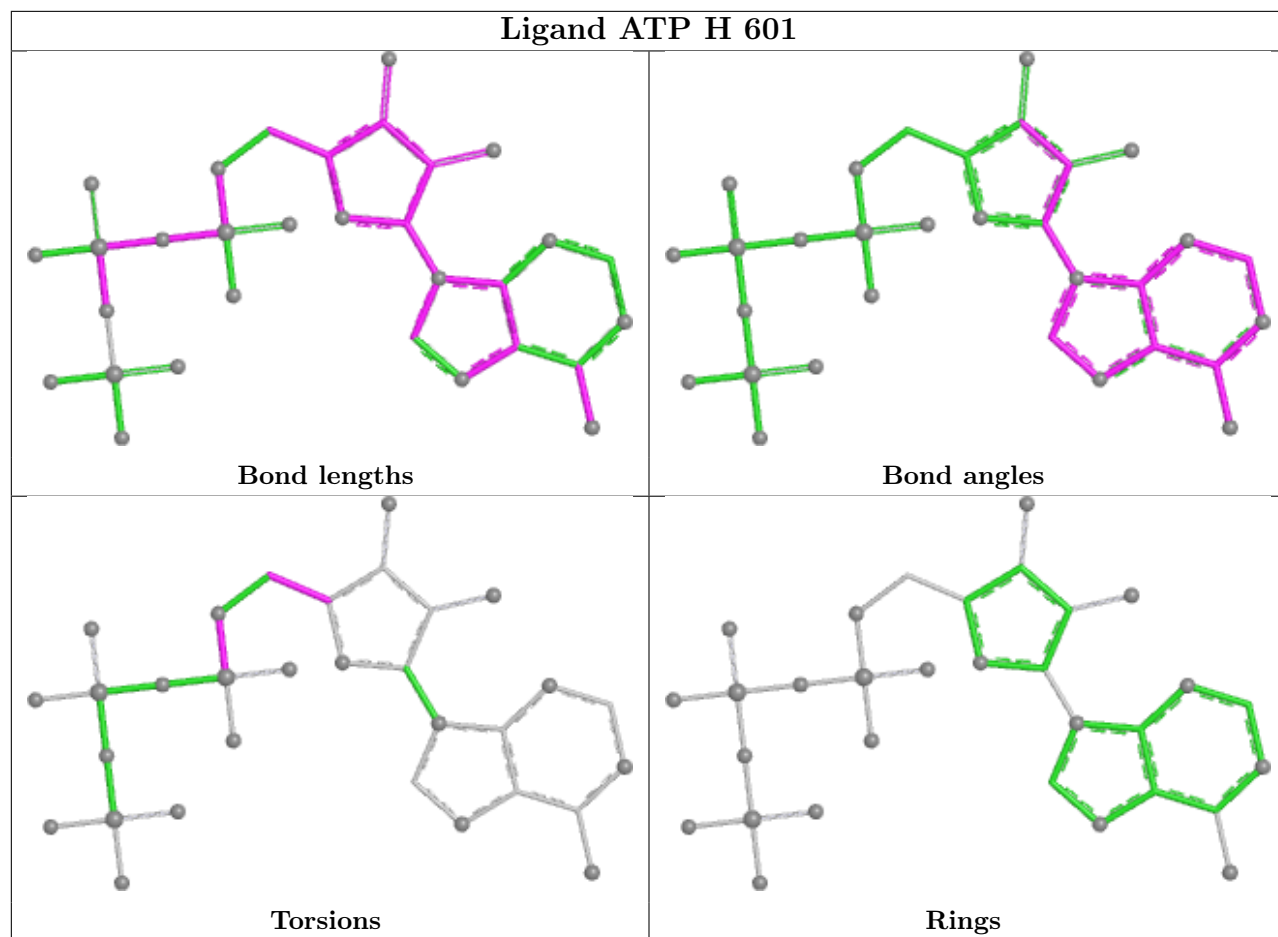
Ligand ATP H 602

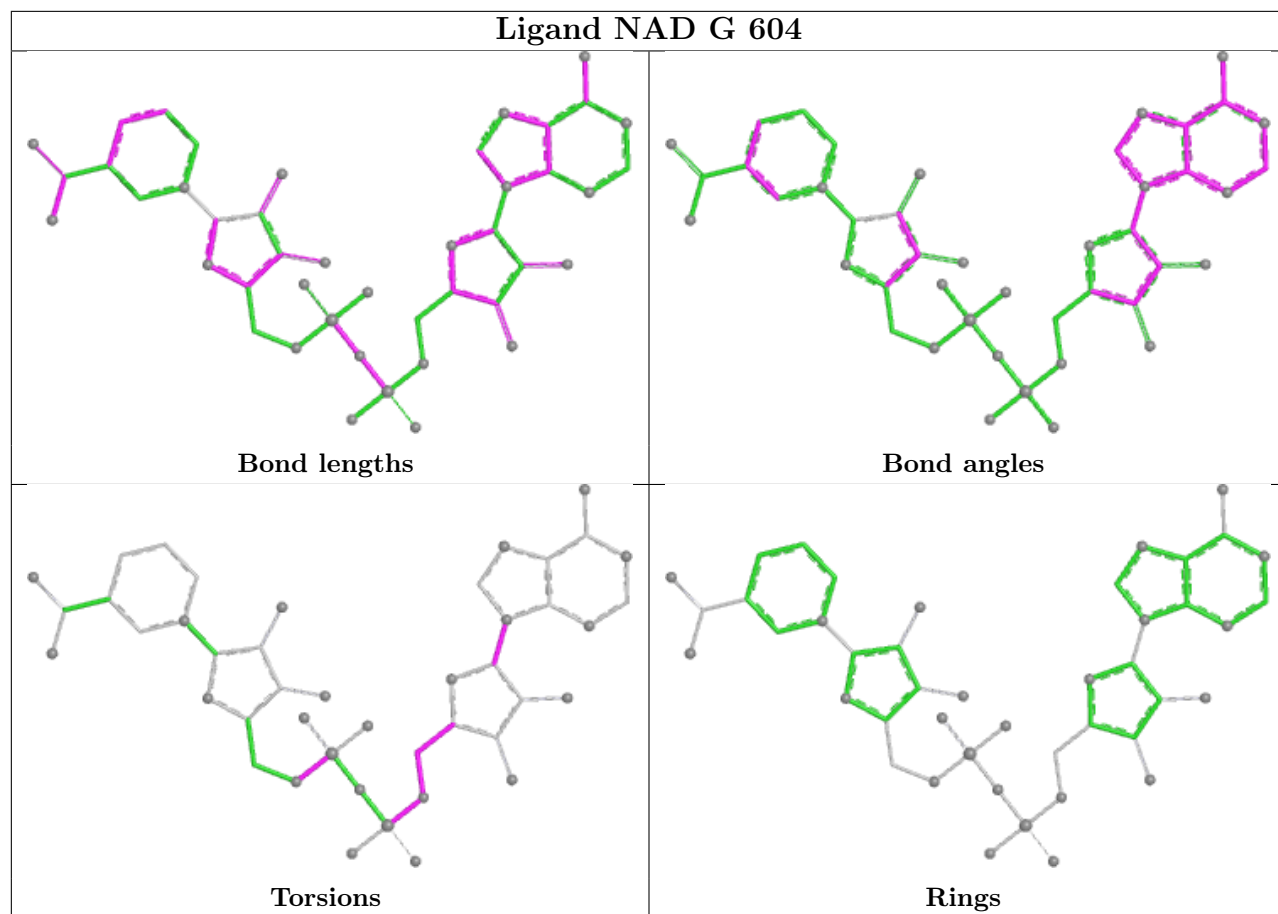


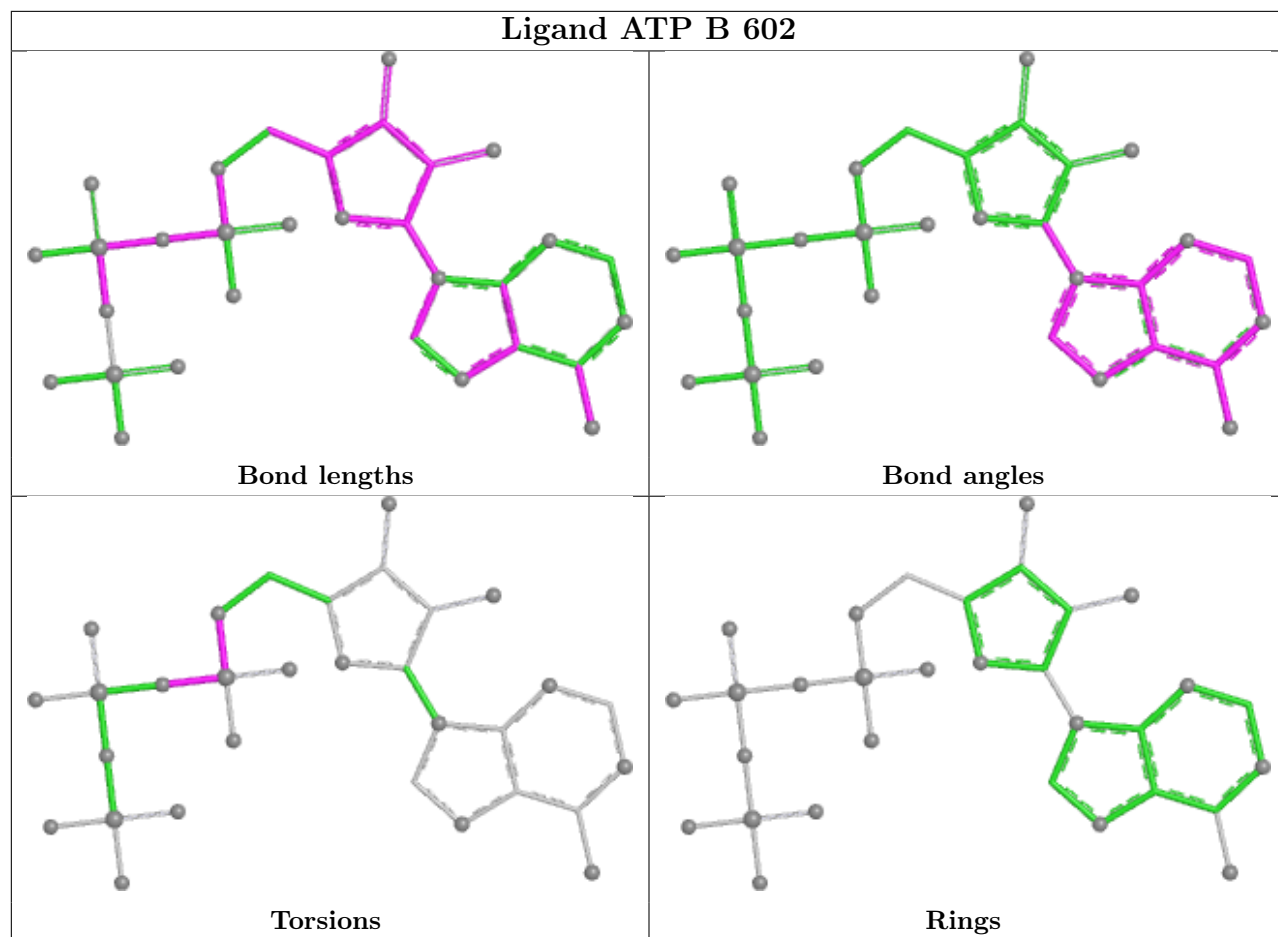
Ligand IMP D 603

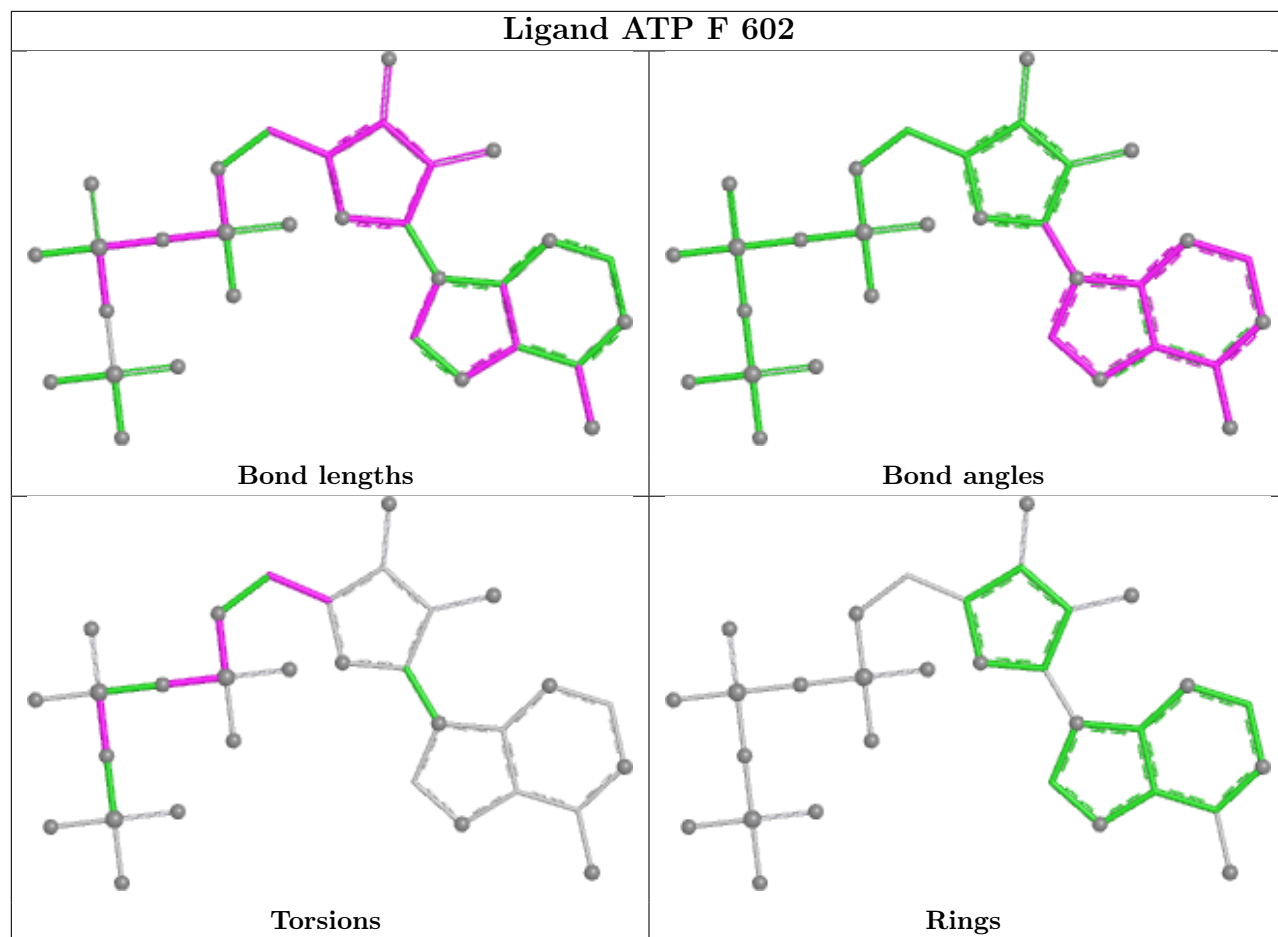


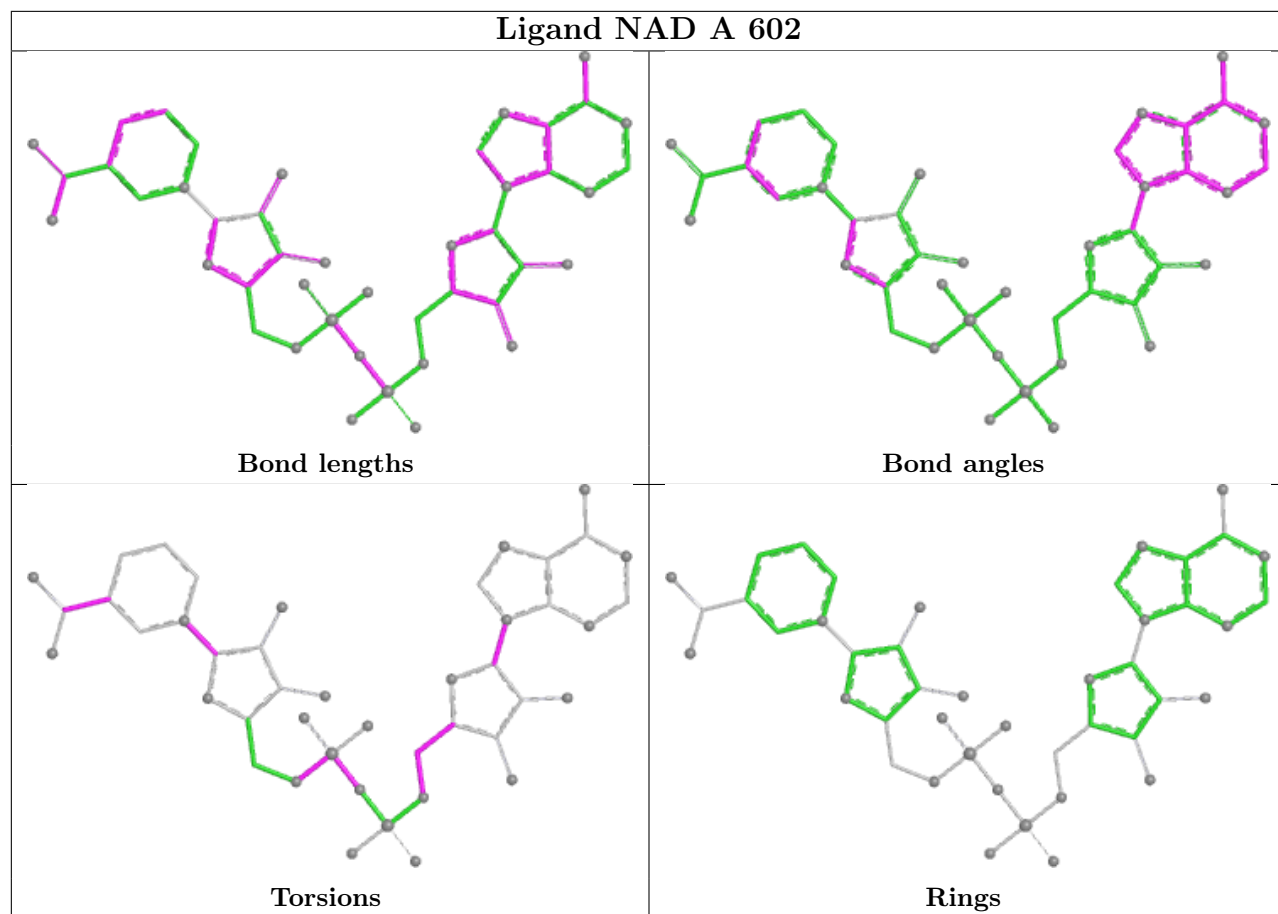


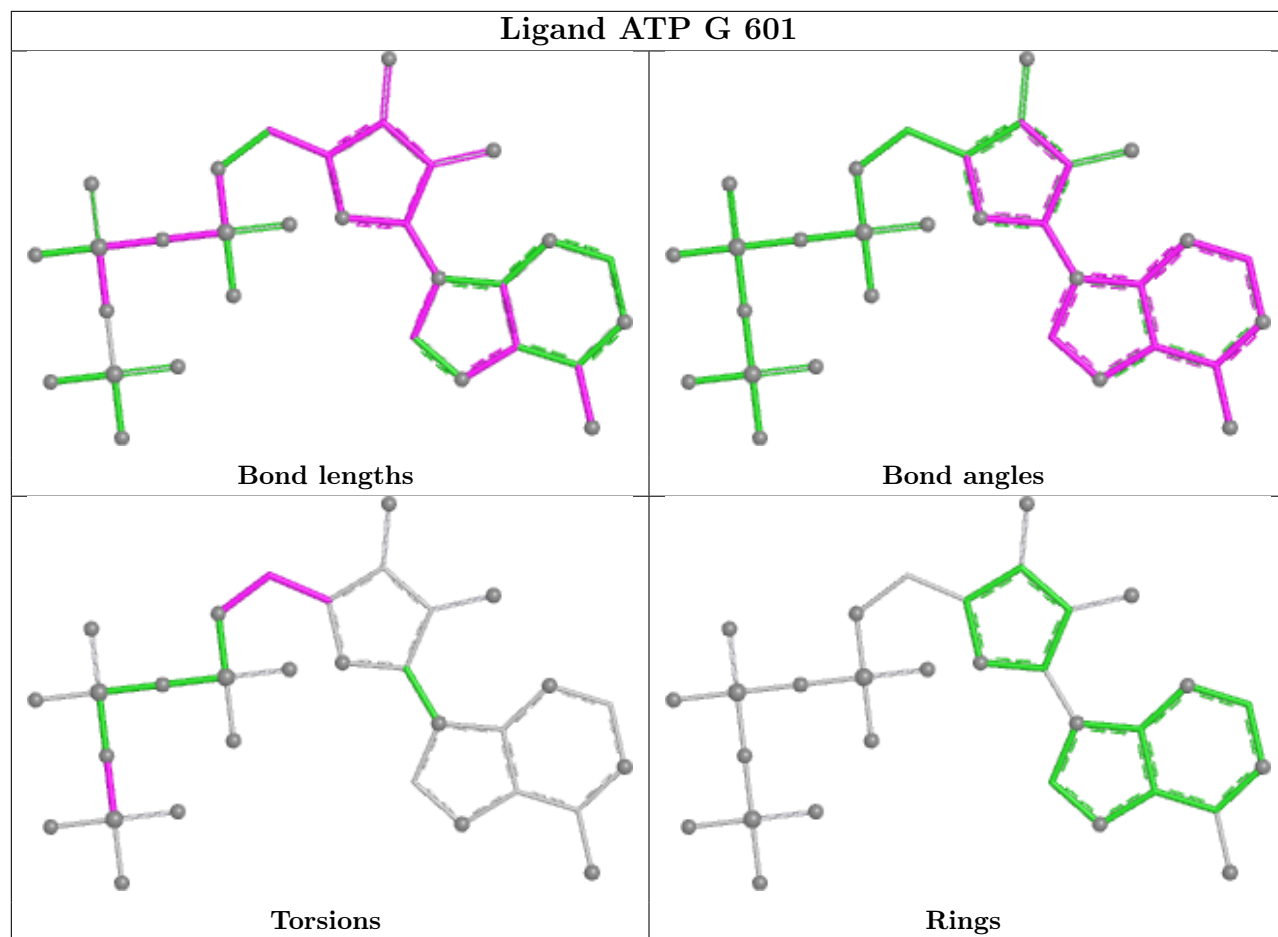


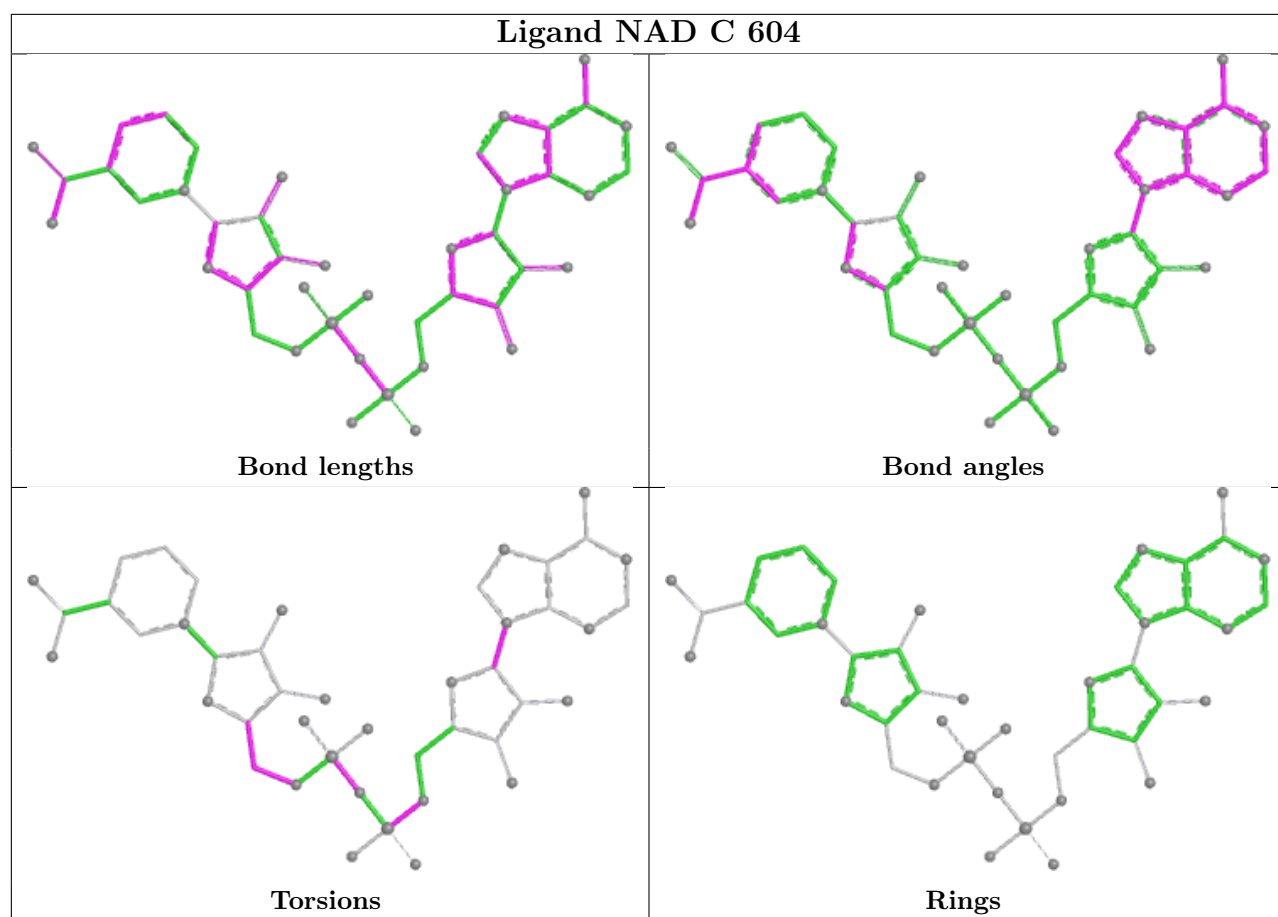


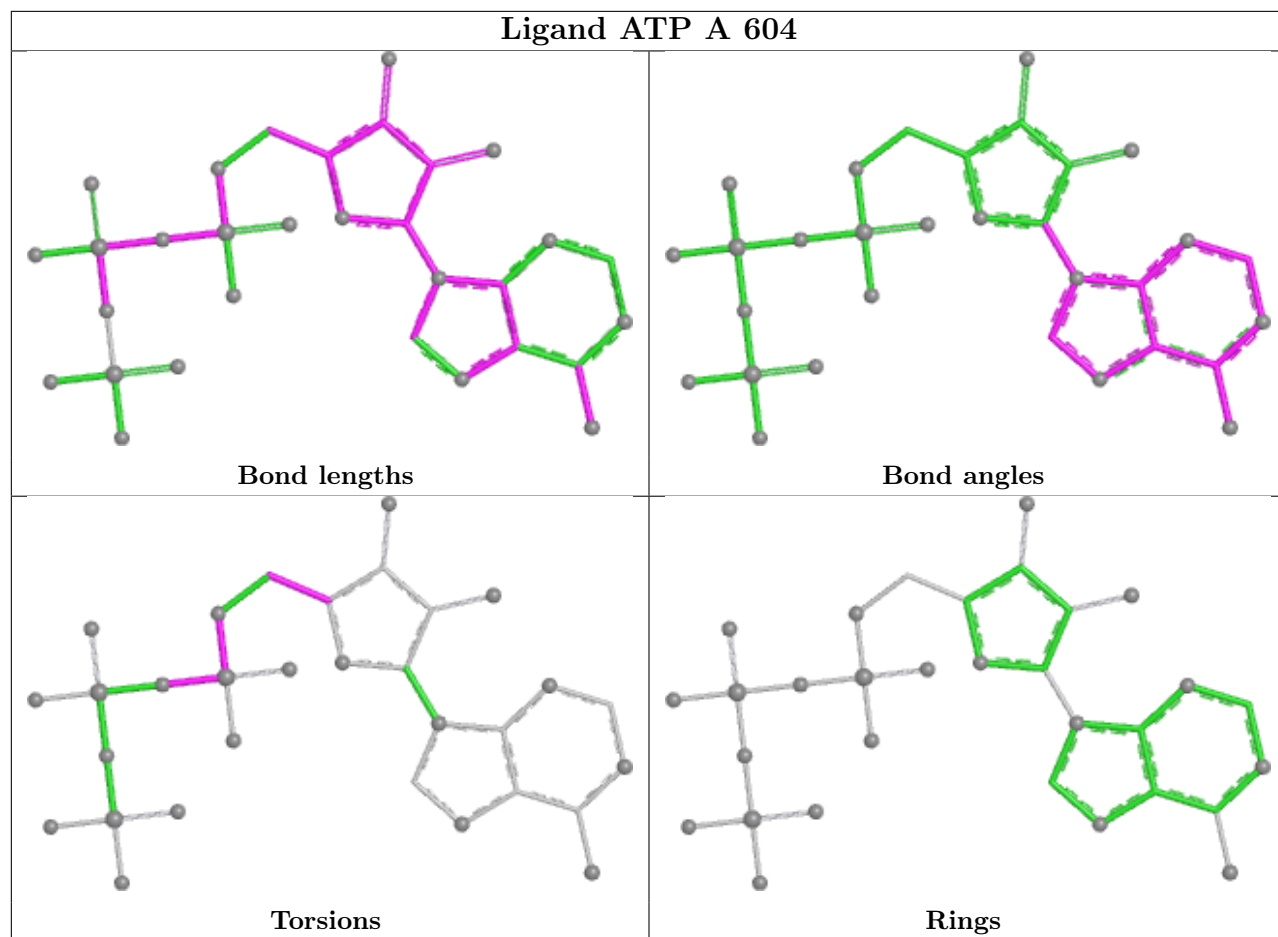




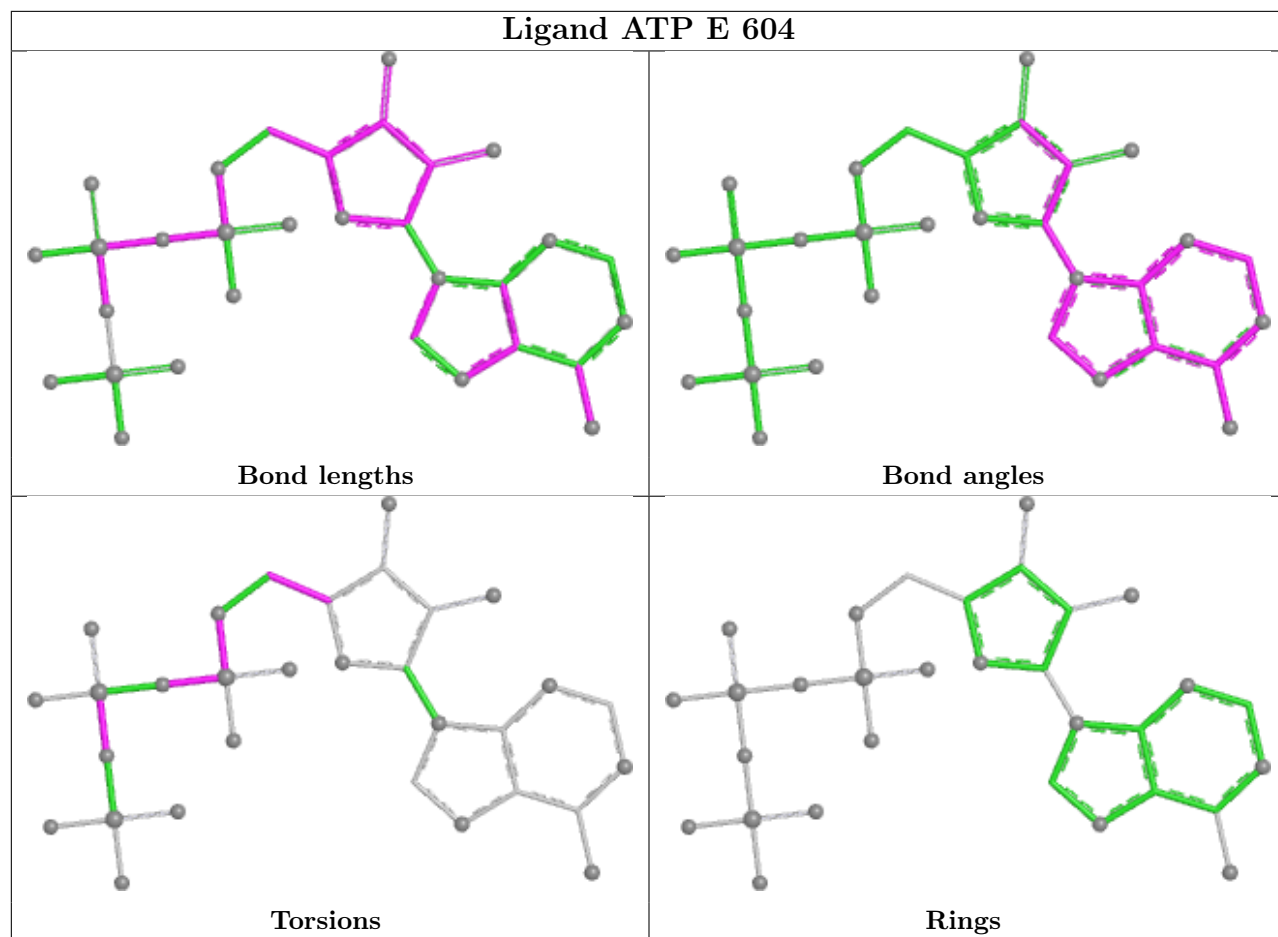




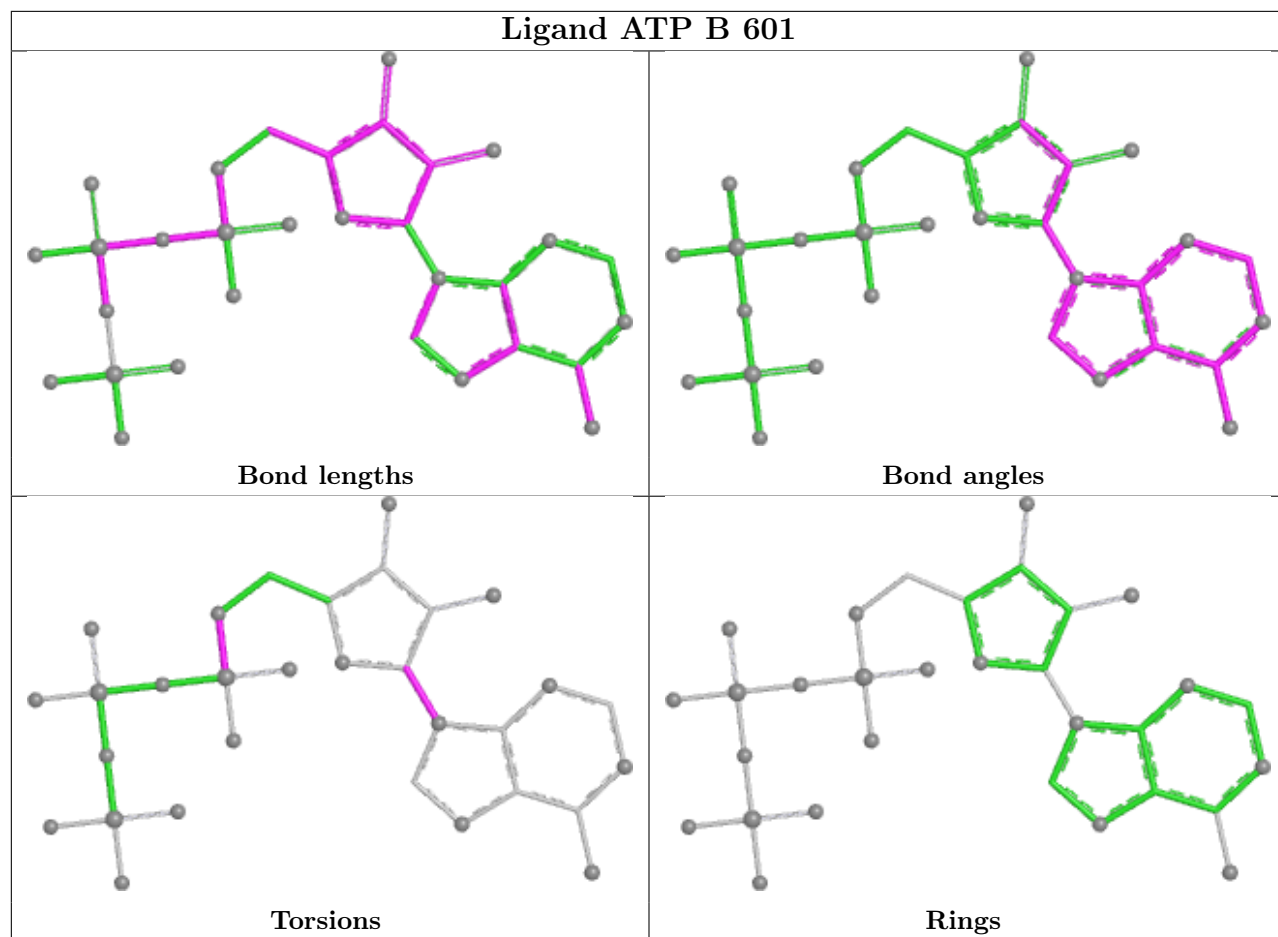




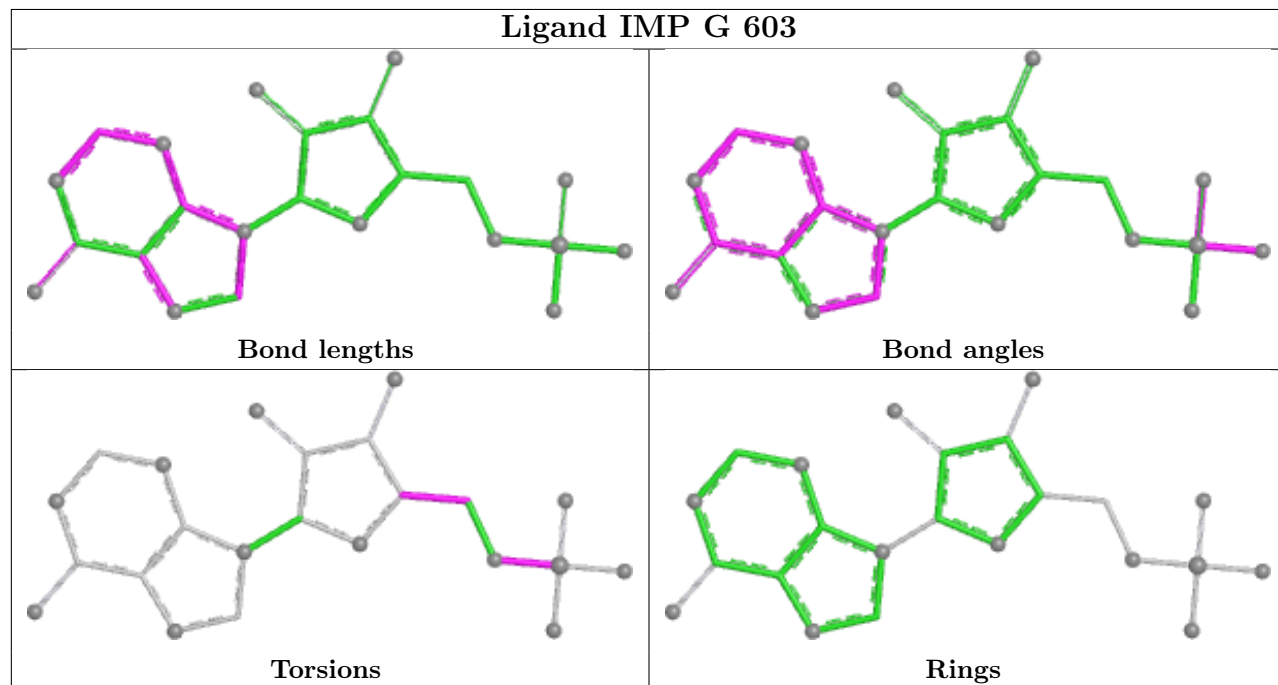
Ligand ATP E 604

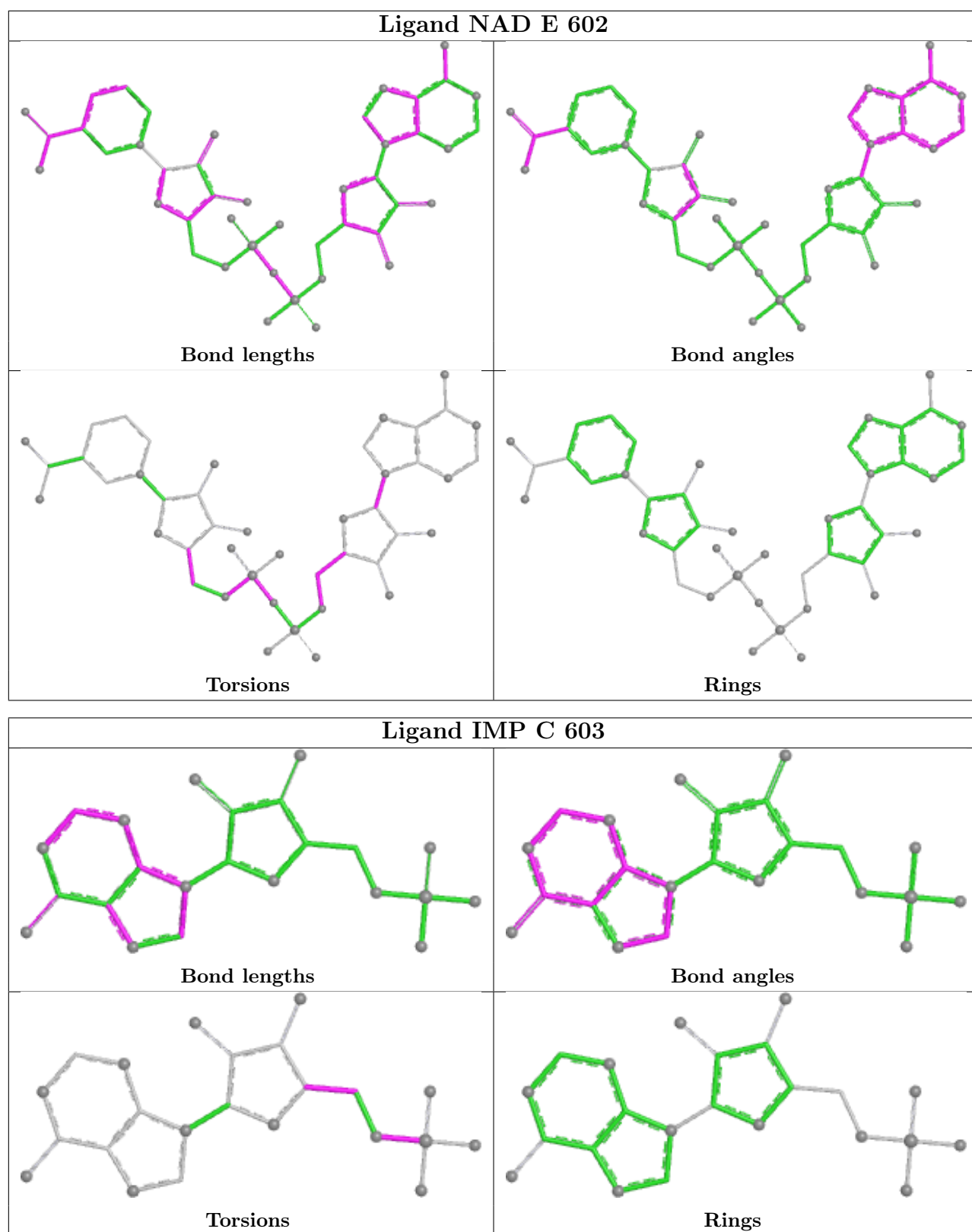


Ligand ATP B 601

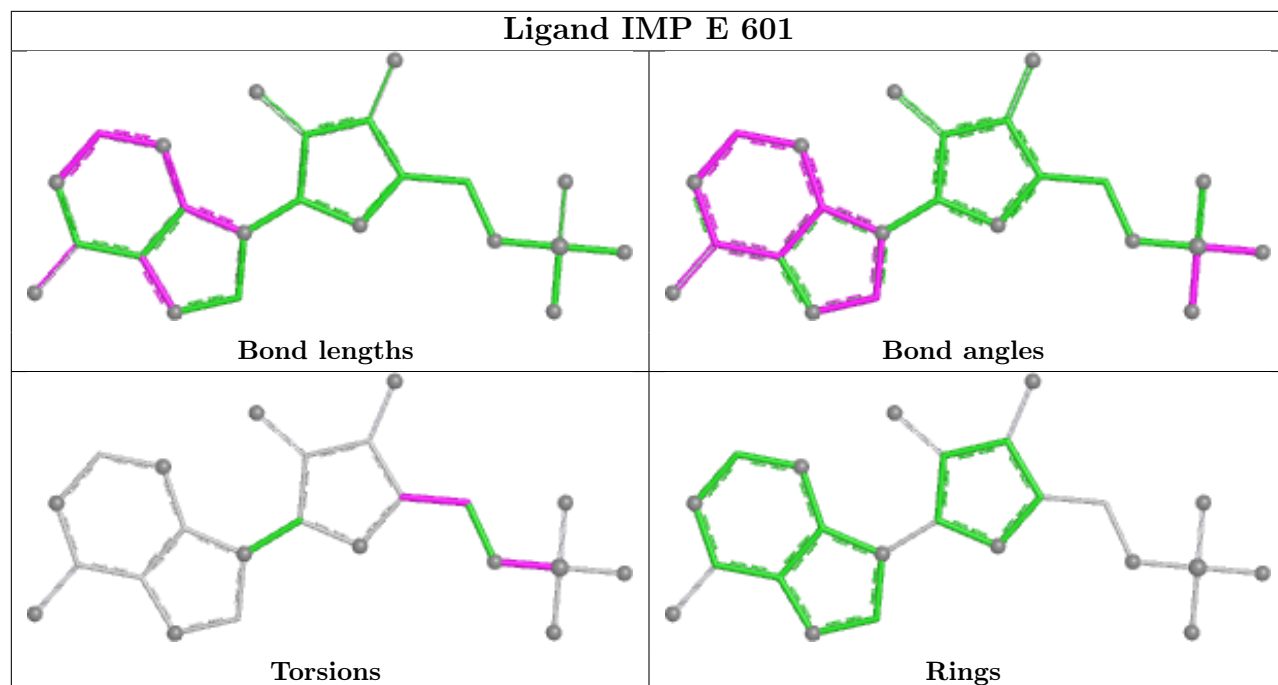


Ligand IMP G 603

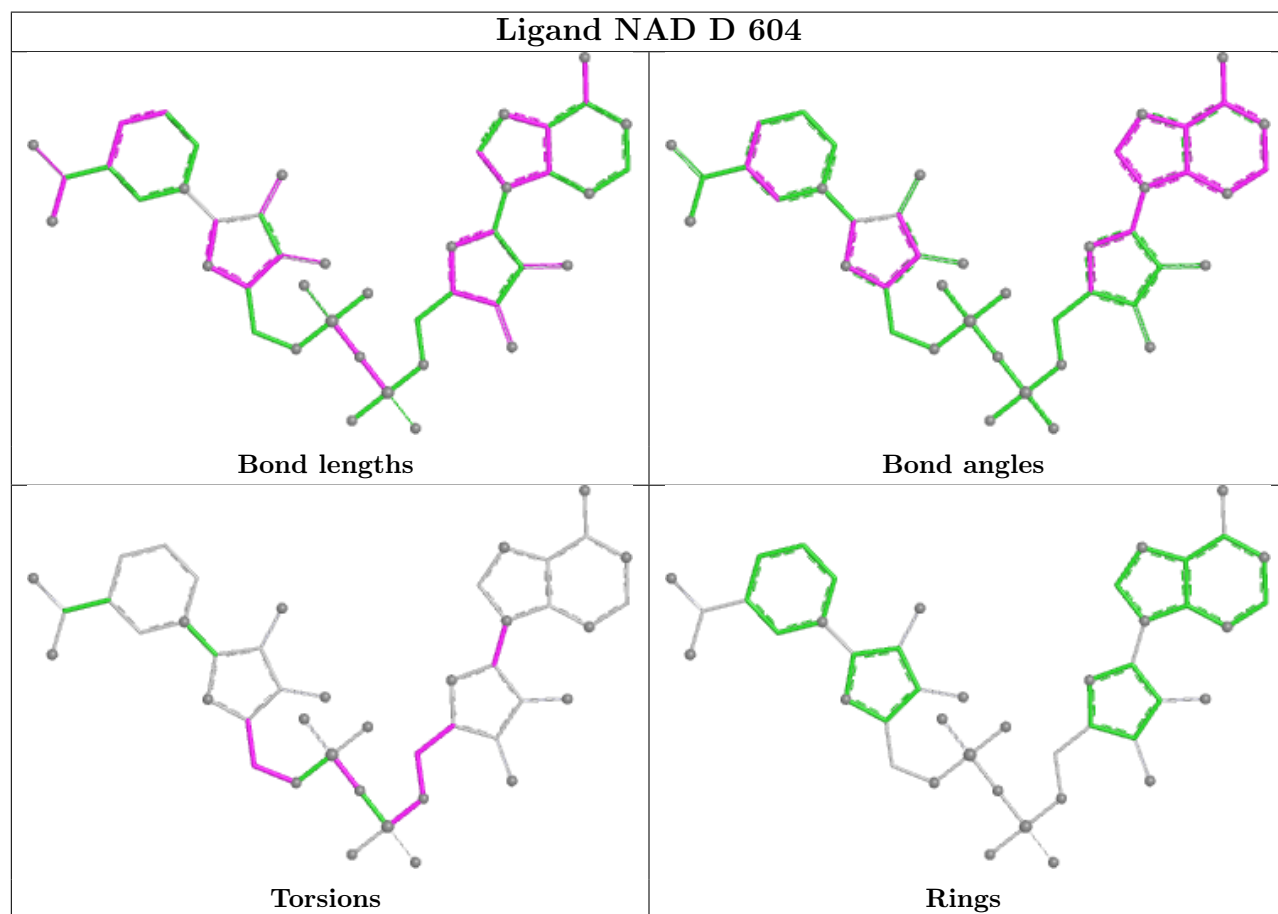


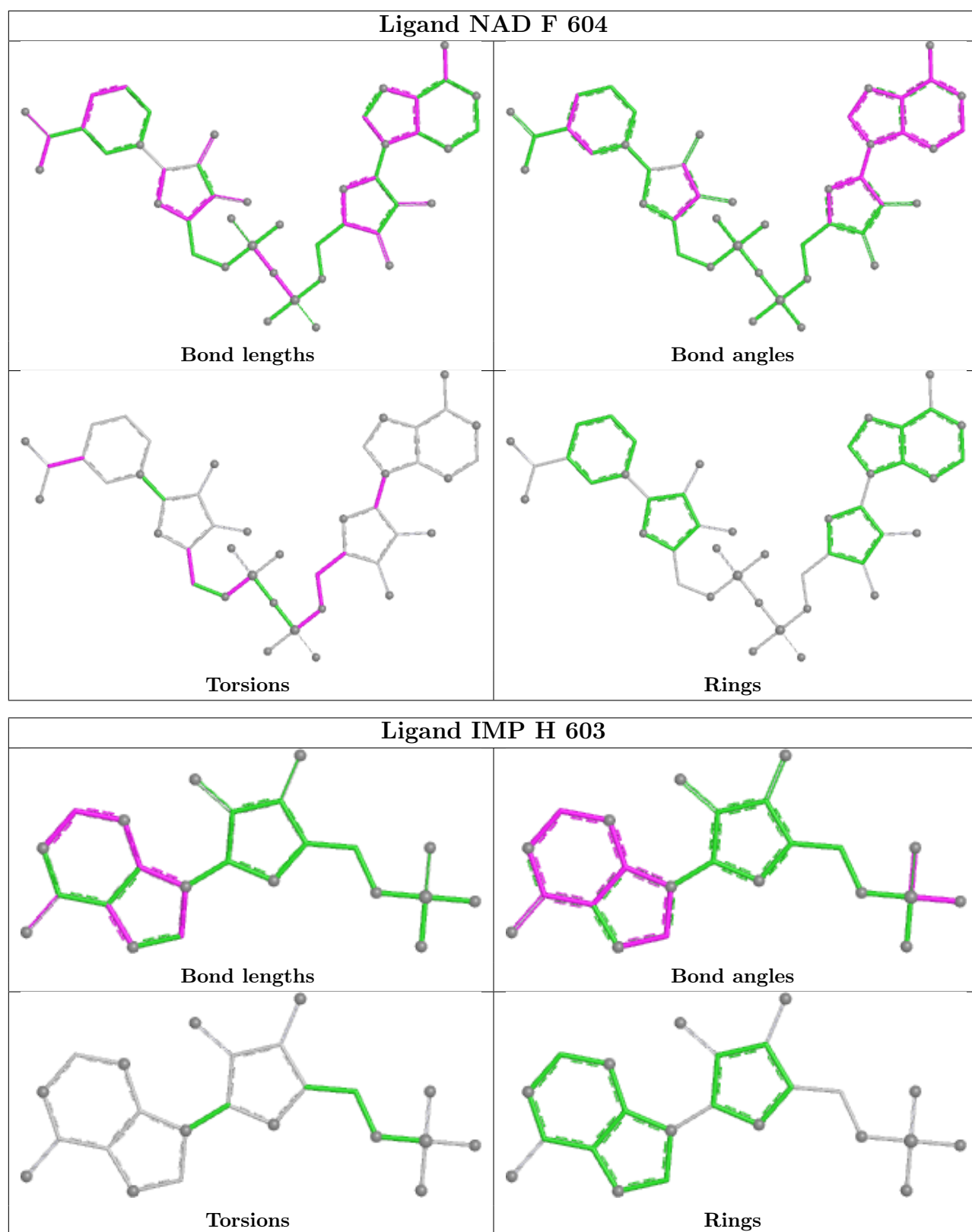


Ligand IMP E 601



Ligand NAD D 604





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

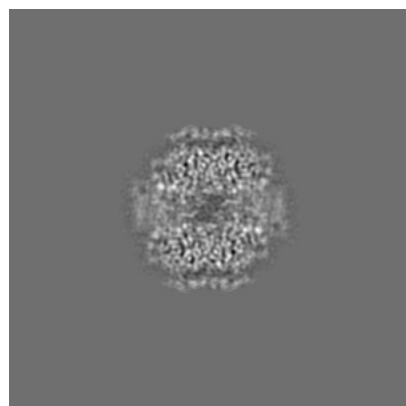
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20690. These allow visual inspection of the internal detail of the map and identification of artifacts.

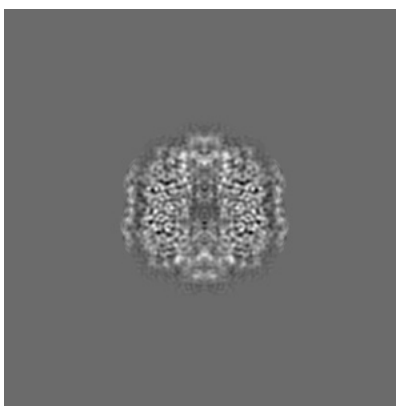
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

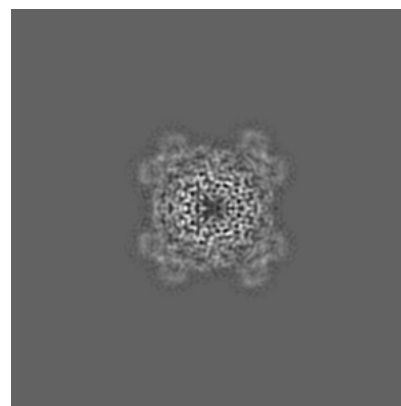
6.1.1 Primary map



X

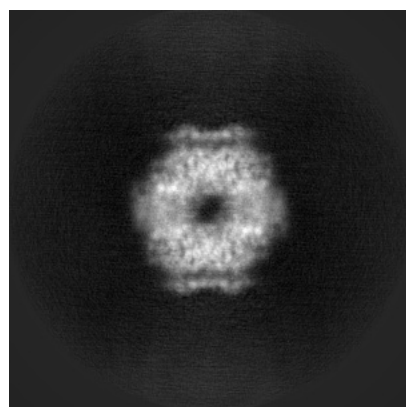


Y

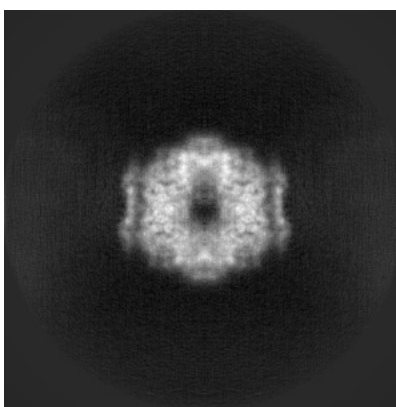


Z

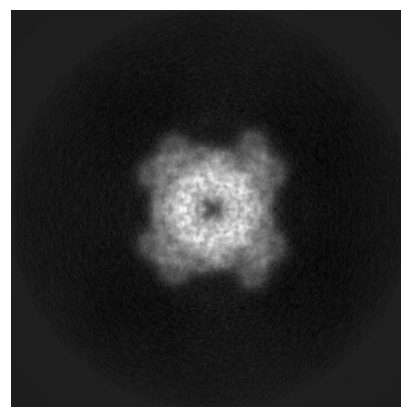
6.1.2 Raw map



X



Y

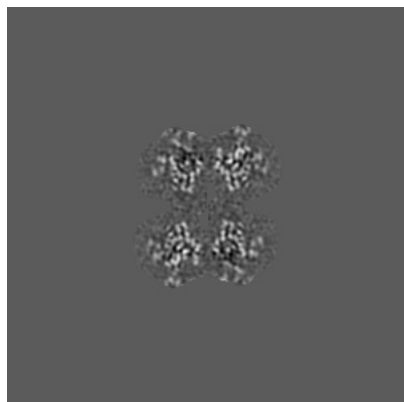


Z

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

6.2 Central slices [i](#)

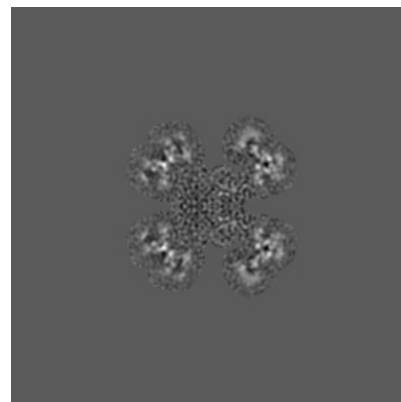
6.2.1 Primary map



X Index: 160

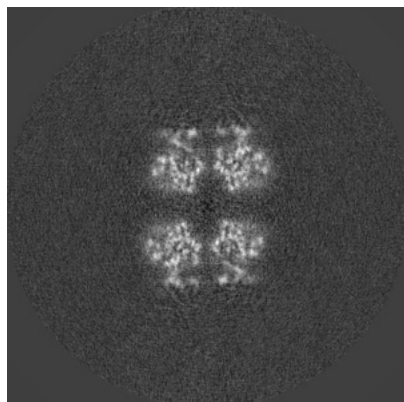


Y Index: 160

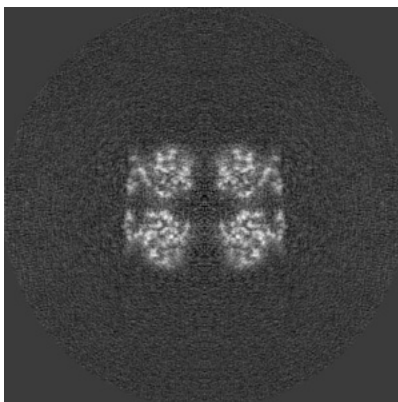


Z Index: 160

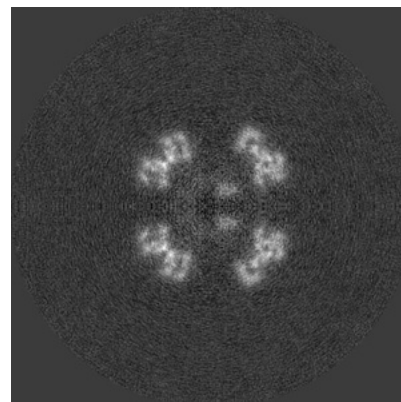
6.2.2 Raw map



X Index: 160



Y Index: 160

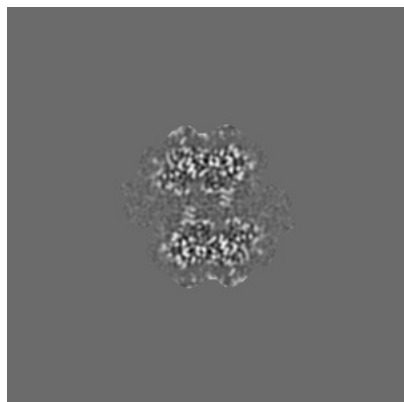


Z Index: 160

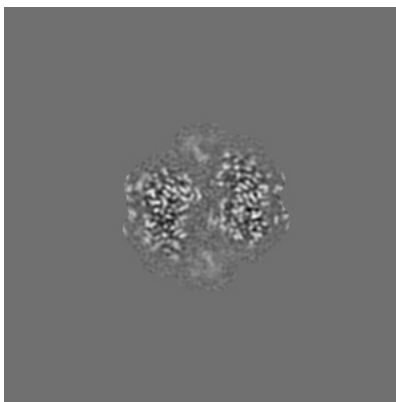
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

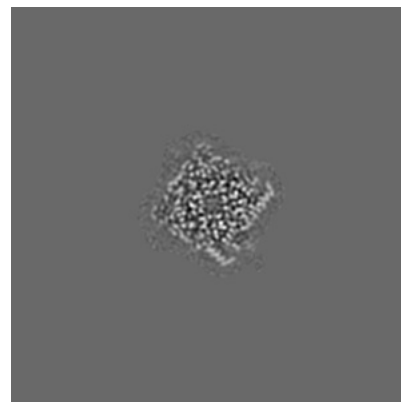
6.3.1 Primary map



X Index: 177

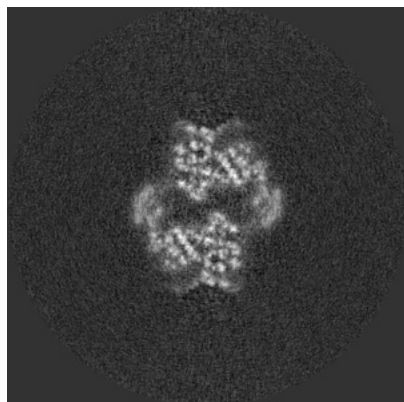


Y Index: 180

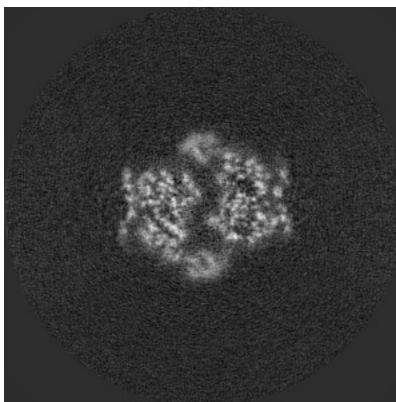


Z Index: 197

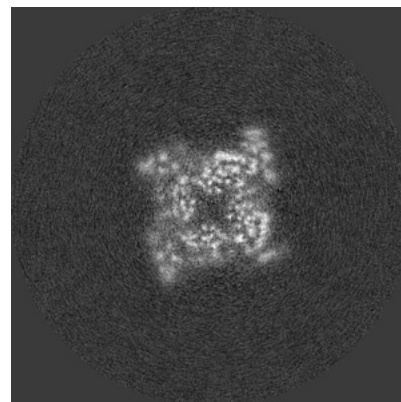
6.3.2 Raw map



X Index: 136



Y Index: 182

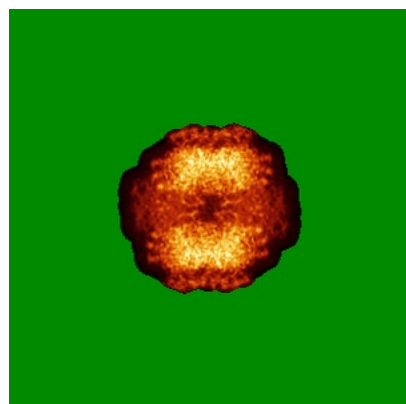


Z Index: 143

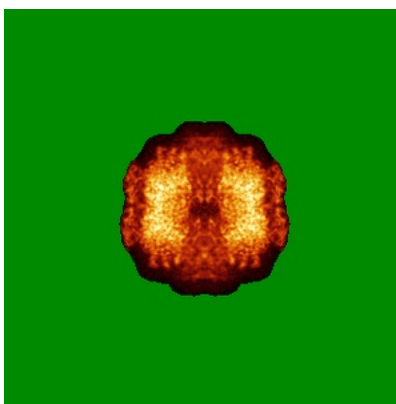
The images above show the largest variance slices of the map in three orthogonal directions.

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

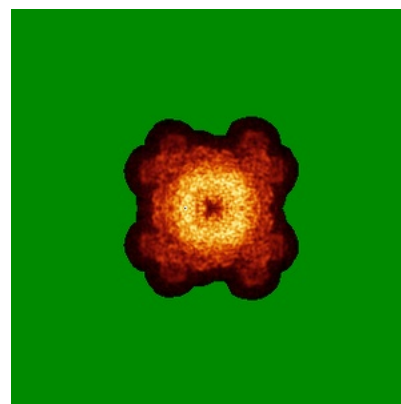
6.4.1 Primary map



X

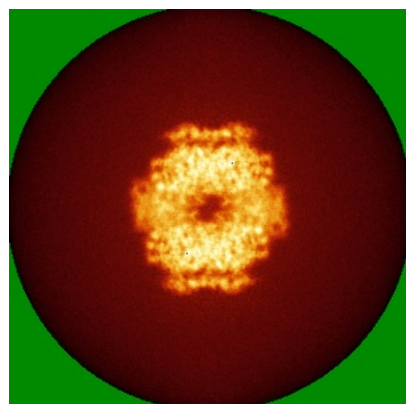


Y

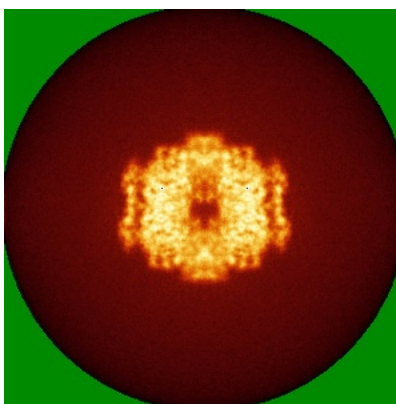


Z

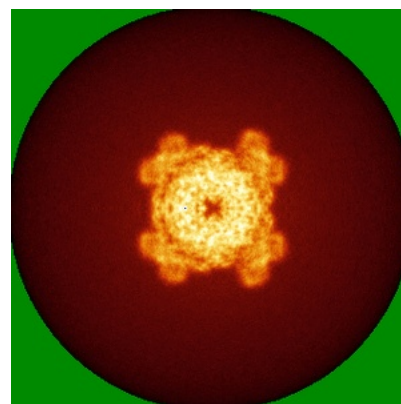
6.4.2 Raw map



X



Y

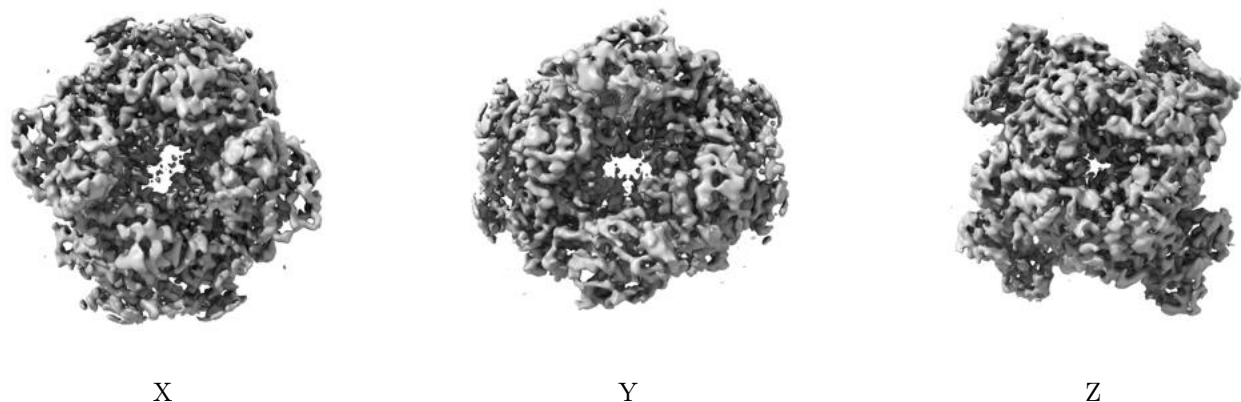


Z

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.

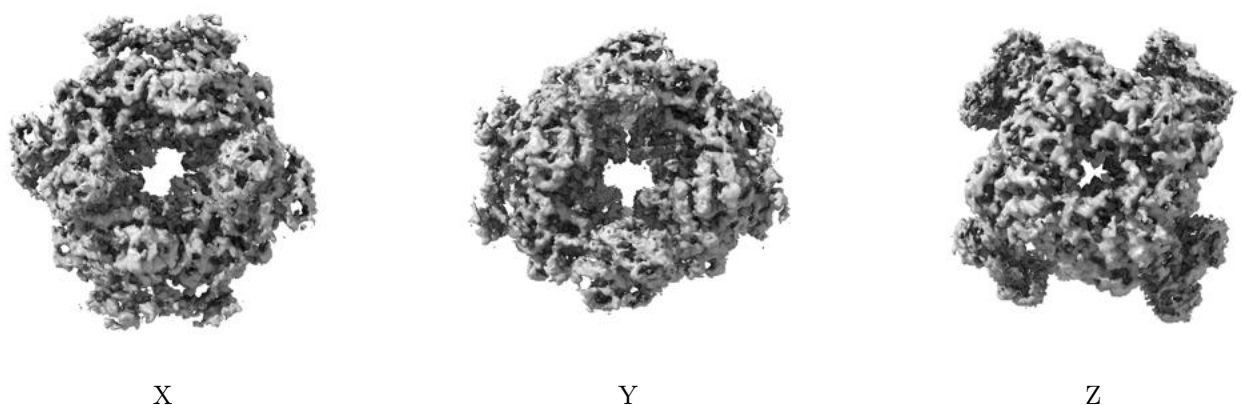
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 17.0. 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.

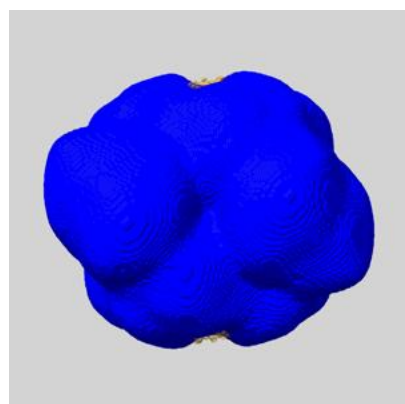
6.6 Mask visualisation [i](#)

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

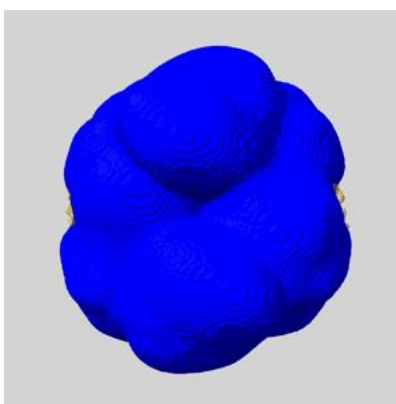
A mask typically either:

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

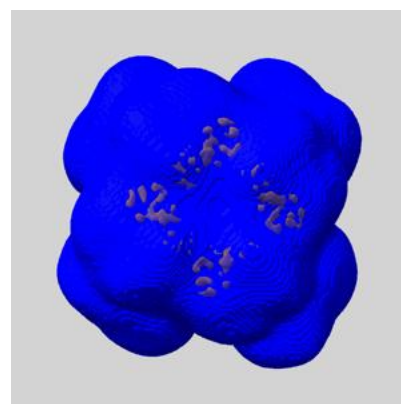
6.6.1 emd_20690_msk_1.map [i](#)



X



Y

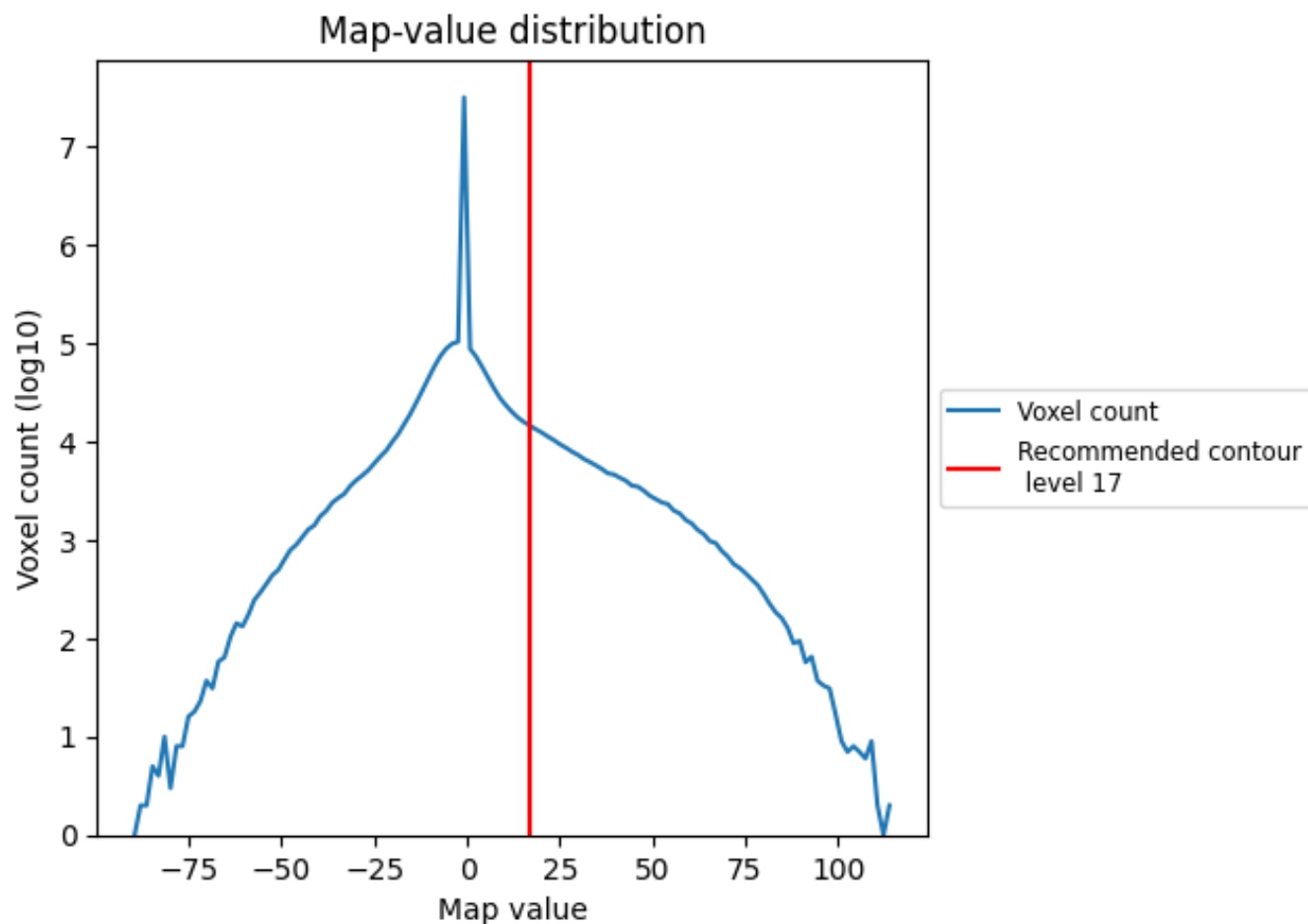


Z

7 Map analysis [i](#)

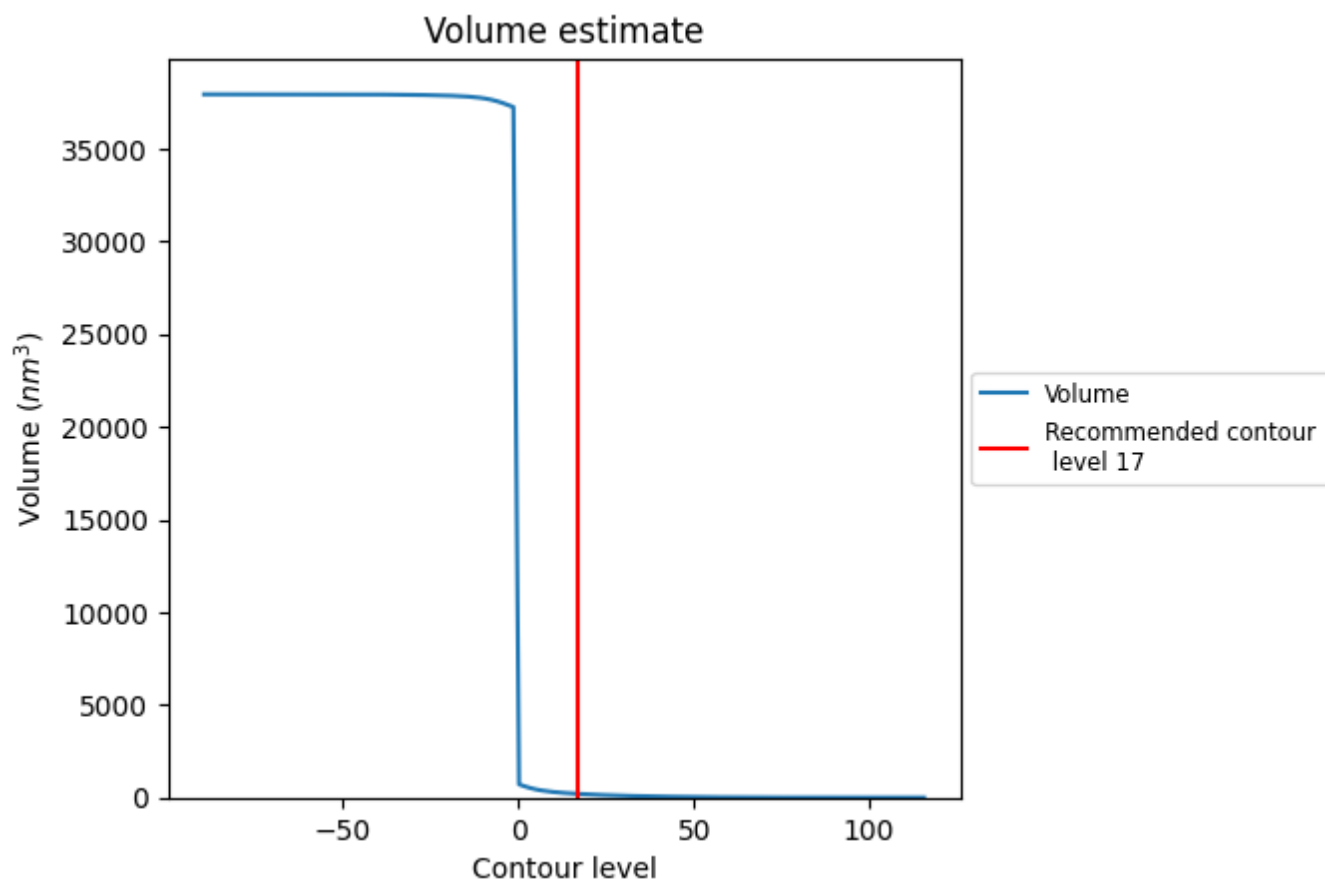
This section contains the results of statistical analysis of the map.

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.

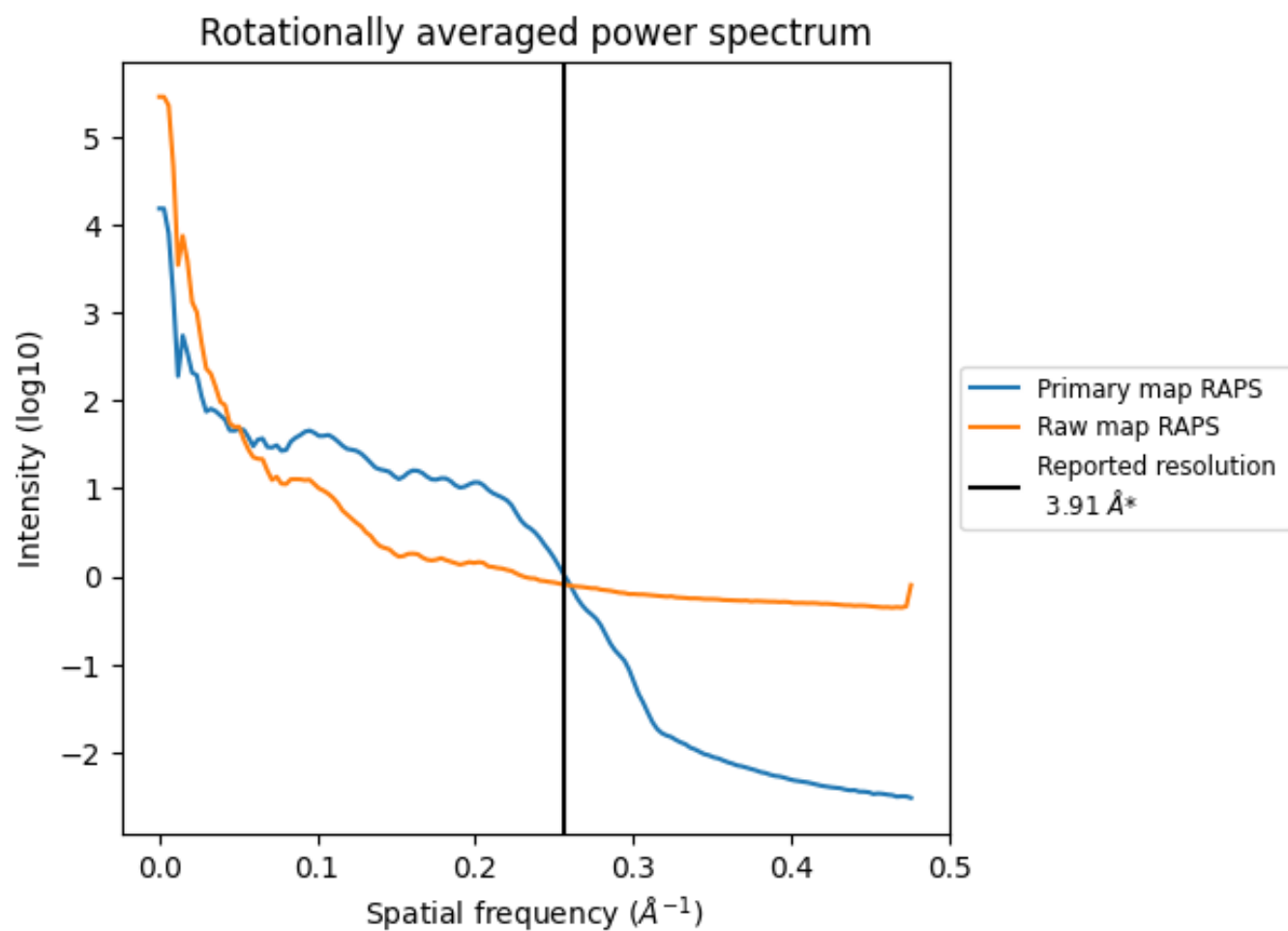
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 181 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

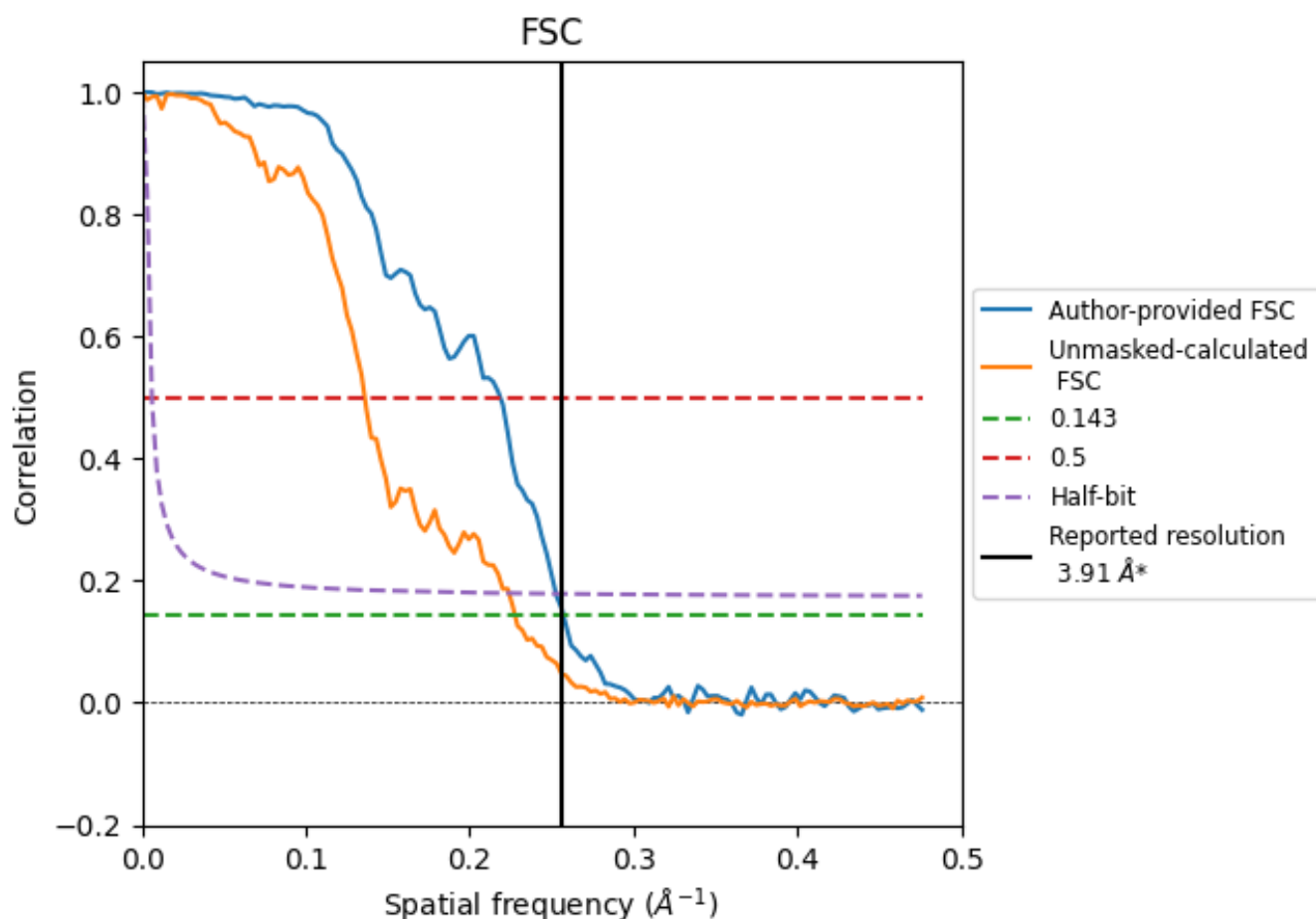


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

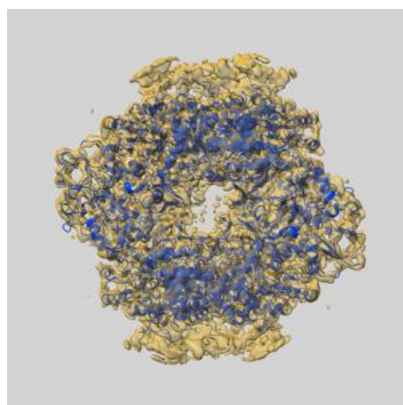
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.89	4.57	3.96
Unmasked-calculated*	4.39	7.36	4.46

*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 4.39 differs from the reported value 3.91 by more than 10 %

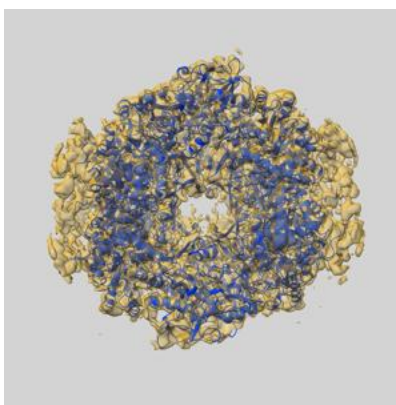
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20690 and PDB model 6U8R. Per-residue inclusion information can be found in section [3](#) on page [9](#).

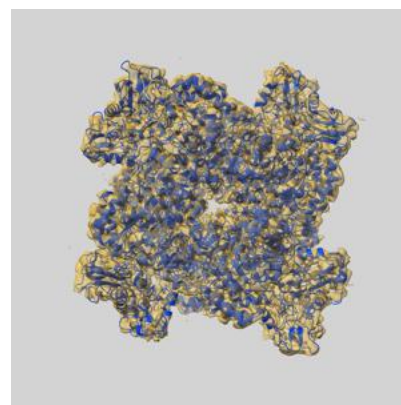
9.1 Map-model overlay [i](#)



X



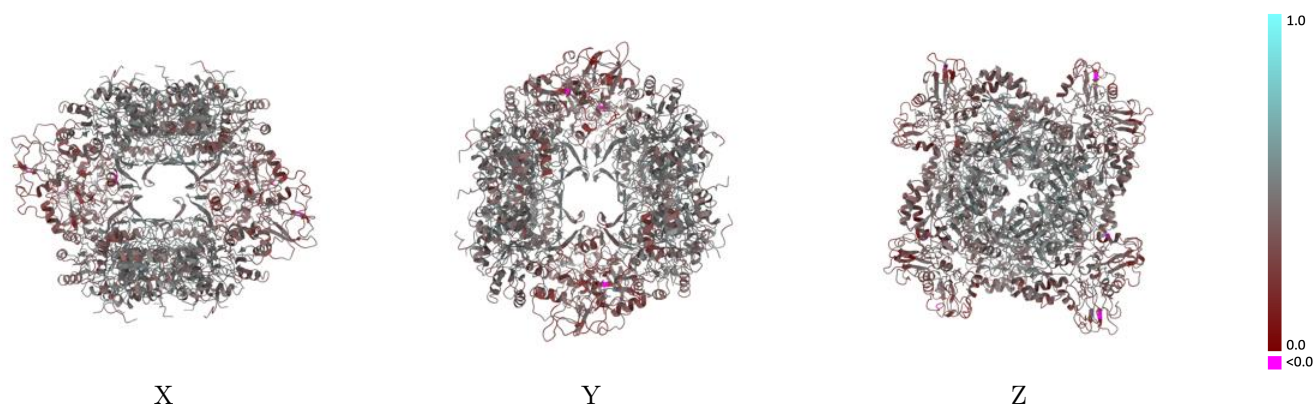
Y



Z

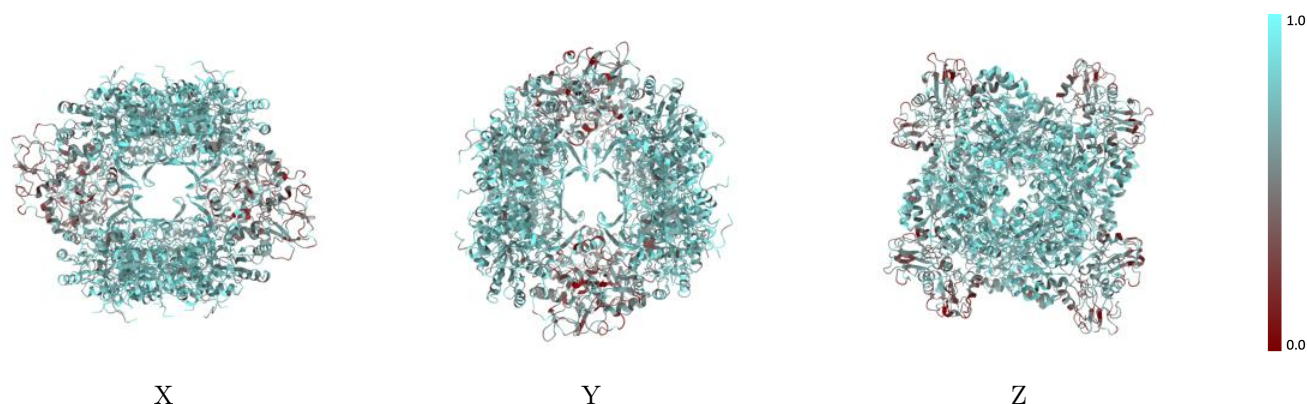
The images above show the 3D surface view of the map at the recommended contour level 17.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



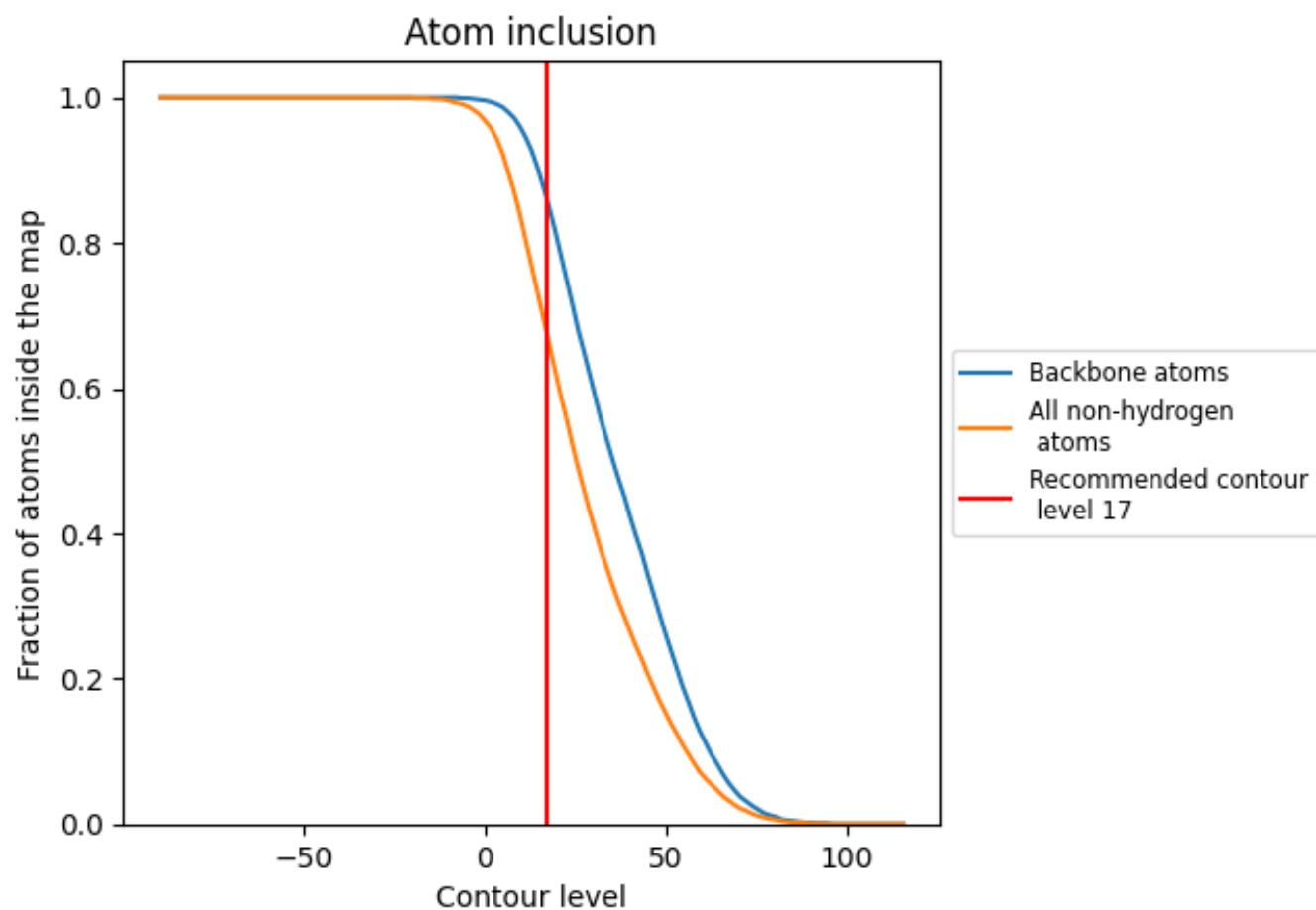
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% 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 (17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.4160
A	 0.6880	 0.4270
B	 0.6720	 0.4090
C	 0.6670	 0.4100
D	 0.6880	 0.4190
E	 0.6860	 0.4260
F	 0.6760	 0.4090
G	 0.6620	 0.4050
H	 0.6860	 0.4210
I	 0.7200	 0.4320
J	 0.6700	 0.4030
K	 0.6900	 0.4280
L	 0.7300	 0.4320
M	 0.7500	 0.4300
N	 0.7200	 0.4120
O	 0.6100	 0.3760
P	 0.7300	 0.4410

