



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 07:35 AM EST

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

This is a 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) : 2.31.2

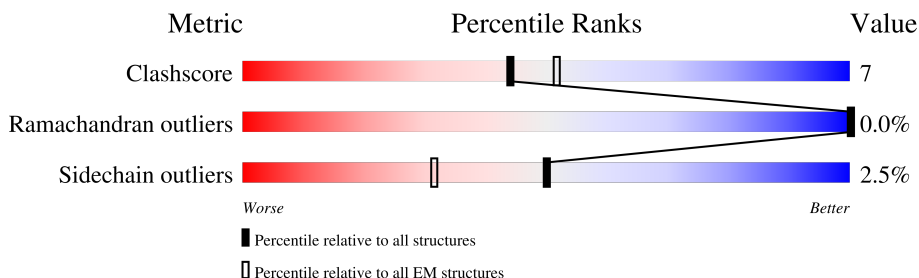
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



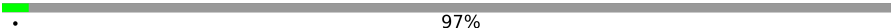
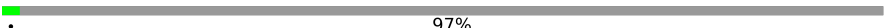
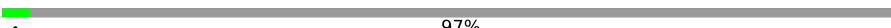
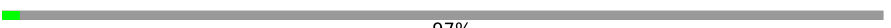
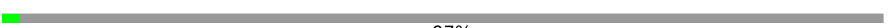



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	519	
1	B	519	
1	C	519	
1	D	519	
1	E	519	
1	F	519	
1	G	519	
1	H	519	

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

## 2 Entry composition [i](#)

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

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

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

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

There are 80 discrepancies between the modelled and reference sequences:

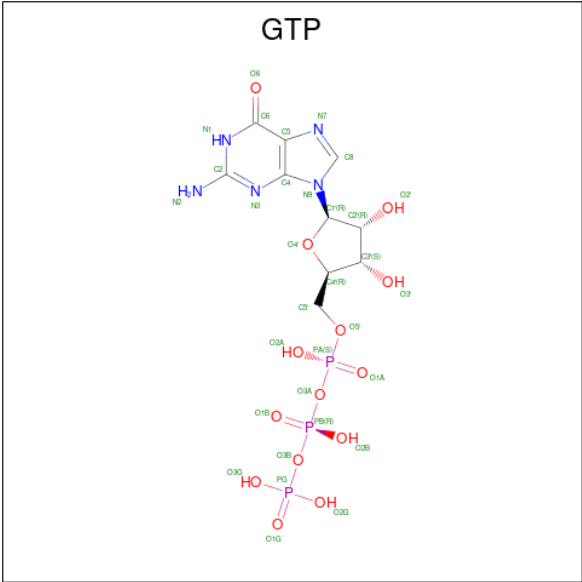
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP P12268
A	-3	GLU	-	expression tag	UNP P12268
A	-2	PHE	-	expression tag	UNP P12268
A	-1	GLU	-	expression tag	UNP P12268
A	0	LEU	-	expression tag	UNP P12268
B	-4	SER	-	expression tag	UNP P12268
B	-3	GLU	-	expression tag	UNP P12268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

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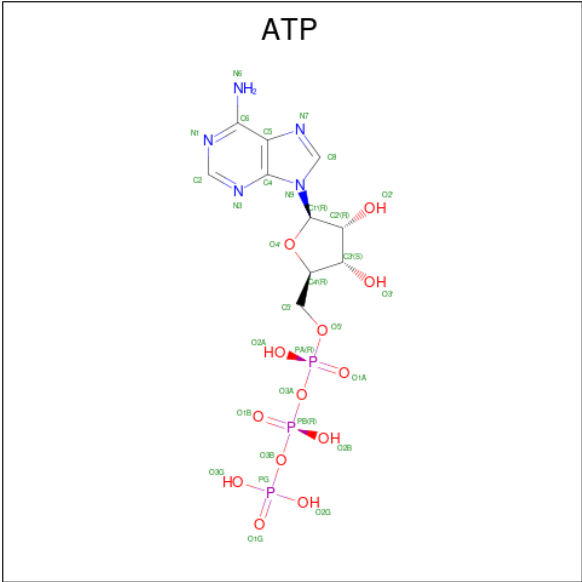
Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	GLU	-	expression tag	UNP P12268
M	0	LEU	-	expression tag	UNP P12268
N	-4	SER	-	expression tag	UNP P12268
N	-3	GLU	-	expression tag	UNP P12268
N	-2	PHE	-	expression tag	UNP P12268
N	-1	GLU	-	expression tag	UNP P12268
N	0	LEU	-	expression tag	UNP P12268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

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



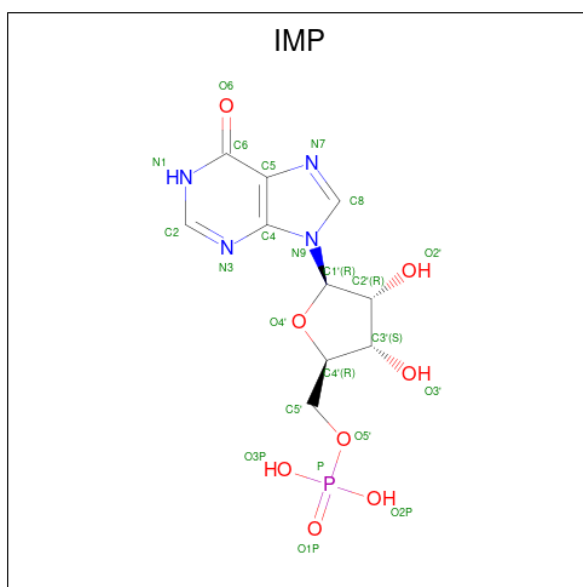
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	A	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	B	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	B	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	D	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	D	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	E	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	E	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	F	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	F	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	H	1	Total	C	N	O	P	0
			64	20	10	28	6	
2	H	1	Total	C	N	O	P	0
			64	20	10	28	6	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



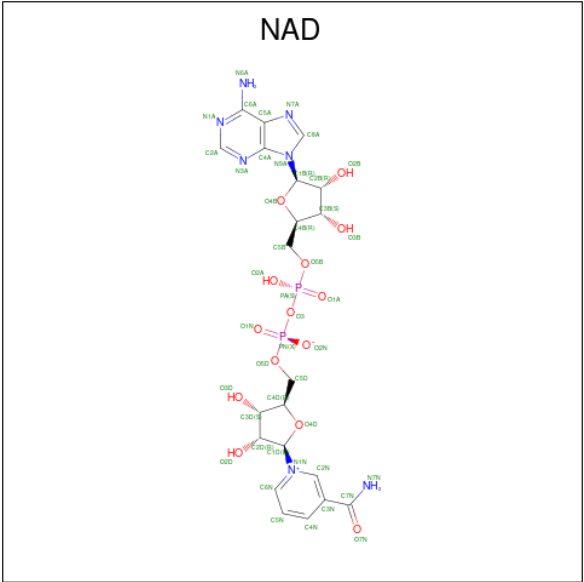
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	G	1	Total	C	N	O	P	0
			62	20	10	26	6	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is INOSINIC ACID (three-letter code: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



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

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

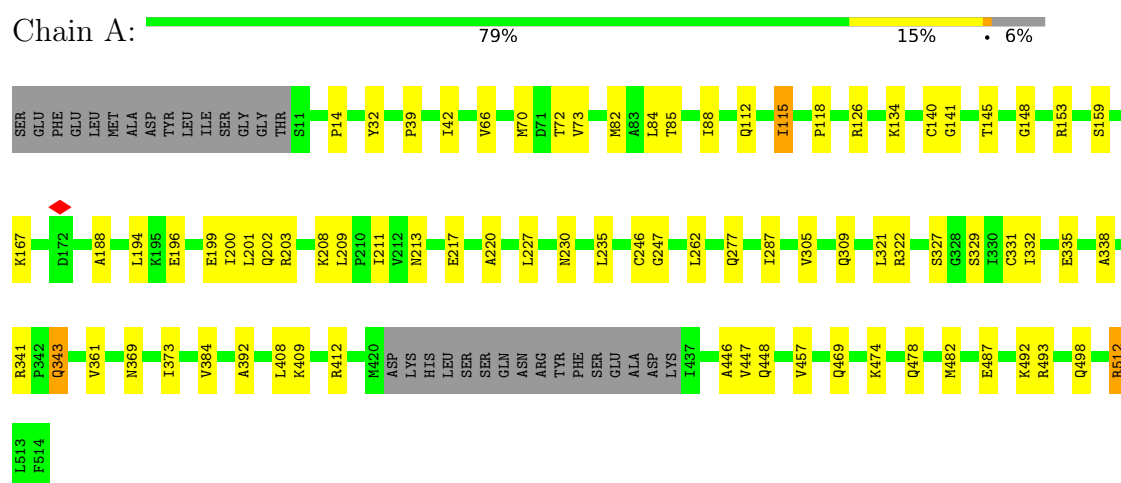


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	D	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	E	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	F	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	G	1	Total	C	N	O	P	0
			44	21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

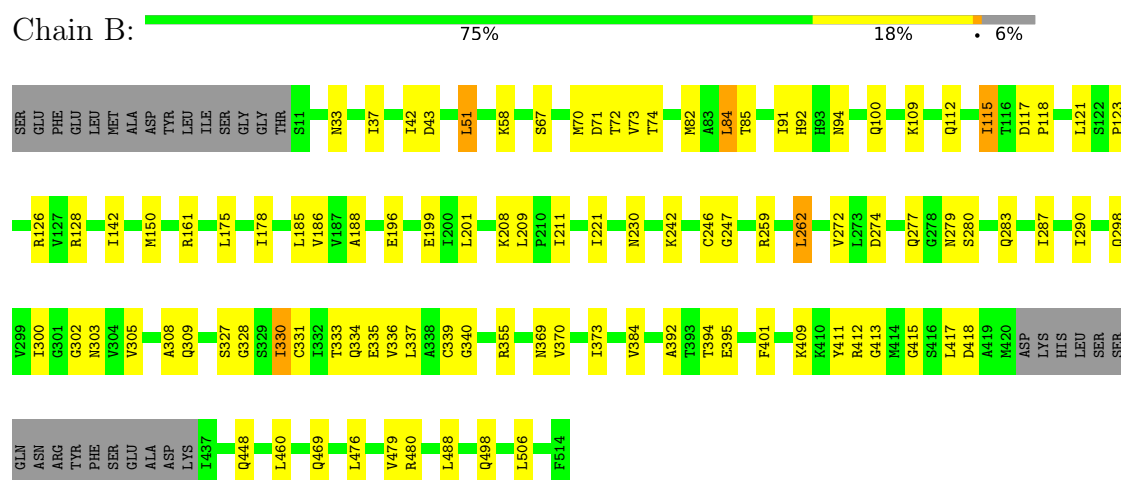
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

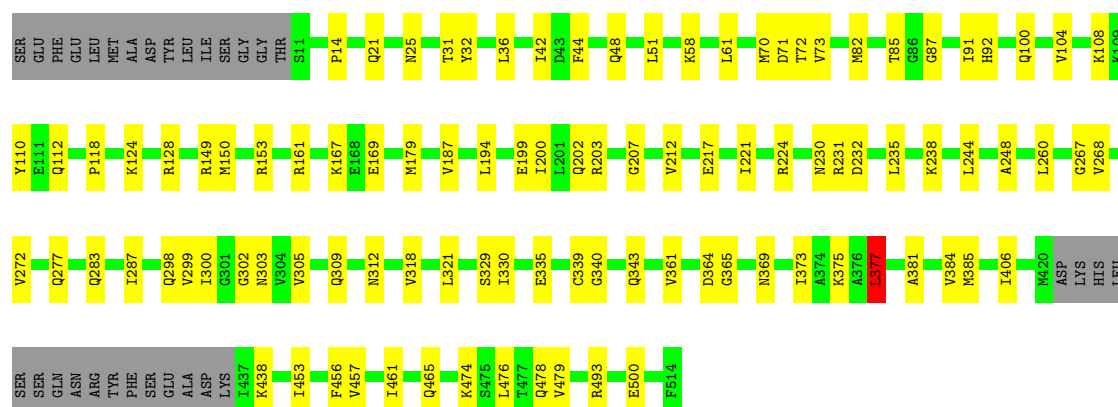


#### • Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



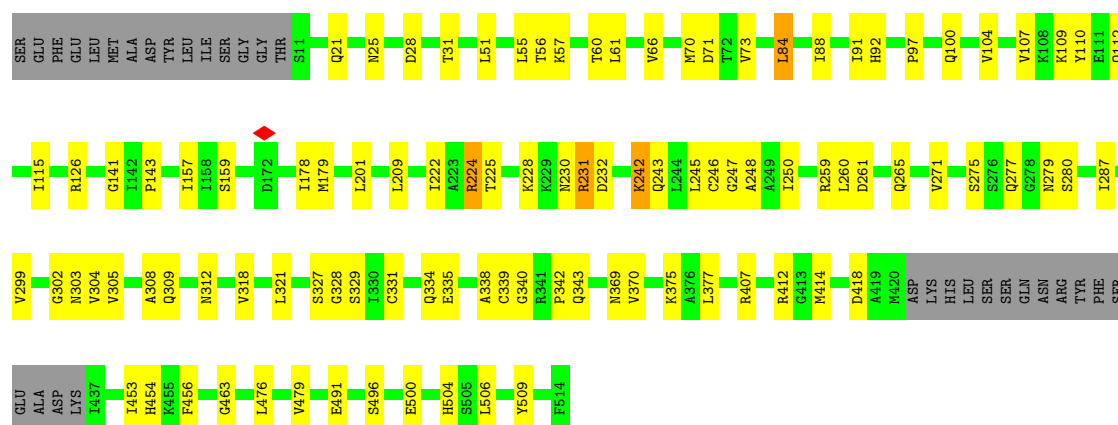
#### • Molecule 1: Inosine-5'-monophosphate dehydrogenase 2





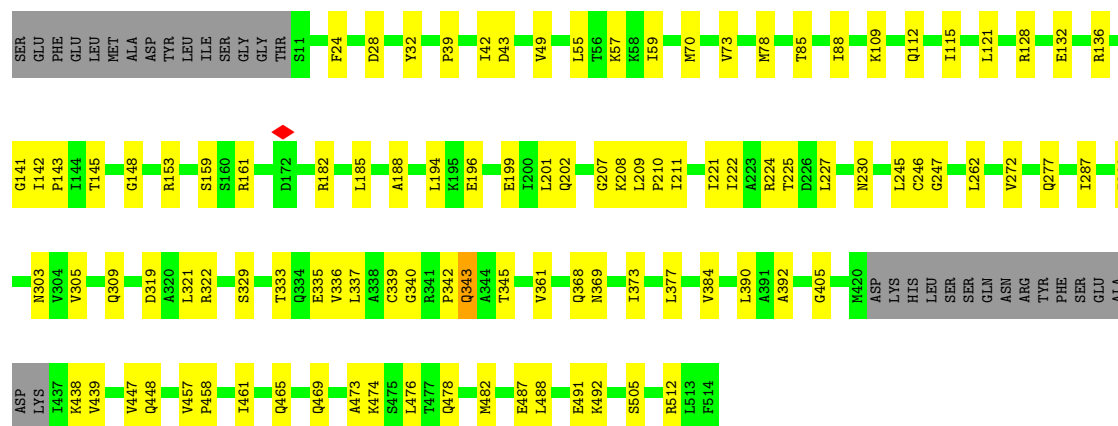
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain D: 75% 18% 6%



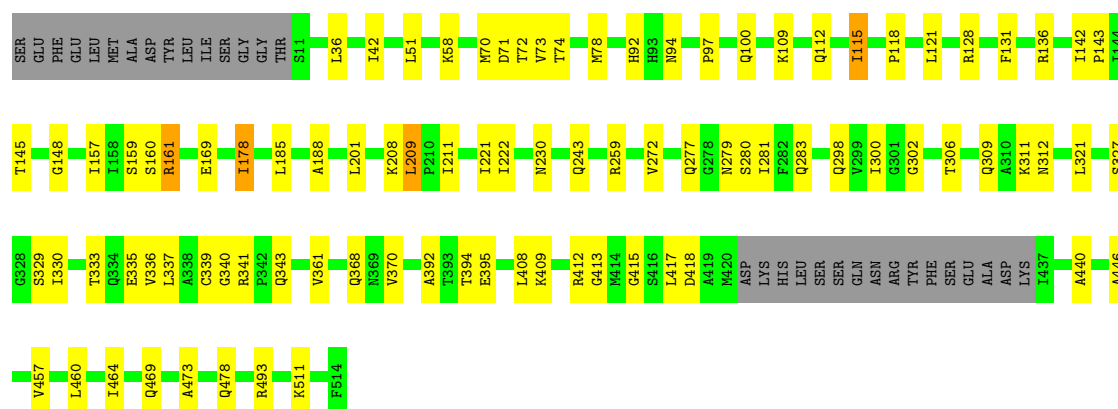
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain E: 74% 19% 6%



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

Chain F: 76% 17% 6%



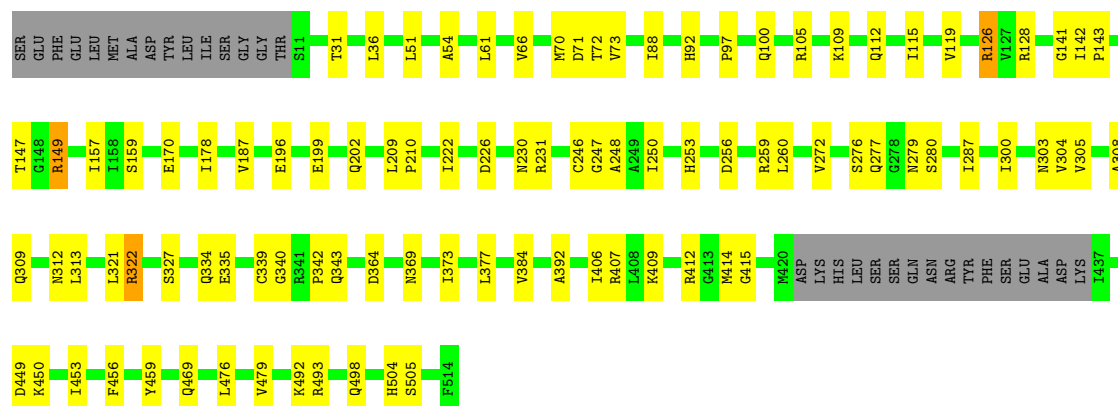
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain G: 77% 17% 6%



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

Chain H: 76% 18% 6%



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

Chain M: 97%

[illegible]

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

Chain N:  97%

[illegible]

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

97%

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

97%







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

## 4 Experimental information

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.43	0/3766	0.66	0/5078
1	B	0.46	0/3766	0.69	4/5078 (0.1%)
1	C	0.42	0/3766	0.66	1/5078 (0.0%)
1	D	0.41	0/3766	0.63	2/5078 (0.0%)
1	E	0.42	0/3766	0.65	0/5078
1	F	0.46	0/3766	0.68	1/5078 (0.0%)
1	G	0.41	0/3766	0.66	2/5078 (0.0%)
1	H	0.41	0/3766	0.63	0/5078
1	I	0.38	0/104	0.82	0/141
1	J	0.35	0/104	0.73	0/141
1	K	0.33	0/104	0.68	0/141
1	L	0.35	0/104	0.72	0/141
1	M	0.39	0/104	0.82	1/141 (0.7%)
1	N	0.33	0/104	0.73	0/141
1	O	0.36	0/104	0.81	1/141 (0.7%)
1	P	0.40	0/104	0.81	0/141
All	All	0.43	0/30960	0.66	12/41752 (0.0%)

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

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	LEU	CA-CB-CG	7.65	132.89	115.30
1	F	209	LEU	CA-CB-CG	6.78	130.90	115.30
1	D	245	LEU	CA-CB-CG	6.29	129.76	115.30
1	G	175	LEU	CA-CB-CG	5.83	128.70	115.30
1	C	377	LEU	CA-CB-CG	5.50	127.95	115.30
1	B	84	LEU	CA-CB-CG	5.41	127.73	115.30
1	G	377	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	209	LEU	CB-CG-CD2	-5.22	102.13	111.00
1	M	13	VAL	CA-CB-CG1	5.15	118.62	110.90
1	D	84	LEU	CA-CB-CG	5.14	127.11	115.30
1	O	13	VAL	CA-CB-CG1	5.07	118.50	110.90
1	B	262	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3710	0	3766	49	0
1	B	3710	0	3766	63	0
1	C	3710	0	3766	56	0
1	D	3710	0	3766	59	0
1	E	3710	0	3766	68	0
1	F	3710	0	3766	62	0
1	G	3710	0	3766	57	0
1	H	3710	0	3766	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	102	0	99	0	0
1	J	102	0	99	1	0
1	K	102	0	99	1	0
1	L	102	0	99	0	0
1	M	102	0	99	1	0
1	N	102	0	99	0	0
1	O	102	0	99	1	0
1	P	102	0	99	0	0
2	A	64	0	22	2	0
2	B	64	0	24	0	0
2	D	64	0	21	1	0
2	E	64	0	23	3	0
2	F	64	0	23	0	0
2	H	64	0	23	1	0
3	A	31	0	12	1	0
3	B	31	0	12	2	0
3	C	62	0	24	1	0
3	D	31	0	12	0	0
3	E	31	0	12	3	0
3	F	31	0	12	3	0
3	G	62	0	24	0	0
3	H	31	0	12	0	0
4	A	23	0	11	1	0
4	B	23	0	11	2	0
4	C	23	0	11	1	0
4	D	23	0	11	1	0
4	E	23	0	11	1	0
4	F	23	0	11	2	0
4	G	23	0	11	2	0
4	H	23	0	11	2	0
5	A	44	0	24	0	0
5	B	44	0	24	4	0
5	C	44	0	24	1	0
5	D	44	0	24	1	0
5	E	44	0	24	2	0
5	F	44	0	24	2	0
5	G	44	0	24	2	0
5	H	44	0	24	2	0
All	All	31726	0	31456	433	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:VAL:H	1:E:309:GLN:HE21	1.34	0.75
1:E:474:LYS:H	1:E:478:GLN:HE21	1.31	0.75
1:C:305:VAL:H	1:C:309:GLN:HE21	1.36	0.72
1:B:305:VAL:H	1:B:309:GLN:HE21	1.38	0.71
1:E:109:LYS:HA	1:E:112:GLN:HE22	1.57	0.70
1:F:72:THR:HG21	1:F:412:ARG:H	1.57	0.70
1:G:474:LYS:H	1:G:478:GLN:HE21	1.37	0.69
1:C:474:LYS:H	1:C:478:GLN:HE21	1.38	0.69
1:G:91:ILE:H	1:G:248:ALA:HA	1.57	0.69
1:B:72:THR:HG21	1:B:412:ARG:H	1.59	0.68
1:H:305:VAL:H	1:H:309:GLN:HE21	1.43	0.66
1:A:373:ILE:HG23	1:A:384:VAL:HG11	1.78	0.65
1:D:109:LYS:HA	1:D:112:GLN:HE22	1.61	0.65
1:B:161:ARG:HD2	3:B:603:ATP:H5'1	1.79	0.65
1:G:305:VAL:H	1:G:309:GLN:HE21	1.44	0.65
1:A:188:ALA:HB3	1:A:211:ILE:HG22	1.78	0.64
1:B:283:GLN:HE22	1:B:302:GLY:H	1.45	0.64
1:E:194:LEU:HD11	2:E:602:GTP:HN22	1.62	0.63
1:A:112:GLN:HB2	1:A:115:ILE:HG22	1.80	0.63
1:A:498:GLN:HE22	1:D:496:SER:HB2	1.63	0.63
1:G:121:LEU:HD23	1:G:142:ILE:HG21	1.80	0.63
1:C:128:ARG:NH2	1:C:169:GLU:O	2.32	0.63
1:G:42:ILE:HB	1:H:280:SER:HA	1.80	0.63
1:C:373:ILE:HG22	1:C:384:VAL:HG11	1.81	0.62
1:B:330:ILE:HG21	1:B:413:GLY:H	1.64	0.62
1:D:305:VAL:H	1:D:309:GLN:HE21	1.46	0.62
1:E:188:ALA:HB3	1:E:211:ILE:HG22	1.80	0.62
1:H:407:ARG:NH2	1:H:449:ASP:OD2	2.33	0.62
1:C:343:GLN:NE2	1:C:365:GLY:O	2.33	0.61
1:G:108:LYS:NZ	1:G:267:GLY:O	2.33	0.61
1:D:61:LEU:HD21	1:D:88:ILE:HB	1.83	0.61
1:B:392:ALA:HA	1:B:409:LYS:HD2	1.83	0.61
1:B:412:ARG:HD2	1:B:418:ASP:HB2	1.83	0.60
1:D:112:GLN:HB2	1:D:115:ILE:HD13	1.82	0.60
1:D:201:LEU:HD13	1:D:209:LEU:HB2	1.84	0.60
1:A:482:MET:HB2	1:A:487:GLU:HB3	1.82	0.60
1:B:373:ILE:HG23	1:B:384:VAL:HG11	1.83	0.60
1:E:246:CYS:SG	1:E:247:GLY:N	2.73	0.60
1:G:339:CYS:SG	1:G:340:GLY:N	2.75	0.60
1:A:39:PRO:HB2	1:B:277:GLN:HE21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ILE:HD11	1:F:118:PRO:HB3	1.83	0.60
1:A:202:GLN:HE21	1:A:227:LEU:HD13	1.68	0.59
1:B:70:MET:HB2	1:B:73:VAL:HG12	1.84	0.59
1:D:279:ASN:HD21	1:D:312:ASN:HD21	1.49	0.59
1:H:112:GLN:HB2	1:H:115:ILE:HG13	1.84	0.59
1:A:14:PRO:HD2	1:B:308:ALA:HA	1.84	0.59
1:F:131:PHE:HE2	1:F:169:GLU:HG2	1.68	0.59
1:F:392:ALA:HA	1:F:409:LYS:HD2	1.84	0.59
1:A:469:GLN:NE2	5:B:605:NAD:O2B	2.35	0.59
1:D:328:GLY:N	1:D:331:CYS:SG	2.72	0.59
1:B:277:GLN:NE2	1:B:309:GLN:OE1	2.36	0.59
1:F:370:VAL:HG12	1:F:460:LEU:HD23	1.84	0.59
1:B:100:GLN:OE1	1:B:259:ARG:NH2	2.34	0.58
1:B:303:ASN:ND2	5:B:605:NAD:O7N	2.35	0.58
1:E:373:ILE:HG23	1:E:384:VAL:HG11	1.84	0.58
1:E:201:LEU:HD23	1:E:209:LEU:HB2	1.85	0.58
1:C:91:ILE:H	1:C:248:ALA:HA	1.68	0.58
1:C:108:LYS:NZ	1:C:267:GLY:O	2.37	0.58
1:E:141:GLY:O	1:E:208:LYS:NZ	2.36	0.58
1:H:70:MET:HB2	1:H:73:VAL:HG12	1.86	0.58
1:C:207:GLY:HA2	1:C:224:ARG:HD2	1.86	0.58
1:F:339:CYS:SG	1:F:340:GLY:N	2.77	0.58
1:E:39:PRO:HB2	1:F:277:GLN:HE21	1.69	0.57
1:B:188:ALA:HB3	1:B:211:ILE:HG22	1.86	0.57
1:G:283:GLN:HE22	1:G:302:GLY:H	1.51	0.57
1:H:303:ASN:ND2	5:H:605:NAD:O7N	2.37	0.57
1:B:115:ILE:HD11	1:B:118:PRO:HB3	1.85	0.57
1:F:161:ARG:NH2	3:F:603:ATP:O1A	2.37	0.57
1:G:303:ASN:ND2	5:G:604:NAD:O7N	2.37	0.57
1:C:493:ARG:NH1	1:D:334:GLN:OE1	2.38	0.57
1:D:209:LEU:HB3	1:D:222:ILE:HB	1.86	0.57
1:D:303:ASN:ND2	5:D:605:NAD:O7N	2.38	0.57
1:F:283:GLN:HE22	1:F:302:GLY:H	1.53	0.57
1:H:72:THR:HG21	1:H:412:ARG:H	1.70	0.57
1:A:246:CYS:SG	1:A:247:GLY:N	2.77	0.57
1:C:339:CYS:SG	1:C:340:GLY:N	2.78	0.57
1:B:412:ARG:NH2	1:B:418:ASP:O	2.37	0.57
1:E:329:SER:OG	1:H:504:HIS:O	2.23	0.56
1:A:199:GLU:OE1	1:A:203:ARG:NH2	2.38	0.56
1:F:109:LYS:HD3	1:F:112:GLN:HE22	1.71	0.56
1:H:128:ARG:HE	1:H:170:GLU:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ALA:HA	1:A:409:LYS:HG3	1.86	0.56
1:C:303:ASN:ND2	5:C:604:NAD:O7N	2.39	0.56
1:C:321:LEU:HB2	1:C:361:VAL:HG23	1.88	0.56
1:H:61:LEU:HD21	1:H:88:ILE:HB	1.86	0.56
1:H:322:ARG:NE	1:H:364:ASP:OD2	2.37	0.56
1:B:328:GLY:N	1:B:331:CYS:SG	2.78	0.56
1:D:112:GLN:HG3	1:D:243:GLN:HG3	1.88	0.56
1:F:100:GLN:OE1	1:F:259:ARG:NH2	2.33	0.56
1:H:226:ASP:OD2	2:H:602:GTP:N1	2.38	0.56
1:B:186:VAL:H	3:B:603:ATP:HN62	1.52	0.55
1:D:453:ILE:HA	1:D:456:PHE:HB3	1.87	0.55
1:E:473:ALA:HB1	1:E:478:GLN:HG3	1.88	0.55
1:D:261:ASP:O	1:D:265:GLN:NE2	2.39	0.55
1:A:72:THR:HG21	1:A:412:ARG:H	1.71	0.55
1:A:201:LEU:HD23	1:A:209:LEU:HB2	1.87	0.55
1:A:329:SER:OG	1:D:504:HIS:O	2.23	0.55
1:D:91:ILE:H	1:D:248:ALA:HA	1.72	0.55
1:B:339:CYS:SG	1:B:340:GLY:N	2.79	0.55
1:E:482:MET:HG3	1:E:488:LEU:HB2	1.88	0.55
1:F:71:ASP:OD2	1:F:412:ARG:NH1	2.40	0.55
1:F:188:ALA:HB3	1:F:211:ILE:HG22	1.89	0.55
1:E:377:LEU:HD13	1:E:476:LEU:HD21	1.89	0.55
1:A:141:GLY:O	1:A:208:LYS:NZ	2.40	0.54
1:G:493:ARG:NH1	1:H:334:GLN:OE1	2.40	0.54
1:G:44:PHE:HB2	1:G:48:GLN:HE21	1.71	0.54
1:D:100:GLN:HE21	1:D:248:ALA:HB1	1.72	0.54
1:E:469:GLN:NE2	5:F:605:NAD:O2B	2.40	0.54
1:C:149:ARG:HE	1:C:150:MET:H	1.53	0.54
1:G:82:MET:HA	1:G:85:THR:HG22	1.90	0.54
1:E:333:THR:HG21	5:E:605:NAD:H5N	1.90	0.54
1:G:369:ASN:ND2	1:H:335:GLU:O	2.41	0.54
1:H:246:CYS:SG	1:H:247:GLY:N	2.80	0.54
1:F:58:LYS:HB3	1:F:298:GLN:HE22	1.73	0.54
1:E:335:GLU:O	1:H:369:ASN:ND2	2.42	0.53
1:G:70:MET:HB2	1:G:73:VAL:HG12	1.90	0.53
1:G:496:SER:HB3	1:H:498:GLN:HE22	1.73	0.53
1:B:82:MET:HA	1:B:85:THR:HG22	1.89	0.53
1:C:21:GLN:O	1:C:25:ASN:ND2	2.41	0.53
1:C:70:MET:HB2	1:C:73:VAL:HG12	1.90	0.53
1:F:70:MET:HB2	1:F:73:VAL:HG12	1.90	0.53
1:C:82:MET:HA	1:C:85:THR:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:VAL:HG13	1:H:142:ILE:HD11	1.90	0.53
1:C:36:LEU:HD21	1:D:342:PRO:HD3	1.89	0.53
1:E:32:TYR:OH	1:E:343:GLN:NE2	2.42	0.53
1:H:209:LEU:HB3	1:H:222:ILE:HB	1.91	0.53
5:E:605:NAD:O2B	1:H:469:GLN:NE2	2.42	0.53
1:G:47:ASP:O	1:G:465:GLN:NE2	2.42	0.53
1:B:71:ASP:OD2	1:B:412:ARG:NH1	2.42	0.53
1:E:161:ARG:NH1	3:E:603:ATP:O3A	2.42	0.52
1:G:453:ILE:HA	1:G:456:PHE:HB3	1.90	0.52
1:A:512:ARG:HD2	1:B:417:LEU:HB2	1.91	0.52
1:D:56:THR:OG1	1:D:57:LYS:N	2.42	0.52
1:A:321:LEU:HB2	1:A:361:VAL:HG23	1.90	0.52
1:E:225:THR:HG1	2:E:601:GTP:HO3'	1.54	0.52
1:F:112:GLN:HG3	1:F:243:GLN:HG2	1.90	0.52
1:F:415:GLY:N	4:F:604:IMP:O6	2.36	0.52
1:C:194:LEU:HD12	1:C:230:ASN:HD21	1.73	0.52
1:C:104:VAL:HG21	1:C:268:VAL:HG22	1.92	0.52
1:A:341:ARG:NH2	1:D:491:GLU:OE1	2.43	0.52
1:E:505:SER:OG	1:F:368:GLN:OE1	2.26	0.52
1:H:100:GLN:OE1	1:H:259:ARG:NH2	2.39	0.52
1:D:141:GLY:HA2	1:D:159:SER:HA	1.92	0.51
1:F:161:ARG:NH1	3:F:603:ATP:O1G	2.43	0.51
1:E:121:LEU:HD13	1:E:142:ILE:HG21	1.93	0.51
1:G:100:GLN:HE21	1:G:248:ALA:HB1	1.75	0.51
1:E:482:MET:HB2	1:E:487:GLU:HB3	1.93	0.51
1:E:342:PRO:HD3	1:H:36:LEU:HD21	1.92	0.51
1:A:66:VAL:HG22	1:A:88:ILE:HG22	1.91	0.51
1:E:369:ASN:ND2	1:F:335:GLU:O	2.44	0.51
1:D:377:LEU:HD13	1:D:476:LEU:HD21	1.92	0.51
1:E:85:THR:HG21	1:E:457:VAL:HG21	1.92	0.51
1:F:160:SER:OG	1:F:161:ARG:NH1	2.44	0.51
1:E:303:ASN:ND2	1:E:322:ARG:O	2.40	0.51
1:F:109:LYS:HA	1:F:112:GLN:HE22	1.75	0.51
1:F:469:GLN:NE2	5:G:604:NAD:O2B	2.44	0.51
1:B:336:VAL:HG12	1:B:337:LEU:HD12	1.93	0.51
1:D:60:THR:HG21	1:O:1:MET:HB2	1.91	0.51
1:B:33:ASN:O	1:B:498:GLN:NE2	2.44	0.51
1:B:401:PHE:HB3	1:E:512:ARG:HD3	1.91	0.51
1:F:36:LEU:HD22	1:F:493:ARG:HD3	1.92	0.51
1:C:500:GLU:OE2	1:D:327:SER:OG	2.29	0.50
1:E:512:ARG:HG2	1:F:417:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:339:CYS:SG	1:H:340:GLY:N	2.84	0.50
1:A:194:LEU:HD11	2:A:602:GTP:HN22	1.76	0.50
1:A:335:GLU:O	1:D:369:ASN:ND2	2.44	0.50
1:B:58:LYS:HB3	1:B:298:GLN:HE22	1.76	0.50
1:D:143:PRO:HA	1:D:157:ILE:HA	1.94	0.50
1:A:493:ARG:NH1	1:B:334:GLN:OE1	2.38	0.50
1:F:333:THR:HG21	5:F:605:NAD:H4N	1.93	0.50
1:B:117:ASP:HA	1:B:150:MET:HG3	1.93	0.50
1:E:143:PRO:HG3	1:E:221:ILE:HG21	1.94	0.50
1:F:36:LEU:HD21	1:G:342:PRO:HD3	1.94	0.50
1:B:112:GLN:HB2	1:B:115:ILE:HG22	1.95	0.49
1:B:415:GLY:N	4:B:604:IMP:O6	2.38	0.49
1:C:58:LYS:HB2	1:C:298:GLN:HE22	1.76	0.49
1:D:277:GLN:NE2	1:D:309:GLN:OE1	2.45	0.49
1:C:36:LEU:HD22	1:C:493:ARG:HD3	1.93	0.49
1:G:500:GLU:OE2	1:H:327:SER:OG	2.29	0.49
1:D:70:MET:HB2	1:D:73:VAL:HG12	1.93	0.49
1:D:476:LEU:HA	1:D:479:VAL:HG12	1.94	0.49
1:H:277:GLN:NE2	1:H:309:GLN:OE1	2.45	0.49
1:B:279:ASN:HB2	1:B:309:GLN:HB2	1.94	0.49
1:H:36:LEU:HD22	1:H:493:ARG:HD3	1.94	0.49
1:G:118:PRO:HB3	1:G:221:ILE:HG21	1.93	0.49
1:E:28:ASP:HA	1:H:492:LYS:HB3	1.95	0.49
1:H:453:ILE:HA	1:H:456:PHE:HB3	1.94	0.49
1:A:331:CYS:SG	1:A:332:ILE:N	2.86	0.49
1:C:118:PRO:HB3	1:C:221:ILE:HG21	1.95	0.49
1:F:42:ILE:HG13	1:G:280:SER:HA	1.95	0.49
1:B:208:LYS:HB3	1:B:221:ILE:HD11	1.94	0.49
1:G:392:ALA:HA	1:G:409:LYS:HD3	1.95	0.49
1:D:31:THR:HG22	1:D:343:GLN:H	1.77	0.49
1:H:476:LEU:HA	1:H:479:VAL:HG12	1.95	0.49
1:E:88:ILE:HD13	1:E:245:LEU:HB3	1.95	0.48
1:G:114:PHE:HD1	1:G:222:ILE:HD13	1.78	0.48
1:H:377:LEU:HD13	1:H:476:LEU:HD21	1.94	0.48
1:E:321:LEU:HB2	1:E:361:VAL:HG12	1.95	0.48
1:C:42:ILE:HG13	1:D:280:SER:HA	1.95	0.48
1:C:364:ASP:HB3	1:C:385:MET:HB3	1.95	0.48
1:G:373:ILE:HG22	1:G:384:VAL:HG11	1.95	0.48
1:H:100:GLN:HE21	1:H:248:ALA:HB1	1.78	0.48
1:E:339:CYS:SG	1:E:340:GLY:N	2.87	0.48
1:E:491:GLU:OE1	1:F:341:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ILE:HA	1:C:456:PHE:HB3	1.94	0.48
1:H:187:VAL:HG23	1:H:210:PRO:HB2	1.96	0.48
1:G:500:GLU:OE1	1:H:31:THR:OG1	2.25	0.48
1:C:44:PHE:HB2	1:C:48:GLN:HE21	1.79	0.48
1:E:55:LEU:HD22	1:E:88:ILE:HG21	1.95	0.48
1:A:159:SER:OG	3:A:603:ATP:O2B	2.31	0.48
1:B:411:TYR:OH	4:B:604:IMP:O1P	2.29	0.48
1:F:457:VAL:HA	1:F:460:LEU:HD12	1.94	0.48
1:A:201:LEU:HB2	1:A:209:LEU:HD22	1.95	0.48
1:G:14:PRO:HD2	1:H:308:ALA:HA	1.96	0.48
1:G:239:ASP:OD1	1:G:243:GLN:N	2.45	0.48
1:A:305:VAL:H	1:A:309:GLN:HE21	1.62	0.47
1:B:480:ARG:NH2	1:M:5:LEU:O	2.46	0.47
1:E:272:VAL:HA	1:E:300:ILE:HB	1.96	0.47
1:E:57:LYS:HE3	1:E:319:ASP:HA	1.95	0.47
1:G:324:GLY:HA3	1:G:343:GLN:HE21	1.78	0.47
1:H:126:ARG:HG2	1:H:170:GLU:HB2	1.96	0.47
1:H:304:VAL:HG21	1:H:321:LEU:HD23	1.96	0.47
1:A:408:LEU:HD13	1:A:446:ALA:HB1	1.97	0.47
1:C:283:GLN:HE22	1:C:302:GLY:H	1.60	0.47
1:G:126:ARG:HD3	1:G:172:ASP:H	1.80	0.47
1:H:54:ALA:HB2	1:K:5:LEU:HD23	1.96	0.47
1:H:279:ASN:HB2	1:H:309:GLN:HB2	1.96	0.47
1:C:100:GLN:HE21	1:C:248:ALA:HB1	1.78	0.47
1:C:231:ARG:NH2	1:C:232:ASP:O	2.48	0.47
1:D:97:PRO:HG3	1:D:259:ARG:HG2	1.95	0.47
1:D:231:ARG:NH2	1:D:232:ASP:OD1	2.47	0.47
1:E:24:PHE:HD1	1:E:345:THR:HG22	1.78	0.47
1:F:329:SER:N	4:F:604:IMP:O1P	2.46	0.47
1:F:336:VAL:HG12	1:F:337:LEU:HD12	1.97	0.47
1:H:97:PRO:HG3	1:H:259:ARG:HG2	1.95	0.47
1:H:147:THR:HG22	1:H:149:ARG:HH21	1.80	0.47
1:H:199:GLU:HA	1:H:202:GLN:HG2	1.97	0.47
1:H:279:ASN:HD21	1:H:312:ASN:HD21	1.62	0.47
1:D:304:VAL:HG21	1:D:321:LEU:HD23	1.96	0.47
1:B:42:ILE:HG12	1:C:277:GLN:HE22	1.78	0.47
1:E:42:ILE:HB	1:F:280:SER:HA	1.97	0.47
1:F:327:SER:HB2	1:F:343:GLN:HG2	1.97	0.47
1:A:82:MET:HA	1:A:85:THR:HG22	1.96	0.46
1:D:299:VAL:HG23	1:D:318:VAL:HG23	1.96	0.46
1:B:369:ASN:HD22	1:C:335:GLU:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LYS:HB3	1:C:244:LEU:HD23	1.96	0.46
1:E:112:GLN:HB2	1:E:115:ILE:HD13	1.96	0.46
1:E:336:VAL:HG12	1:E:337:LEU:HD12	1.96	0.46
1:F:51:LEU:HD22	1:F:464:ILE:HD11	1.97	0.46
1:H:272:VAL:HA	1:H:300:ILE:HB	1.97	0.46
1:A:85:THR:HG21	1:A:457:VAL:HG21	1.97	0.46
1:C:375:LYS:HG3	1:D:338:ALA:HB1	1.96	0.46
1:B:196:GLU:HA	1:B:199:GLU:HG3	1.97	0.46
1:B:272:VAL:HA	1:B:300:ILE:HB	1.97	0.46
1:G:187:VAL:HG11	1:G:212:VAL:HG22	1.98	0.46
1:H:143:PRO:HA	1:H:157:ILE:HG22	1.97	0.46
1:A:134:LYS:HG3	1:A:140:CYS:HB3	1.97	0.46
1:E:128:ARG:NH2	1:E:132:GLU:OE2	2.47	0.46
1:H:196:GLU:HA	1:H:199:GLU:HG2	1.98	0.46
1:C:61:LEU:HD23	1:C:87:GLY:HA2	1.97	0.46
1:B:121:LEU:HD23	1:B:142:ILE:HG21	1.98	0.46
1:F:178:ILE:H	1:F:178:ILE:HG13	1.65	0.46
1:H:105:ARG:O	1:H:109:LYS:N	2.41	0.46
1:A:196:GLU:HA	1:A:199:GLU:HG3	1.98	0.46
1:D:250:ILE:HD13	1:D:260:LEU:HD12	1.97	0.46
1:G:36:LEU:HD22	1:G:493:ARG:HD3	1.98	0.46
2:A:602:GTP:H3'	2:A:602:GTP:PB	2.56	0.46
1:C:31:THR:OG1	1:C:32:TYR:N	2.48	0.46
1:C:369:ASN:ND2	1:D:335:GLU:O	2.50	0.46
1:C:461:ILE:O	1:C:465:GLN:HB2	2.15	0.46
1:E:70:MET:SD	4:E:604:IMP:H8	2.56	0.45
1:B:175:LEU:HD13	1:B:178:ILE:HD11	1.98	0.45
1:C:32:TYR:HE2	1:C:343:GLN:HE21	1.64	0.45
1:E:458:PRO:HA	1:E:461:ILE:HG12	1.97	0.45
1:A:188:ALA:HB2	1:A:200:ILE:HD11	1.96	0.45
1:E:145:THR:OG1	1:E:153:ARG:O	2.28	0.45
1:G:201:LEU:HD22	1:G:209:LEU:HD13	1.99	0.45
1:H:141:GLY:HA2	1:H:159:SER:HA	1.98	0.45
1:C:71:ASP:OD1	1:C:72:THR:OG1	2.33	0.45
1:F:408:LEU:HD23	1:F:446:ALA:HB3	1.98	0.45
1:D:84:LEU:HD12	1:D:454:HIS:HE1	1.81	0.45
1:F:330:ILE:HD13	1:F:413:GLY:HA3	1.97	0.45
1:F:412:ARG:NH2	1:F:418:ASP:O	2.50	0.45
1:E:182:ARG:HE	1:E:185:LEU:HD21	1.82	0.45
1:H:109:LYS:HA	1:H:112:GLN:HE22	1.80	0.45
1:E:78:MET:HE1	1:E:390:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:ARG:H	1:H:149:ARG:HD2	1.82	0.45
1:D:21:GLN:O	1:D:25:ASN:ND2	2.50	0.45
1:E:209:LEU:HB3	1:E:222:ILE:HB	1.98	0.45
1:G:305:VAL:H	1:G:309:GLN:NE2	2.11	0.45
1:E:196:GLU:HA	1:E:199:GLU:HG2	1.98	0.44
1:F:321:LEU:HB2	1:F:361:VAL:HG12	1.98	0.44
1:G:36:LEU:HD21	1:H:342:PRO:HD3	1.98	0.44
1:E:161:ARG:HD2	3:E:603:ATP:H5'1	1.99	0.44
1:F:306:THR:HG23	1:F:309:GLN:H	1.83	0.44
1:G:511:LYS:NZ	1:H:335:GLU:OE2	2.45	0.44
1:B:123:PRO:HA	1:B:175:LEU:HB2	1.99	0.44
1:C:406:ILE:HG13	1:H:406:ILE:HG13	2.00	0.44
1:C:476:LEU:HA	1:C:479:VAL:HG12	1.99	0.44
1:C:153:ARG:NH2	1:C:217:GLU:OE2	2.50	0.44
1:G:367:ILE:HG12	1:G:373:ILE:HG22	1.99	0.44
1:G:126:ARG:HH21	1:G:170:GLU:HA	1.83	0.44
1:C:377:LEU:HA	1:C:381:ALA:HB3	1.98	0.44
1:G:461:ILE:O	1:G:465:GLN:HB2	2.17	0.44
1:A:145:THR:HG23	1:A:148:GLY:H	1.82	0.44
1:F:109:LYS:HA	1:F:112:GLN:NE2	2.32	0.44
1:H:71:ASP:HA	1:H:92:HIS:CD2	2.53	0.44
1:F:74:THR:HA	1:F:78:MET:HG3	2.00	0.44
1:A:70:MET:SD	4:A:604:IMP:H8	2.57	0.43
1:B:394:THR:OG1	1:B:395:GLU:OE1	2.31	0.43
1:F:209:LEU:HG	1:F:222:ILE:HD11	1.99	0.43
1:H:109:LYS:HA	1:H:112:GLN:NE2	2.33	0.43
1:A:115:ILE:HD11	1:A:118:PRO:HB3	1.99	0.43
1:B:71:ASP:HA	1:B:92:HIS:CD2	2.53	0.43
1:B:246:CYS:SG	1:B:247:GLY:N	2.91	0.43
1:B:327:SER:N	1:B:331:CYS:SG	2.91	0.43
1:B:476:LEU:HA	1:B:479:VAL:HG12	2.00	0.43
1:G:364:ASP:OD1	4:G:603:IMP:O3'	2.32	0.43
1:A:369:ASN:ND2	1:B:335:GLU:O	2.51	0.43
1:B:369:ASN:OD1	1:B:369:ASN:N	2.50	0.43
1:C:299:VAL:HG23	1:C:318:VAL:HG23	1.99	0.43
1:D:224:ARG:NH2	1:G:164:ASP:OD2	2.50	0.43
1:F:208:LYS:HB3	1:F:221:ILE:HD11	2.00	0.43
1:A:211:ILE:HD11	1:A:220:ALA:HB3	2.00	0.43
1:C:272:VAL:HA	1:C:300:ILE:HB	2.01	0.43
1:A:492:LYS:HE3	1:A:492:LYS:HB2	1.84	0.43
1:G:476:LEU:HA	1:G:479:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:415:GLY:N	4:H:604:IMP:O6	2.39	0.43
1:B:370:VAL:HG12	1:B:460:LEU:HD23	2.01	0.43
1:H:70:MET:SD	4:H:604:IMP:H8	2.58	0.43
1:D:28:ASP:OD1	1:D:28:ASP:N	2.51	0.43
1:E:392:ALA:HB2	1:E:447:VAL:HG13	2.01	0.43
1:A:327:SER:OG	1:D:500:GLU:OE2	2.36	0.43
1:D:100:GLN:OE1	1:D:259:ARG:NH2	2.40	0.43
1:G:465:GLN:O	1:G:469:GLN:HB2	2.19	0.43
1:H:343:GLN:NE2	1:H:364:ASP:O	2.52	0.43
1:A:70:MET:HB2	1:A:73:VAL:HG12	2.00	0.42
1:D:104:VAL:HA	1:D:107:VAL:HG12	2.00	0.42
1:G:200:ILE:O	1:G:204:SER:HB2	2.19	0.42
1:A:42:ILE:HB	1:B:280:SER:HA	2.02	0.42
1:A:474:LYS:H	1:A:478:GLN:HE21	1.67	0.42
1:D:506:LEU:HD11	1:D:509:TYR:HB3	2.00	0.42
1:E:145:THR:HG23	1:E:148:GLY:H	1.84	0.42
1:F:121:LEU:HD23	1:F:142:ILE:HG21	2.01	0.42
1:G:68:SER:OG	1:G:70:MET:SD	2.73	0.42
1:G:415:GLY:N	4:G:603:IMP:O6	2.40	0.42
1:F:394:THR:OG1	1:F:395:GLU:OE1	2.30	0.42
1:G:377:LEU:HA	1:G:381:ALA:HB3	2.00	0.42
1:B:448:GLN:NE2	1:E:405:GLY:O	2.50	0.42
1:C:329:SER:N	4:C:603:IMP:O3P	2.43	0.42
1:F:143:PRO:HB3	1:F:157:ILE:HG22	2.02	0.42
1:B:73:VAL:HG13	1:B:74:THR:HG23	2.02	0.42
1:B:91:ILE:H	1:B:91:ILE:HG13	1.74	0.42
1:A:338:ALA:HB1	1:D:375:LYS:HG3	2.00	0.42
1:C:71:ASP:HA	1:C:92:HIS:CD2	2.55	0.42
1:D:271:VAL:HG13	1:D:299:VAL:HG12	2.01	0.42
1:E:70:MET:HB2	1:E:73:VAL:HG12	2.01	0.42
1:E:368:GLN:HE22	1:H:505:SER:HB2	1.84	0.42
1:G:71:ASP:OD2	1:G:412:ARG:NH2	2.51	0.42
1:G:71:ASP:HA	1:G:92:HIS:CD2	2.55	0.42
1:A:32:TYR:OH	1:A:343:GLN:NE2	2.52	0.42
1:B:43:ASP:N	1:B:43:ASP:OD1	2.53	0.42
1:C:14:PRO:HD2	1:D:308:ALA:HA	2.02	0.42
2:E:602:GTP:H3'	2:E:602:GTP:O3B	2.20	0.42
1:F:97:PRO:HG3	1:F:259:ARG:HG2	2.02	0.42
1:C:167:LYS:HD3	1:C:167:LYS:HA	1.89	0.42
1:D:339:CYS:SG	1:D:340:GLY:N	2.93	0.42
1:E:448:GLN:H	1:E:448:GLN:HG2	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:SER:N	5:H:605:NAD:O1N	2.50	0.42
1:A:145:THR:OG1	1:A:153:ARG:O	2.26	0.41
1:E:305:VAL:H	1:E:309:GLN:NE2	2.11	0.41
1:H:449:ASP:OD1	1:H:450:LYS:N	2.53	0.41
1:C:199:GLU:HA	1:C:202:GLN:HG2	2.01	0.41
1:G:55:LEU:HB2	1:G:61:LEU:HD13	2.02	0.41
1:E:49:VAL:HG13	1:E:465:GLN:HG2	2.01	0.41
1:E:55:LEU:HD23	1:E:59:ILE:HD11	2.01	0.41
1:F:71:ASP:HA	1:F:92:HIS:CD2	2.55	0.41
1:F:112:GLN:HB2	1:F:115:ILE:HG22	2.02	0.41
1:F:161:ARG:HH12	3:F:603:ATP:PB	2.43	0.41
1:G:101:ALA:HA	1:G:104:VAL:HG12	2.02	0.41
1:B:37:ILE:HG23	1:B:488:LEU:HD21	2.02	0.41
1:C:161:ARG:HD3	3:C:601:ATP:H5'2	2.02	0.41
1:D:242:LYS:HD3	2:D:602:GTP:C5	2.55	0.41
1:E:202:GLN:HE21	1:E:227:LEU:HD13	1.85	0.41
1:E:210:PRO:HA	1:E:221:ILE:HA	2.02	0.41
1:G:51:LEU:H	1:G:51:LEU:HG	1.75	0.41
1:A:213:ASN:HD21	1:A:217:GLU:HB3	1.86	0.41
1:A:392:ALA:HB2	1:A:447:VAL:HG13	2.03	0.41
1:B:506:LEU:HD11	1:C:330:ILE:HG22	2.03	0.41
1:D:225:THR:HA	1:D:228:LYS:HD3	2.02	0.41
1:F:473:ALA:HB1	1:F:478:GLN:HB3	2.01	0.41
1:G:321:LEU:HB2	1:G:361:VAL:HG12	2.01	0.41
1:H:373:ILE:HG23	1:H:384:VAL:HG21	2.03	0.41
1:F:145:THR:HG23	1:F:148:GLY:H	1.86	0.41
1:B:126:ARG:HD2	1:B:128:ARG:HH22	1.85	0.41
1:B:333:THR:HG21	5:B:605:NAD:H4N	2.02	0.41
1:E:57:LYS:HA	1:J:2:ALA:HB3	2.02	0.41
1:F:417:LEU:HG	1:F:440:ALA:HB2	2.03	0.41
1:G:396:ALA:HB3	1:G:409:LYS:HE2	2.03	0.41
1:D:246:CYS:SG	1:D:247:GLY:N	2.93	0.41
1:E:492:LYS:HB2	1:E:492:LYS:HE3	1.87	0.41
1:F:511:LYS:HE2	1:F:511:LYS:HB3	1.93	0.41
1:G:482:MET:HB3	1:G:488:LEU:HB2	2.03	0.41
1:A:448:GLN:H	1:A:448:GLN:HG2	1.63	0.41
1:B:51:LEU:H	1:B:51:LEU:HG	1.61	0.41
1:D:55:LEU:HB2	1:D:61:LEU:HD13	2.03	0.41
1:D:412:ARG:HD2	1:D:418:ASP:HB3	2.02	0.41
1:E:43:ASP:HA	1:F:281:ILE:HG12	2.03	0.41
1:E:159:SER:OG	3:E:603:ATP:O2B	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:ASN:HB2	1:F:309:GLN:HG3	2.02	0.41
1:F:311:LYS:HE2	1:F:311:LYS:HB2	1.92	0.41
1:G:221:ILE:HD12	1:G:221:ILE:HA	1.95	0.41
1:H:66:VAL:HB	1:H:88:ILE:HG22	2.01	0.41
1:H:253:HIS:N	1:H:256:ASP:OD2	2.54	0.41
1:B:287:ILE:HA	1:B:290:ILE:HG12	2.03	0.41
1:C:187:VAL:HG11	1:C:212:VAL:HG22	2.02	0.41
1:C:200:ILE:HD12	1:C:203:ARG:HH11	1.86	0.41
1:C:453:ILE:HB	1:C:457:VAL:HG13	2.01	0.41
1:D:71:ASP:HA	1:D:92:HIS:CD2	2.55	0.41
1:D:329:SER:N	4:D:604:IMP:O2P	2.54	0.41
1:E:439:VAL:HG23	1:H:459:TYR:HE1	1.86	0.41
1:H:313:LEU:HD23	1:H:313:LEU:HA	1.92	0.41
1:H:250:ILE:HD13	1:H:260:LEU:HD12	2.03	0.40
1:H:392:ALA:HA	1:H:409:LYS:HD2	2.02	0.40
1:B:67:SER:HB3	1:B:82:MET:SD	2.61	0.40
1:D:275:SER:OG	1:D:302:GLY:O	2.37	0.40
1:E:207:GLY:HA2	1:E:224:ARG:HD2	2.04	0.40
1:F:272:VAL:HA	1:F:300:ILE:HB	2.02	0.40
1:F:73:VAL:O	1:F:78:MET:HG3	2.22	0.40
1:G:66:VAL:HG13	1:G:385:MET:HA	2.03	0.40
1:B:274:ASP:OD2	5:B:605:NAD:O3D	2.38	0.40
1:D:370:VAL:HG11	1:D:463:GLY:HA3	2.04	0.40
1:F:159:SER:OG	1:F:160:SER:N	2.52	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	484/519 (93%)	447 (92%)	37 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	484/519 (93%)	453 (94%)	31 (6%)	0	100	100
1	C	484/519 (93%)	454 (94%)	29 (6%)	1 (0%)	47	78
1	D	484/519 (93%)	451 (93%)	33 (7%)	0	100	100
1	E	484/519 (93%)	447 (92%)	37 (8%)	0	100	100
1	F	484/519 (93%)	450 (93%)	34 (7%)	0	100	100
1	G	484/519 (93%)	449 (93%)	35 (7%)	0	100	100
1	H	484/519 (93%)	453 (94%)	31 (6%)	0	100	100
1	I	12/519 (2%)	6 (50%)	6 (50%)	0	100	100
1	J	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	K	12/519 (2%)	9 (75%)	3 (25%)	0	100	100
1	L	12/519 (2%)	5 (42%)	7 (58%)	0	100	100
1	M	12/519 (2%)	6 (50%)	6 (50%)	0	100	100
1	N	12/519 (2%)	6 (50%)	6 (50%)	0	100	100
1	O	12/519 (2%)	7 (58%)	5 (42%)	0	100	100
1	P	12/519 (2%)	8 (67%)	4 (33%)	0	100	100
All	All	3968/8304 (48%)	3658 (92%)	309 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	110	TYR

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/425 (94%)	386 (97%)	12 (3%)	41	66
1	B	398/425 (94%)	385 (97%)	13 (3%)	38	64
1	C	398/425 (94%)	388 (98%)	10 (2%)	47	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	398/425 (94%)	386 (97%)	12 (3%)	41	66
1	E	398/425 (94%)	391 (98%)	7 (2%)	59	77
1	F	398/425 (94%)	388 (98%)	10 (2%)	47	69
1	G	398/425 (94%)	392 (98%)	6 (2%)	65	81
1	H	398/425 (94%)	389 (98%)	9 (2%)	50	71
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%)	10 (91%)	1 (9%)	9	37
1	M	11/425 (3%)	11 (100%)	0	100	100
1	N	11/425 (3%)	11 (100%)	0	100	100
1	O	11/425 (3%)	11 (100%)	0	100	100
1	P	11/425 (3%)	10 (91%)	1 (9%)	9	37
All	All	3272/6800 (48%)	3191 (98%)	81 (2%)	50	69

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	115	ILE
1	A	126	ARG
1	A	167	LYS
1	A	230	ASN
1	A	235	LEU
1	A	262	LEU
1	A	277	GLN
1	A	287	ILE
1	A	322	ARG
1	A	343	GLN
1	A	512	ARG
1	B	51	LEU
1	B	84	LEU
1	B	94	ASN
1	B	109	LYS
1	B	115	ILE
1	B	185	LEU
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	230	ASN
1	B	242	LYS
1	B	262	LEU
1	B	330	ILE
1	B	355	ARG
1	B	469	GLN
1	C	51	LEU
1	C	112	GLN
1	C	124	LYS
1	C	179	MET
1	C	235	LEU
1	C	260	LEU
1	C	287	ILE
1	C	312	ASN
1	C	377	LEU
1	C	438	LYS
1	D	51	LEU
1	D	66	VAL
1	D	126	ARG
1	D	178	ILE
1	D	179	MET
1	D	224	ARG
1	D	230	ASN
1	D	231	ARG
1	D	242	LYS
1	D	287	ILE
1	D	407	ARG
1	D	414	MET
1	E	136	ARG
1	E	230	ASN
1	E	262	LEU
1	E	277	GLN
1	E	287	ILE
1	E	343	GLN
1	E	438	LYS
1	F	94	ASN
1	F	115	ILE
1	F	128	ARG
1	F	136	ARG
1	F	161	ARG
1	F	178	ILE
1	F	185	LEU

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Mol	Chain	Res	Type
1	F	201	LEU
1	F	230	ASN
1	F	312	ASN
1	G	124	LYS
1	G	128	ARG
1	G	179	MET
1	G	287	ILE
1	G	312	ASN
1	G	377	LEU
1	H	51	LEU
1	H	126	ARG
1	H	149	ARG
1	H	178	ILE
1	H	230	ASN
1	H	231	ARG
1	H	287	ILE
1	H	322	ARG
1	H	414	MET
1	P	1	MET
1	L	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	202	GLN
1	A	230	ASN
1	A	343	GLN
1	A	498	GLN
1	B	94	ASN
1	B	112	GLN
1	B	230	ASN
1	B	277	GLN
1	B	309	GLN
1	B	498	GLN
1	C	48	GLN
1	C	100	GLN
1	C	112	GLN
1	C	230	ASN
1	C	283	GLN
1	C	303	ASN
1	C	309	GLN

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Mol	Chain	Res	Type
1	C	312	ASN
1	C	343	GLN
1	C	478	GLN
1	D	112	GLN
1	D	265	GLN
1	D	277	GLN
1	D	283	GLN
1	D	309	GLN
1	D	312	ASN
1	D	454	HIS
1	E	112	GLN
1	E	137	HIS
1	E	309	GLN
1	E	343	GLN
1	E	478	GLN
1	F	94	ASN
1	F	112	GLN
1	F	198	ASN
1	G	48	GLN
1	G	100	GLN
1	G	283	GLN
1	G	309	GLN
1	G	312	ASN
1	G	478	GLN
1	G	498	GLN
1	H	277	GLN
1	H	279	ASN
1	H	309	GLN
1	H	312	ASN
1	H	343	GLN
1	H	498	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

38 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GTP	D	601	-	26,34,34	3.95	15 (57%)	32,54,54	1.59	8 (25%)
5	NAD	D	605	-	42,48,48	3.51	16 (38%)	50,73,73	2.59	9 (18%)
2	GTP	F	601	-	26,34,34	3.90	15 (57%)	32,54,54	1.58	7 (21%)
2	GTP	E	601	-	26,34,34	3.90	15 (57%)	32,54,54	1.74	7 (21%)
2	GTP	B	601	-	26,34,34	3.89	15 (57%)	32,54,54	1.63	7 (21%)
4	IMP	A	604	-	21,25,25	2.53	6 (28%)	24,38,38	1.33	4 (16%)
3	ATP	F	603	-	26,33,33	3.39	12 (46%)	31,52,52	3.99	7 (22%)
3	ATP	G	601	-	26,33,33	3.32	12 (46%)	31,52,52	4.03	8 (25%)
5	NAD	B	605	-	42,48,48	3.50	16 (38%)	50,73,73	2.66	8 (16%)
2	GTP	E	602	-	26,34,34	3.92	15 (57%)	32,54,54	1.62	7 (21%)
2	GTP	B	602	-	26,34,34	3.90	15 (57%)	32,54,54	1.59	8 (25%)
5	NAD	C	604	-	42,48,48	3.48	16 (38%)	50,73,73	2.66	7 (14%)
3	ATP	C	601	-	26,33,33	3.34	12 (46%)	31,52,52	3.92	7 (22%)
4	IMP	G	603	-	21,25,25	2.54	7 (33%)	24,38,38	1.41	5 (20%)
4	IMP	B	604	-	21,25,25	2.58	7 (33%)	24,38,38	1.47	4 (16%)
4	IMP	C	603	-	21,25,25	2.58	7 (33%)	24,38,38	1.44	5 (20%)
4	IMP	E	604	-	21,25,25	2.52	7 (33%)	24,38,38	1.37	4 (16%)
2	GTP	H	602	-	26,34,34	3.96	15 (57%)	32,54,54	1.56	8 (25%)
5	NAD	G	604	-	42,48,48	3.49	16 (38%)	50,73,73	2.68	10 (20%)
2	GTP	H	601	-	26,34,34	3.99	15 (57%)	32,54,54	1.58	7 (21%)
2	GTP	D	602	-	26,34,34	3.98	15 (57%)	32,54,54	1.74	8 (25%)
3	ATP	B	603	-	26,33,33	3.40	12 (46%)	31,52,52	3.97	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	D	603	-	26,33,33	3.37	12 (46%)	31,52,52	3.88	6 (19%)
3	ATP	E	603	-	26,33,33	3.39	12 (46%)	31,52,52	3.97	7 (22%)
5	NAD	E	605	-	42,48,48	3.51	15 (35%)	50,73,73	2.61	9 (18%)
3	ATP	C	602	-	26,33,33	3.35	12 (46%)	31,52,52	3.92	7 (22%)
5	NAD	F	605	-	42,48,48	3.50	16 (38%)	50,73,73	2.67	9 (18%)
2	GTP	A	602	-	26,34,34	3.95	15 (57%)	32,54,54	1.76	8 (25%)
3	ATP	A	603	-	26,33,33	3.39	12 (46%)	31,52,52	4.02	7 (22%)
3	ATP	H	603	-	26,33,33	3.36	12 (46%)	31,52,52	3.93	7 (22%)
4	IMP	H	604	-	21,25,25	2.59	7 (33%)	24,38,38	1.40	4 (16%)
5	NAD	A	605	-	42,48,48	3.48	15 (35%)	50,73,73	2.58	8 (16%)
2	GTP	F	602	-	26,34,34	3.94	15 (57%)	32,54,54	1.61	9 (28%)
4	IMP	F	604	-	21,25,25	2.59	6 (28%)	24,38,38	1.40	5 (20%)
4	IMP	D	604	-	21,25,25	2.62	7 (33%)	24,38,38	1.34	4 (16%)
3	ATP	G	602	-	26,33,33	3.37	12 (46%)	31,52,52	3.90	7 (22%)
5	NAD	H	605	-	42,48,48	3.51	16 (38%)	50,73,73	2.58	8 (16%)
2	GTP	A	601	-	26,34,34	3.88	15 (57%)	32,54,54	1.75	8 (25%)

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
2	GTP	D	601	-	-	5/18/38/38	0/3/3/3
5	NAD	D	605	-	-	9/26/62/62	0/5/5/5
2	GTP	F	601	-	-	5/18/38/38	0/3/3/3
2	GTP	E	601	-	-	7/18/38/38	0/3/3/3
2	GTP	B	601	-	-	5/18/38/38	0/3/3/3
4	IMP	A	604	-	-	1/6/26/26	0/3/3/3
3	ATP	F	603	-	-	2/18/38/38	0/3/3/3
3	ATP	G	601	-	-	5/18/38/38	0/3/3/3
5	NAD	B	605	-	-	15/26/62/62	0/5/5/5
2	GTP	E	602	-	-	9/18/38/38	0/3/3/3
2	GTP	B	602	-	-	2/18/38/38	0/3/3/3
5	NAD	C	604	-	-	8/26/62/62	0/5/5/5
3	ATP	C	601	-	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMP	G	603	-	-	5/6/26/26	0/3/3/3
4	IMP	B	604	-	-	2/6/26/26	0/3/3/3
4	IMP	C	603	-	-	5/6/26/26	0/3/3/3
4	IMP	E	604	-	-	5/6/26/26	0/3/3/3
2	GTP	H	602	-	-	3/18/38/38	0/3/3/3
5	NAD	G	604	-	-	7/26/62/62	0/5/5/5
2	GTP	H	601	-	-	5/18/38/38	0/3/3/3
2	GTP	D	602	-	-	6/18/38/38	0/3/3/3
3	ATP	B	603	-	-	6/18/38/38	0/3/3/3
3	ATP	D	603	-	-	10/18/38/38	0/3/3/3
3	ATP	E	603	-	-	5/18/38/38	0/3/3/3
5	NAD	E	605	-	-	11/26/62/62	0/5/5/5
3	ATP	C	602	-	-	4/18/38/38	0/3/3/3
5	NAD	F	605	-	-	8/26/62/62	0/5/5/5
2	GTP	A	602	-	-	4/18/38/38	0/3/3/3
3	ATP	A	603	-	-	5/18/38/38	0/3/3/3
3	ATP	H	603	-	-	0/18/38/38	0/3/3/3
4	IMP	H	604	-	-	0/6/26/26	0/3/3/3
5	NAD	A	605	-	-	4/26/62/62	0/5/5/5
2	GTP	F	602	-	-	2/18/38/38	0/3/3/3
4	IMP	F	604	-	-	3/6/26/26	0/3/3/3
4	IMP	D	604	-	-	0/6/26/26	0/3/3/3
3	ATP	G	602	-	-	7/18/38/38	0/3/3/3
5	NAD	H	605	-	-	10/26/62/62	0/5/5/5
2	GTP	A	601	-	-	6/18/38/38	0/3/3/3

All (480) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GTP	C2'-C3'	-10.93	1.23	1.53
2	F	601	GTP	C2'-C3'	-10.85	1.23	1.53
2	E	601	GTP	C2'-C3'	-10.84	1.23	1.53
2	A	601	GTP	C2'-C3'	-10.81	1.23	1.53
2	F	602	GTP	C2'-C3'	-10.80	1.23	1.53
2	H	601	GTP	C2'-C3'	-10.68	1.24	1.53
2	D	601	GTP	C2'-C3'	-10.68	1.24	1.53
2	E	602	GTP	C2'-C3'	-10.56	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	603	ATP	C2'-C3'	-10.56	1.24	1.53
2	B	602	GTP	C2'-C3'	-10.52	1.24	1.53
3	E	603	ATP	C2'-C3'	-10.49	1.24	1.53
2	A	602	GTP	C2'-C3'	-10.48	1.24	1.53
2	H	602	GTP	C2'-C3'	-10.48	1.24	1.53
2	D	602	GTP	C2'-C3'	-10.44	1.24	1.53
3	B	603	ATP	C2'-C3'	-10.44	1.24	1.53
3	A	603	ATP	C2'-C3'	-10.36	1.25	1.53
3	D	603	ATP	C2'-C3'	-10.26	1.25	1.53
3	C	601	ATP	C2'-C3'	-10.24	1.25	1.53
3	C	602	ATP	C2'-C3'	-10.18	1.25	1.53
3	H	603	ATP	C2'-C3'	-10.12	1.25	1.53
3	G	602	ATP	C2'-C3'	-10.02	1.25	1.53
3	G	601	ATP	C2'-C3'	-9.96	1.26	1.53
5	A	605	NAD	C3B-C4B	-9.02	1.29	1.53
4	H	604	IMP	C2-N3	8.96	1.46	1.29
5	A	605	NAD	C3D-C4D	-8.96	1.30	1.53
5	D	605	NAD	C3D-C4D	-8.95	1.30	1.53
5	E	605	NAD	C3B-C4B	-8.95	1.30	1.53
5	F	605	NAD	C3B-C4B	-8.93	1.30	1.53
4	D	604	IMP	C2-N3	8.92	1.46	1.29
5	B	605	NAD	C3B-C4B	-8.90	1.30	1.53
5	F	605	NAD	C3D-C4D	-8.90	1.30	1.53
5	H	605	NAD	C3D-C4D	-8.87	1.30	1.53
4	F	604	IMP	C2-N3	8.85	1.45	1.29
5	C	604	NAD	C3B-C4B	-8.85	1.30	1.53
5	E	605	NAD	C3D-C4D	-8.81	1.30	1.53
5	D	605	NAD	C3B-C4B	-8.80	1.30	1.53
5	G	604	NAD	C3D-C4D	-8.77	1.30	1.53
5	H	605	NAD	C3B-C4B	-8.76	1.30	1.53
4	C	603	IMP	C2-N3	8.75	1.45	1.29
5	B	605	NAD	C3D-C4D	-8.71	1.30	1.53
4	A	604	IMP	C2-N3	8.62	1.45	1.29
5	G	604	NAD	C3B-C4B	-8.62	1.31	1.53
5	C	604	NAD	C3D-C4D	-8.60	1.31	1.53
4	B	604	IMP	C2-N3	8.59	1.45	1.29
4	E	604	IMP	C2-N3	8.57	1.45	1.29
4	G	603	IMP	C2-N3	8.38	1.45	1.29
3	H	603	ATP	C2'-C1'	8.23	1.66	1.53
3	B	603	ATP	C2'-C1'	8.18	1.66	1.53
3	C	602	ATP	C2'-C1'	8.17	1.66	1.53
3	G	602	ATP	C2'-C1'	8.12	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	601	ATP	C2'-C1'	8.08	1.66	1.53
3	A	603	ATP	C2'-C1'	8.04	1.66	1.53
5	E	605	NAD	O4D-C1D	-8.00	1.29	1.41
3	C	601	ATP	C2'-C1'	7.96	1.65	1.53
3	D	603	ATP	C2'-C1'	7.94	1.65	1.53
5	D	605	NAD	O4B-C1B	-7.86	1.30	1.41
3	E	603	ATP	C2'-C1'	7.84	1.65	1.53
5	G	604	NAD	O4D-C1D	-7.83	1.30	1.41
5	B	605	NAD	O4D-C1D	-7.82	1.30	1.41
5	H	605	NAD	O4D-C1D	-7.79	1.30	1.41
5	F	605	NAD	O4D-C1D	-7.75	1.30	1.41
5	H	605	NAD	O4B-C1B	-7.74	1.30	1.41
3	F	603	ATP	C2'-C1'	7.70	1.65	1.53
5	G	604	NAD	O4B-C4B	7.67	1.62	1.45
5	C	604	NAD	O4B-C4B	7.66	1.62	1.45
5	A	605	NAD	O4D-C1D	-7.65	1.30	1.41
5	C	604	NAD	O4D-C1D	-7.60	1.30	1.41
5	B	605	NAD	O4B-C4B	7.53	1.61	1.45
5	G	604	NAD	O4B-C1B	-7.51	1.30	1.41
5	H	605	NAD	O4B-C4B	7.48	1.61	1.45
2	E	602	GTP	O4'-C1'	7.47	1.51	1.41
5	D	605	NAD	O4D-C1D	-7.45	1.30	1.41
5	D	605	NAD	O4D-C4D	7.42	1.61	1.45
5	D	605	NAD	O4B-C4B	7.42	1.61	1.45
5	E	605	NAD	O4B-C4B	7.39	1.61	1.45
5	F	605	NAD	O4B-C4B	7.39	1.61	1.45
5	E	605	NAD	O4D-C4D	7.39	1.61	1.45
5	B	605	NAD	O4D-C4D	7.37	1.61	1.45
5	C	604	NAD	O4B-C1B	-7.36	1.30	1.41
5	C	604	NAD	O4D-C4D	7.36	1.61	1.45
5	F	605	NAD	O4D-C4D	7.32	1.61	1.45
5	A	605	NAD	O4B-C4B	7.31	1.61	1.45
5	B	605	NAD	O4B-C1B	-7.27	1.30	1.41
5	E	605	NAD	O4B-C1B	-7.27	1.30	1.41
5	H	605	NAD	O4D-C4D	7.27	1.61	1.45
5	F	605	NAD	O4B-C1B	-7.25	1.31	1.41
5	G	604	NAD	O4D-C4D	7.25	1.61	1.45
5	A	605	NAD	O4D-C4D	7.25	1.61	1.45
5	A	605	NAD	O4B-C1B	-7.22	1.31	1.41
2	H	602	GTP	O4'-C1'	7.15	1.51	1.41
2	D	602	GTP	O4'-C1'	7.07	1.51	1.41
2	H	601	GTP	O4'-C1'	7.04	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	602	GTP	O4'-C1'	7.02	1.50	1.41
2	A	602	GTP	O4'-C1'	7.01	1.50	1.41
2	E	601	GTP	O4'-C1'	6.87	1.50	1.41
2	B	602	GTP	O4'-C4'	-6.86	1.29	1.45
2	B	601	GTP	O4'-C1'	6.83	1.50	1.41
2	D	601	GTP	O4'-C1'	6.79	1.50	1.41
2	F	601	GTP	O4'-C1'	6.71	1.50	1.41
5	F	605	NAD	C7N-N7N	6.65	1.45	1.33
2	F	601	GTP	O4'-C4'	-6.65	1.30	1.45
3	B	603	ATP	O4'-C1'	-6.64	1.31	1.41
2	B	601	GTP	O4'-C4'	-6.64	1.30	1.45
5	H	605	NAD	C7N-N7N	6.61	1.45	1.33
2	B	602	GTP	O4'-C1'	6.60	1.50	1.41
2	A	601	GTP	O4'-C1'	6.60	1.50	1.41
5	D	605	NAD	C7N-N7N	6.60	1.45	1.33
2	H	601	GTP	O4'-C4'	-6.59	1.30	1.45
5	C	604	NAD	C7N-N7N	6.58	1.45	1.33
2	E	601	GTP	O4'-C4'	-6.58	1.30	1.45
3	G	602	ATP	O4'-C1'	-6.57	1.31	1.41
5	B	605	NAD	C7N-N7N	6.57	1.45	1.33
5	G	604	NAD	C7N-N7N	6.56	1.45	1.33
5	E	605	NAD	C7N-N7N	6.55	1.45	1.33
2	A	601	GTP	O4'-C4'	-6.54	1.30	1.45
3	A	603	ATP	O4'-C1'	-6.53	1.32	1.41
5	A	605	NAD	C7N-N7N	6.52	1.45	1.33
3	E	603	ATP	O4'-C1'	-6.49	1.32	1.41
2	D	601	GTP	O4'-C4'	-6.46	1.30	1.45
2	H	602	GTP	O4'-C4'	-6.45	1.30	1.45
2	A	602	GTP	O4'-C4'	-6.45	1.30	1.45
2	E	602	GTP	O4'-C4'	-6.45	1.30	1.45
3	F	603	ATP	O4'-C1'	-6.43	1.32	1.41
3	D	603	ATP	O4'-C1'	-6.37	1.32	1.41
2	D	602	GTP	O4'-C4'	-6.36	1.30	1.45
2	F	602	GTP	O4'-C4'	-6.29	1.30	1.45
3	G	601	ATP	O4'-C1'	-6.24	1.32	1.41
3	C	601	ATP	O4'-C1'	-6.18	1.32	1.41
3	H	603	ATP	O4'-C1'	-6.15	1.32	1.41
3	C	602	ATP	O4'-C1'	-6.06	1.32	1.41
2	A	602	GTP	C2-N3	5.82	1.47	1.33
2	D	602	GTP	C2-N3	5.75	1.47	1.33
2	D	601	GTP	C3'-C4'	5.65	1.67	1.53
2	H	602	GTP	C2-N3	5.59	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	GTP	C2-N3	5.58	1.46	1.33
2	D	601	GTP	C2-N3	5.56	1.46	1.33
2	F	602	GTP	C2-N3	5.55	1.46	1.33
2	F	601	GTP	C2-N3	5.51	1.46	1.33
2	A	602	GTP	C2'-C1'	5.51	1.62	1.53
2	D	602	GTP	C3'-C4'	5.50	1.67	1.53
2	B	601	GTP	C2-N3	5.46	1.46	1.33
2	F	602	GTP	C3'-C4'	5.45	1.66	1.53
2	B	602	GTP	C2-N3	5.44	1.46	1.33
2	A	601	GTP	C2-N3	5.42	1.46	1.33
2	A	602	GTP	C3'-C4'	5.41	1.66	1.53
2	H	602	GTP	C3'-C4'	5.41	1.66	1.53
2	A	601	GTP	C3'-C4'	5.40	1.66	1.53
2	D	602	GTP	C2'-C1'	5.40	1.62	1.53
2	H	601	GTP	C3'-C4'	5.38	1.66	1.53
2	E	601	GTP	C2-N3	5.37	1.46	1.33
2	E	602	GTP	C3'-C4'	5.32	1.66	1.53
2	H	601	GTP	C2-N2	5.28	1.46	1.34
2	E	602	GTP	C2-N3	5.26	1.46	1.33
2	H	602	GTP	C2'-C1'	5.25	1.61	1.53
2	E	601	GTP	C3'-C4'	5.19	1.66	1.53
2	D	601	GTP	C2-N2	5.18	1.46	1.34
2	B	602	GTP	C3'-C4'	5.18	1.66	1.53
2	H	602	GTP	C2-N2	5.17	1.46	1.34
2	D	602	GTP	C2-N2	5.15	1.46	1.34
2	D	601	GTP	C4-N3	5.12	1.49	1.37
2	D	602	GTP	C4-N3	5.12	1.49	1.37
2	F	602	GTP	C2-N2	5.08	1.46	1.34
2	H	602	GTP	C4-N3	5.08	1.49	1.37
2	B	601	GTP	C3'-C4'	5.08	1.66	1.53
2	B	602	GTP	C2-N2	5.07	1.46	1.34
2	F	601	GTP	C2-N2	5.06	1.46	1.34
2	E	601	GTP	C2-N2	5.06	1.46	1.34
2	A	602	GTP	C2-N2	5.03	1.46	1.34
2	F	601	GTP	C3'-C4'	5.02	1.65	1.53
2	H	601	GTP	C4-N3	5.02	1.49	1.37
2	B	601	GTP	C2-N2	5.02	1.46	1.34
2	A	602	GTP	C4-N3	5.01	1.49	1.37
2	A	601	GTP	C2-N2	5.00	1.46	1.34
2	B	602	GTP	C2'-C1'	4.94	1.61	1.53
2	H	601	GTP	C2'-C1'	4.88	1.61	1.53
2	F	602	GTP	C4-N3	4.86	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	GTP	C4-N3	4.86	1.49	1.37
2	A	601	GTP	C4-N3	4.85	1.49	1.37
2	E	602	GTP	C2-N2	4.81	1.45	1.34
2	F	601	GTP	C4-N3	4.80	1.49	1.37
2	E	601	GTP	C4-N3	4.78	1.49	1.37
2	F	602	GTP	C2'-C1'	4.77	1.61	1.53
2	E	602	GTP	C2'-C1'	4.77	1.61	1.53
2	E	602	GTP	C4-N3	4.76	1.48	1.37
2	B	601	GTP	C4-N3	4.67	1.48	1.37
4	D	604	IMP	C2-N1	4.64	1.43	1.35
2	F	601	GTP	C2'-C1'	4.60	1.60	1.53
4	G	603	IMP	C2-N1	4.58	1.43	1.35
4	B	604	IMP	C2-N1	4.57	1.43	1.35
4	C	603	IMP	C2-N1	4.52	1.43	1.35
2	B	601	GTP	C2'-C1'	4.47	1.60	1.53
2	E	601	GTP	C2'-C1'	4.41	1.60	1.53
4	F	604	IMP	C2-N1	4.39	1.43	1.35
2	D	601	GTP	C2'-C1'	4.38	1.60	1.53
4	E	604	IMP	C2-N1	4.29	1.43	1.35
4	A	604	IMP	C2-N1	4.26	1.43	1.35
4	H	604	IMP	C2-N1	4.17	1.43	1.35
2	A	601	GTP	C2'-C1'	4.12	1.60	1.53
2	D	601	GTP	C6-N1	3.99	1.43	1.37
2	H	601	GTP	C6-N1	3.89	1.43	1.37
3	F	603	ATP	C5'-C4'	-3.70	1.40	1.51
3	E	603	ATP	C5'-C4'	-3.65	1.40	1.51
2	D	602	GTP	C6-N1	3.57	1.43	1.37
4	C	603	IMP	C4-N3	3.57	1.48	1.37
4	D	604	IMP	C4-N3	3.57	1.48	1.37
2	D	602	GTP	O2'-C2'	3.57	1.51	1.43
2	H	602	GTP	O2'-C2'	3.56	1.51	1.43
2	F	601	GTP	C6-N1	3.56	1.43	1.37
3	A	603	ATP	C5'-C4'	-3.56	1.40	1.51
2	E	602	GTP	C6-N1	3.55	1.43	1.37
2	E	601	GTP	C6-N1	3.55	1.43	1.37
4	H	604	IMP	C4-N3	3.53	1.48	1.37
2	H	601	GTP	O2'-C2'	3.53	1.51	1.43
4	F	604	IMP	C4-N3	3.52	1.48	1.37
3	B	603	ATP	C5'-C4'	-3.51	1.40	1.51
2	A	601	GTP	C6-N1	3.51	1.43	1.37
2	F	602	GTP	C6-N1	3.49	1.43	1.37
2	D	601	GTP	O2'-C2'	3.49	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	603	ATP	C5'-C4'	-3.49	1.40	1.51
2	B	602	GTP	C6-N1	3.49	1.43	1.37
2	A	602	GTP	O2'-C2'	3.46	1.51	1.43
2	B	601	GTP	C6-N1	3.45	1.43	1.37
2	A	601	GTP	O2'-C2'	3.44	1.51	1.43
2	F	602	GTP	O2'-C2'	3.44	1.51	1.43
2	H	602	GTP	C6-N1	3.44	1.43	1.37
2	E	602	GTP	O2'-C2'	3.43	1.51	1.43
4	B	604	IMP	C5-C4	-3.43	1.34	1.43
3	G	602	ATP	C5'-C4'	-3.43	1.40	1.51
2	B	602	GTP	O2'-C2'	3.40	1.51	1.43
4	B	604	IMP	C4-N3	3.39	1.48	1.37
3	C	602	ATP	C5'-C4'	-3.39	1.41	1.51
4	A	604	IMP	C4-N3	3.39	1.48	1.37
3	C	601	ATP	C5'-C4'	-3.36	1.41	1.51
2	E	601	GTP	O2'-C2'	3.35	1.50	1.43
2	F	601	GTP	O2'-C2'	3.35	1.50	1.43
3	D	603	ATP	C5'-C4'	-3.34	1.41	1.51
4	E	604	IMP	C4-N3	3.34	1.47	1.37
3	G	602	ATP	O3'-C3'	3.32	1.50	1.43
3	C	602	ATP	O3'-C3'	3.32	1.50	1.43
3	D	603	ATP	O3'-C3'	3.31	1.50	1.43
4	G	603	IMP	C4-N3	3.31	1.47	1.37
4	G	603	IMP	C5-C4	-3.31	1.34	1.43
3	H	603	ATP	O3'-C3'	3.28	1.50	1.43
3	C	601	ATP	O3'-C3'	3.27	1.50	1.43
2	D	602	GTP	C5-C6	3.25	1.54	1.47
4	F	604	IMP	C5-C4	-3.24	1.34	1.43
3	G	602	ATP	C3'-C4'	3.24	1.61	1.53
3	D	603	ATP	C3'-C4'	3.24	1.61	1.53
2	H	601	GTP	C5-C6	3.24	1.54	1.47
3	G	601	ATP	C5'-C4'	-3.23	1.41	1.51
4	E	604	IMP	C5-C4	-3.22	1.34	1.43
2	B	601	GTP	O2'-C2'	3.21	1.50	1.43
3	G	601	ATP	O3'-C3'	3.21	1.50	1.43
3	F	603	ATP	O3'-C3'	3.20	1.50	1.43
3	A	603	ATP	O3'-C3'	3.20	1.50	1.43
3	C	601	ATP	C3'-C4'	3.20	1.61	1.53
3	G	601	ATP	C3'-C4'	3.18	1.61	1.53
3	E	603	ATP	O3'-C3'	3.18	1.50	1.43
5	D	605	NAD	O2D-C2D	-3.17	1.35	1.43
4	A	604	IMP	C5-C4	-3.17	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	ATP	O3'-C3'	3.16	1.50	1.43
5	E	605	NAD	O2D-C2D	-3.13	1.35	1.43
5	D	605	NAD	O2B-C2B	-3.13	1.35	1.43
5	B	605	NAD	O7N-C7N	-3.12	1.18	1.24
3	H	603	ATP	C3'-C4'	3.12	1.61	1.53
5	H	605	NAD	O2B-C2B	-3.10	1.35	1.43
5	F	605	NAD	O7N-C7N	-3.10	1.18	1.24
3	C	602	ATP	C3'-C4'	3.09	1.60	1.53
4	C	603	IMP	C5-C4	-3.09	1.35	1.43
5	G	604	NAD	O2D-C2D	-3.09	1.35	1.43
5	H	605	NAD	O2D-C2D	-3.07	1.35	1.43
5	E	605	NAD	O7N-C7N	-3.07	1.18	1.24
5	A	605	NAD	O2B-C2B	-3.07	1.35	1.43
5	E	605	NAD	O2B-C2B	-3.06	1.35	1.43
5	B	605	NAD	O2D-C2D	-3.05	1.35	1.43
5	A	605	NAD	O2D-C2D	-3.05	1.35	1.43
5	F	605	NAD	O2D-C2D	-3.05	1.35	1.43
5	B	605	NAD	O2B-C2B	-3.05	1.35	1.43
5	C	604	NAD	O2D-C2D	-3.05	1.35	1.43
5	E	605	NAD	C6A-N6A	3.03	1.45	1.34
5	A	605	NAD	O7N-C7N	-3.01	1.18	1.24
4	H	604	IMP	C5-C4	-3.01	1.35	1.43
5	G	604	NAD	C6A-N6A	3.01	1.45	1.34
2	A	602	GTP	C5-C6	3.01	1.53	1.47
5	F	605	NAD	C6A-N6A	3.00	1.45	1.34
5	A	605	NAD	C6A-N6A	3.00	1.45	1.34
2	D	601	GTP	C5-C6	3.00	1.53	1.47
5	H	605	NAD	C6A-N6A	3.00	1.45	1.34
5	C	604	NAD	O2B-C2B	-3.00	1.35	1.43
5	D	605	NAD	C6A-N6A	2.99	1.45	1.34
2	E	602	GTP	C5-C6	2.99	1.53	1.47
2	H	602	GTP	C5-C6	2.99	1.53	1.47
3	D	603	ATP	PA-O5'	2.99	1.71	1.59
5	F	605	NAD	O2B-C2B	-2.99	1.35	1.43
5	C	604	NAD	C6A-N6A	2.98	1.44	1.34
5	B	605	NAD	C6A-N6A	2.97	1.44	1.34
3	F	603	ATP	C5-C4	-2.97	1.33	1.40
5	H	605	NAD	O7N-C7N	-2.97	1.18	1.24
3	G	601	ATP	PA-O5'	2.96	1.71	1.59
5	G	604	NAD	O7N-C7N	-2.96	1.18	1.24
4	D	604	IMP	C5-C4	-2.95	1.35	1.43
3	E	603	ATP	C3'-C4'	2.95	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	ATP	PA-O5'	2.95	1.71	1.59
5	G	604	NAD	O2B-C2B	-2.95	1.36	1.43
3	G	602	ATP	PA-O5'	2.94	1.71	1.59
3	H	603	ATP	PA-O5'	2.93	1.71	1.59
3	C	601	ATP	PA-O5'	2.91	1.71	1.59
3	A	603	ATP	PA-O5'	2.90	1.71	1.59
2	E	602	GTP	C5-C4	-2.90	1.35	1.43
2	H	601	GTP	C2-N1	2.89	1.44	1.37
3	F	603	ATP	PA-O5'	2.89	1.71	1.59
5	C	604	NAD	O7N-C7N	-2.88	1.18	1.24
3	E	603	ATP	C5-C4	-2.88	1.33	1.40
5	B	605	NAD	C5A-C4A	-2.87	1.33	1.40
2	A	602	GTP	C6-N1	2.87	1.42	1.37
5	D	605	NAD	O7N-C7N	-2.86	1.18	1.24
2	F	602	GTP	C5-C6	2.86	1.53	1.47
3	F	603	ATP	C3'-C4'	2.85	1.60	1.53
3	G	601	ATP	C5-C4	-2.85	1.33	1.40
5	E	605	NAD	C5A-C4A	-2.85	1.33	1.40
3	A	603	ATP	C5-C4	-2.85	1.33	1.40
5	F	605	NAD	C5A-C4A	-2.85	1.33	1.40
2	A	601	GTP	C5-C6	2.84	1.53	1.47
2	D	601	GTP	C2-N1	2.84	1.44	1.37
3	B	603	ATP	C5-C4	-2.84	1.33	1.40
2	E	601	GTP	C5-C6	2.84	1.53	1.47
5	G	604	NAD	O3B-C3B	2.84	1.49	1.43
5	F	605	NAD	O3B-C3B	2.83	1.49	1.43
5	B	605	NAD	O3B-C3B	2.83	1.49	1.43
3	C	602	ATP	O4'-C4'	2.83	1.51	1.45
5	C	604	NAD	C5A-C4A	-2.83	1.33	1.40
5	D	605	NAD	C5A-C4A	-2.82	1.33	1.40
2	B	601	GTP	C5-C6	2.82	1.53	1.47
2	E	601	GTP	C5-C4	-2.82	1.35	1.43
5	G	604	NAD	C5A-C4A	-2.82	1.33	1.40
5	A	605	NAD	C5A-C4A	-2.82	1.33	1.40
2	A	602	GTP	C5-C4	-2.81	1.35	1.43
5	D	605	NAD	O3B-C3B	2.81	1.49	1.43
5	G	604	NAD	O3D-C3D	2.81	1.49	1.43
5	C	604	NAD	O3B-C3B	2.80	1.49	1.43
2	B	602	GTP	C5-C6	2.80	1.53	1.47
5	H	605	NAD	O3B-C3B	2.80	1.49	1.43
3	C	601	ATP	O4'-C4'	2.80	1.51	1.45
3	D	603	ATP	O4'-C4'	2.80	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	605	NAD	O3B-C3B	2.80	1.49	1.43
3	B	603	ATP	C3'-C4'	2.80	1.60	1.53
5	C	604	NAD	O3D-C3D	2.79	1.49	1.43
3	A	603	ATP	C3'-C4'	2.79	1.60	1.53
5	H	605	NAD	C5A-C4A	-2.79	1.33	1.40
3	E	603	ATP	PA-O5'	2.79	1.70	1.59
5	A	605	NAD	O3B-C3B	2.79	1.49	1.43
3	H	603	ATP	O4'-C4'	2.79	1.51	1.45
2	F	601	GTP	C5-C6	2.78	1.53	1.47
2	B	602	GTP	C5-C4	-2.78	1.36	1.43
3	D	603	ATP	C5-C4	-2.76	1.33	1.40
2	F	602	GTP	C5-C4	-2.76	1.36	1.43
5	B	605	NAD	O3D-C3D	2.75	1.49	1.43
3	G	602	ATP	O4'-C4'	2.75	1.51	1.45
5	D	605	NAD	O3D-C3D	2.75	1.49	1.43
3	C	601	ATP	C5-C4	-2.75	1.33	1.40
4	H	604	IMP	O6-C6	-2.74	1.17	1.23
3	B	603	ATP	PA-O5'	2.74	1.70	1.59
3	H	603	ATP	C6-N6	2.74	1.44	1.34
5	E	605	NAD	O3D-C3D	2.74	1.49	1.43
3	D	603	ATP	C6-N6	2.73	1.44	1.34
5	H	605	NAD	O3D-C3D	2.72	1.49	1.43
3	H	603	ATP	C5-C4	-2.72	1.33	1.40
3	G	602	ATP	C5-C4	-2.71	1.33	1.40
3	B	603	ATP	O4'-C4'	2.71	1.51	1.45
2	A	601	GTP	C5-C4	-2.71	1.36	1.43
2	D	602	GTP	C2-N1	2.71	1.44	1.37
3	C	601	ATP	C6-N6	2.70	1.43	1.34
3	G	601	ATP	O4'-C4'	2.70	1.51	1.45
5	A	605	NAD	O3D-C3D	2.70	1.49	1.43
5	F	605	NAD	O3D-C3D	2.70	1.49	1.43
3	C	602	ATP	C6-N6	2.70	1.43	1.34
4	A	604	IMP	O6-C6	-2.69	1.17	1.23
2	F	601	GTP	C5-C4	-2.69	1.36	1.43
3	C	602	ATP	C5-C4	-2.68	1.33	1.40
3	G	602	ATP	C6-N6	2.68	1.43	1.34
4	E	604	IMP	O6-C6	-2.68	1.17	1.23
3	G	601	ATP	C6-N6	2.67	1.43	1.34
3	A	603	ATP	O4'-C4'	2.65	1.50	1.45
3	E	603	ATP	C6-N6	2.65	1.43	1.34
2	A	601	GTP	C2-N1	2.64	1.44	1.37
2	F	602	GTP	C2-N1	2.64	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	IMP	O6-C6	-2.64	1.17	1.23
3	B	603	ATP	C6-N6	2.64	1.43	1.34
3	F	603	ATP	C6-N6	2.63	1.43	1.34
3	E	603	ATP	O4'-C4'	2.63	1.50	1.45
3	A	603	ATP	C6-N6	2.63	1.43	1.34
2	H	602	GTP	C2-N1	2.62	1.44	1.37
4	F	604	IMP	O6-C6	-2.62	1.18	1.23
2	F	601	GTP	C2-N1	2.62	1.44	1.37
2	B	601	GTP	C5-C4	-2.61	1.36	1.43
2	B	601	GTP	C2-N1	2.61	1.44	1.37
2	E	602	GTP	C2-N1	2.59	1.44	1.37
2	B	602	GTP	C2-N1	2.59	1.44	1.37
2	E	601	GTP	C2-N1	2.57	1.44	1.37
3	F	603	ATP	O4'-C4'	2.56	1.50	1.45
4	G	603	IMP	O6-C6	-2.54	1.18	1.23
3	C	602	ATP	O2'-C2'	2.54	1.49	1.43
3	G	601	ATP	O2'-C2'	2.52	1.48	1.43
4	C	603	IMP	O6-C6	-2.51	1.18	1.23
2	D	602	GTP	O3'-C3'	2.50	1.48	1.43
3	G	602	ATP	O2'-C2'	2.50	1.48	1.43
3	D	603	ATP	O2'-C2'	2.50	1.48	1.43
2	D	601	GTP	O3'-C3'	2.49	1.48	1.43
3	H	603	ATP	O2'-C2'	2.48	1.48	1.43
4	G	603	IMP	C6-N1	2.48	1.43	1.38
2	A	602	GTP	C2-N1	2.46	1.43	1.37
2	A	602	GTP	O3'-C3'	2.45	1.48	1.43
3	A	603	ATP	O2'-C2'	2.45	1.48	1.43
4	D	604	IMP	O6-C6	-2.44	1.18	1.23
2	H	601	GTP	O3'-C3'	2.44	1.48	1.43
2	D	602	GTP	C5-C4	-2.44	1.36	1.43
2	H	602	GTP	O3'-C3'	2.44	1.48	1.43
2	H	602	GTP	C5-C4	-2.43	1.36	1.43
2	D	601	GTP	C5-C4	-2.42	1.36	1.43
2	H	601	GTP	C5-C4	-2.42	1.36	1.43
4	D	604	IMP	C6-N1	2.41	1.42	1.38
3	F	603	ATP	O2'-C2'	2.40	1.48	1.43
3	C	601	ATP	O2'-C2'	2.40	1.48	1.43
5	B	605	NAD	C4N-C3N	-2.38	1.35	1.39
2	B	602	GTP	O3'-C3'	2.38	1.48	1.43
2	F	602	GTP	O3'-C3'	2.38	1.48	1.43
2	E	602	GTP	O6-C6	-2.37	1.18	1.23
2	E	602	GTP	O3'-C3'	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	GTP	O6-C6	-2.37	1.18	1.23
5	H	605	NAD	C4N-C3N	-2.37	1.35	1.39
3	E	603	ATP	O2'-C2'	2.35	1.48	1.43
4	G	603	IMP	C5-C6	2.35	1.52	1.47
2	A	601	GTP	O3'-C3'	2.34	1.48	1.43
4	D	604	IMP	C5-C6	2.33	1.52	1.47
4	H	604	IMP	C5-C6	2.33	1.52	1.47
2	F	601	GTP	O6-C6	-2.31	1.18	1.23
2	F	602	GTP	O6-C6	-2.31	1.18	1.23
2	A	602	GTP	O6-C6	-2.31	1.18	1.23
3	C	602	ATP	C2-N3	2.31	1.35	1.32
5	D	605	NAD	C4N-C3N	-2.30	1.35	1.39
4	C	603	IMP	C6-N1	2.29	1.42	1.38
3	G	602	ATP	C2-N3	2.29	1.35	1.32
4	B	604	IMP	C6-N1	2.28	1.42	1.38
2	B	601	GTP	O3'-C3'	2.27	1.48	1.43
2	A	601	GTP	O6-C6	-2.27	1.18	1.23
5	F	605	NAD	C4N-C3N	-2.26	1.35	1.39
2	F	601	GTP	O3'-C3'	2.26	1.48	1.43
5	A	605	NAD	C4N-C3N	-2.25	1.35	1.39
5	E	605	NAD	C4N-C3N	-2.24	1.35	1.39
2	E	601	GTP	O3'-C3'	2.23	1.48	1.43
2	B	601	GTP	O6-C6	-2.22	1.18	1.23
5	G	604	NAD	C4N-C3N	-2.21	1.35	1.39
2	B	602	GTP	O6-C6	-2.21	1.18	1.23
3	H	603	ATP	C2-N3	2.20	1.35	1.32
3	B	603	ATP	O2'-C2'	2.20	1.48	1.43
3	D	603	ATP	C2-N3	2.19	1.35	1.32
4	C	603	IMP	C5-C6	2.19	1.51	1.47
2	D	602	GTP	O6-C6	-2.18	1.18	1.23
4	E	604	IMP	C6-N1	2.17	1.42	1.38
3	B	603	ATP	C2-N3	2.16	1.35	1.32
5	C	604	NAD	C4N-C3N	-2.15	1.35	1.39
3	G	601	ATP	C2-N3	2.15	1.35	1.32
3	C	601	ATP	C2-N3	2.13	1.35	1.32
4	F	604	IMP	C6-N1	2.13	1.42	1.38
4	A	604	IMP	C6-N1	2.12	1.42	1.38
2	H	602	GTP	O6-C6	-2.11	1.19	1.23
5	B	605	NAD	C2A-N3A	2.09	1.35	1.32
2	H	601	GTP	O6-C6	-2.08	1.19	1.23
2	D	601	GTP	O6-C6	-2.06	1.19	1.23
4	H	604	IMP	C6-N1	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	ATP	C2-N3	2.05	1.35	1.32
3	F	603	ATP	C2-N3	2.04	1.35	1.32
5	G	604	NAD	C2A-N3A	2.04	1.35	1.32
4	E	604	IMP	C5-C6	2.04	1.51	1.47
5	C	604	NAD	C2A-N3A	2.03	1.35	1.32
5	H	605	NAD	C2A-N3A	2.03	1.35	1.32
4	B	604	IMP	C5-C6	2.02	1.51	1.47
3	A	603	ATP	C2-N3	2.01	1.35	1.32
5	D	605	NAD	C2A-N3A	2.00	1.35	1.32
5	F	605	NAD	C2A-N3A	2.00	1.35	1.32

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	603	ATP	C5-C6-N6	14.52	142.42	120.35
3	B	603	ATP	C5-C6-N6	14.52	142.41	120.35
3	D	603	ATP	C5-C6-N6	14.48	142.35	120.35
3	A	603	ATP	C5-C6-N6	14.47	142.35	120.35
3	F	603	ATP	C5-C6-N6	14.47	142.34	120.35
3	C	602	ATP	C5-C6-N6	14.47	142.34	120.35
3	E	603	ATP	C5-C6-N6	14.41	142.24	120.35
3	G	602	ATP	C5-C6-N6	14.29	142.06	120.35
3	C	601	ATP	C5-C6-N6	14.20	141.94	120.35
3	G	601	ATP	C5-C6-N6	14.03	141.68	120.35
5	G	604	NAD	C5A-C6A-N6A	11.04	137.12	120.35
5	C	604	NAD	C5A-C6A-N6A	11.02	137.10	120.35
5	F	605	NAD	C5A-C6A-N6A	10.96	137.01	120.35
5	B	605	NAD	C5A-C6A-N6A	10.96	137.01	120.35
5	A	605	NAD	C5A-C6A-N6A	10.85	136.84	120.35
5	E	605	NAD	C5A-C6A-N6A	10.80	136.76	120.35
5	D	605	NAD	C5A-C6A-N6A	10.78	136.73	120.35
5	H	605	NAD	C5A-C6A-N6A	10.74	136.67	120.35
3	G	601	ATP	C1'-N9-C4	-10.67	107.89	126.64
3	F	603	ATP	C1'-N9-C4	-10.31	108.53	126.64
3	B	603	ATP	N6-C6-N1	-10.21	97.37	118.57
3	A	603	ATP	N6-C6-N1	-10.15	97.50	118.57
3	C	602	ATP	N6-C6-N1	-10.15	97.51	118.57
3	C	601	ATP	C1'-N9-C4	-10.08	108.93	126.64
3	F	603	ATP	N6-C6-N1	-10.08	97.66	118.57
3	D	603	ATP	N6-C6-N1	-10.04	97.73	118.57
3	H	603	ATP	N6-C6-N1	-10.00	97.82	118.57
3	C	601	ATP	N6-C6-N1	-9.98	97.86	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	603	ATP	C1'-N9-C4	-9.96	109.14	126.64
3	G	601	ATP	N6-C6-N1	-9.96	97.90	118.57
3	G	602	ATP	N6-C6-N1	-9.95	97.92	118.57
3	E	603	ATP	N6-C6-N1	-9.87	98.08	118.57
3	D	603	ATP	C1'-N9-C4	-9.73	109.55	126.64
3	H	603	ATP	C1'-N9-C4	-9.70	109.60	126.64
3	C	602	ATP	C1'-N9-C4	-9.69	109.61	126.64
3	A	603	ATP	C1'-N9-C4	-9.64	109.71	126.64
3	B	603	ATP	C1'-N9-C4	-9.59	109.80	126.64
3	G	602	ATP	C1'-N9-C4	-9.57	109.83	126.64
5	C	604	NAD	C1B-N9A-C4A	-8.97	110.88	126.64
5	B	605	NAD	C1B-N9A-C4A	-8.95	110.92	126.64
5	G	604	NAD	C1B-N9A-C4A	-8.89	111.01	126.64
5	D	605	NAD	C1B-N9A-C4A	-8.57	111.59	126.64
5	F	605	NAD	C1B-N9A-C4A	-8.44	111.82	126.64
5	E	605	NAD	C1B-N9A-C4A	-8.41	111.86	126.64
5	H	605	NAD	C1B-N9A-C4A	-8.26	112.14	126.64
5	A	605	NAD	C1B-N9A-C4A	-7.96	112.65	126.64
5	F	605	NAD	N6A-C6A-N1A	-7.67	102.65	118.57
5	G	604	NAD	N6A-C6A-N1A	-7.64	102.71	118.57
5	B	605	NAD	N6A-C6A-N1A	-7.63	102.74	118.57
5	A	605	NAD	N6A-C6A-N1A	-7.61	102.79	118.57
5	C	604	NAD	N6A-C6A-N1A	-7.60	102.81	118.57
5	D	605	NAD	N6A-C6A-N1A	-7.57	102.86	118.57
5	E	605	NAD	N6A-C6A-N1A	-7.55	102.89	118.57
5	H	605	NAD	N6A-C6A-N1A	-7.54	102.93	118.57
3	G	601	ATP	N3-C2-N1	-6.14	119.09	128.68
3	G	602	ATP	N3-C2-N1	-6.04	119.23	128.68
3	C	601	ATP	N3-C2-N1	-6.00	119.29	128.68
3	C	602	ATP	N3-C2-N1	-5.97	119.34	128.68
3	E	603	ATP	N3-C2-N1	-5.90	119.46	128.68
5	A	605	NAD	N3A-C2A-N1A	-5.90	119.46	128.68
5	D	605	NAD	N3A-C2A-N1A	-5.82	119.58	128.68
5	E	605	NAD	N3A-C2A-N1A	-5.80	119.61	128.68
5	F	605	NAD	N3A-C2A-N1A	-5.80	119.61	128.68
3	B	603	ATP	N3-C2-N1	-5.76	119.67	128.68
5	H	605	NAD	N3A-C2A-N1A	-5.76	119.68	128.68
5	B	605	NAD	N3A-C2A-N1A	-5.75	119.69	128.68
3	D	603	ATP	N3-C2-N1	-5.72	119.74	128.68
3	H	603	ATP	N3-C2-N1	-5.71	119.75	128.68
5	G	604	NAD	N3A-C2A-N1A	-5.69	119.78	128.68
5	C	604	NAD	N3A-C2A-N1A	-5.69	119.79	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	603	ATP	N3-C2-N1	-5.69	119.79	128.68
3	A	603	ATP	N3-C2-N1	-5.66	119.82	128.68
2	D	602	GTP	C3'-C2'-C1'	4.48	107.72	100.98
2	B	601	GTP	PB-O3B-PG	-4.29	118.09	132.83
3	G	601	ATP	C3'-C2'-C1'	4.27	107.41	100.98
2	A	602	GTP	C5-C6-N1	4.22	121.39	113.95
3	A	603	ATP	PA-O3A-PB	-4.07	118.86	132.83
3	E	603	ATP	PB-O3B-PG	-4.07	118.87	132.83
2	E	601	GTP	PB-O3B-PG	-4.07	118.88	132.83
3	A	603	ATP	C3'-C2'-C1'	4.04	107.06	100.98
2	A	601	GTP	PB-O3B-PG	-4.02	119.05	132.83
4	H	604	IMP	C5-C6-N1	3.99	121.00	113.95
4	B	604	IMP	C5-C6-N1	3.97	120.96	113.95
3	A	603	ATP	PB-O3B-PG	-3.93	119.33	132.83
2	H	602	GTP	C3'-C2'-C1'	3.91	106.86	100.98
2	A	602	GTP	C2-N1-C6	-3.89	117.93	125.10
3	B	603	ATP	PB-O3B-PG	-3.89	119.48	132.83
5	F	605	NAD	PN-O3-PA	-3.89	119.49	132.83
4	G	603	IMP	C5-C6-N1	3.86	120.77	113.95
5	B	605	NAD	PN-O3-PA	-3.84	119.63	132.83
4	F	604	IMP	C5-C6-N1	3.80	120.66	113.95
5	E	605	NAD	PN-O3-PA	-3.72	120.05	132.83
4	C	603	IMP	C5-C6-N1	3.70	120.48	113.95
2	F	602	GTP	C5-C6-N1	3.69	120.47	113.95
2	E	601	GTP	C5-C6-N1	3.68	120.45	113.95
4	E	604	IMP	C5-C6-N1	3.68	120.45	113.95
4	A	604	IMP	C5-C6-N1	3.67	120.43	113.95
4	D	604	IMP	C5-C6-N1	3.64	120.38	113.95
2	A	601	GTP	C5-C6-N1	3.64	120.37	113.95
2	A	602	GTP	C3'-C2'-C1'	3.63	106.44	100.98
5	C	604	NAD	C3D-C2D-C1D	3.62	106.43	100.98
2	E	602	GTP	C5-C6-N1	3.61	120.33	113.95
2	D	602	GTP	C5-C6-N1	3.61	120.32	113.95
3	F	603	ATP	PB-O3B-PG	-3.61	120.45	132.83
2	E	602	GTP	C2-N1-C6	-3.59	118.48	125.10
5	F	605	NAD	C3D-C2D-C1D	3.58	106.36	100.98
2	B	602	GTP	C3'-C2'-C1'	3.56	106.34	100.98
3	G	602	ATP	C3'-C2'-C1'	3.56	106.34	100.98
2	F	601	GTP	C5-C6-N1	3.55	120.22	113.95
2	B	602	GTP	C5-C6-N1	3.54	120.20	113.95
2	E	601	GTP	C3'-C2'-C1'	3.51	106.26	100.98
3	E	603	ATP	PA-O3A-PB	-3.50	120.83	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	IMP	O6-C6-C5	-3.48	117.57	124.37
3	H	603	ATP	PB-O3B-PG	-3.48	120.90	132.83
5	A	605	NAD	PN-O3-PA	-3.46	120.94	132.83
2	H	601	GTP	PB-O3B-PG	-3.45	120.99	132.83
2	H	601	GTP	C5-C6-N1	3.43	120.01	113.95
2	F	602	GTP	C2-N1-C6	-3.39	118.85	125.10
3	H	603	ATP	C3'-C2'-C1'	3.39	106.08	100.98
3	B	603	ATP	PA-O3A-PB	-3.38	121.21	132.83
2	F	601	GTP	PB-O3B-PG	-3.38	121.24	132.83
2	D	601	GTP	C5-C6-N1	3.33	119.83	113.95
5	C	604	NAD	PN-O3-PA	-3.32	121.43	132.83
2	E	601	GTP	PA-O3A-PB	-3.30	121.50	132.83
2	E	602	GTP	C8-N7-C5	3.29	109.25	102.99
5	G	604	NAD	PN-O3-PA	-3.29	121.55	132.83
2	A	601	GTP	PA-O3A-PB	-3.28	121.58	132.83
3	C	601	ATP	PB-O3B-PG	-3.27	121.59	132.83
3	G	601	ATP	PB-O3B-PG	-3.27	121.61	132.83
4	F	604	IMP	O6-C6-C5	-3.26	118.01	124.37
2	B	601	GTP	C5-C6-N1	3.25	119.69	113.95
2	B	601	GTP	PA-O3A-PB	-3.25	121.69	132.83
2	D	602	GTP	C2-N1-C6	-3.24	119.12	125.10
2	F	601	GTP	C2-N1-C6	-3.23	119.14	125.10
2	A	601	GTP	C2-N1-C6	-3.22	119.17	125.10
2	H	602	GTP	C5-C6-N1	3.21	119.63	113.95
2	H	601	GTP	C3'-C2'-C1'	3.21	105.81	100.98
3	F	603	ATP	C3'-C2'-C1'	3.20	105.80	100.98
5	A	605	NAD	C3D-C2D-C1D	3.17	105.76	100.98
2	B	602	GTP	C2-N1-C6	-3.16	119.27	125.10
5	E	605	NAD	C3D-C2D-C1D	3.16	105.74	100.98
3	C	602	ATP	C3'-C2'-C1'	3.15	105.72	100.98
2	E	601	GTP	C2-N1-C6	-3.14	119.31	125.10
2	E	602	GTP	C3'-C2'-C1'	3.14	105.70	100.98
2	A	601	GTP	C3'-C2'-C1'	3.13	105.69	100.98
3	C	601	ATP	C3'-C2'-C1'	3.12	105.67	100.98
2	B	601	GTP	C2-N1-C6	-3.11	119.38	125.10
2	D	601	GTP	C3'-C2'-C1'	3.10	105.64	100.98
4	C	603	IMP	O6-C6-C5	-3.09	118.34	124.37
2	D	602	GTP	C2'-C3'-C4'	3.09	108.64	102.64
4	D	604	IMP	O6-C6-C5	-3.08	118.36	124.37
2	A	601	GTP	C2'-C3'-C4'	3.07	108.61	102.64
4	E	604	IMP	O6-C6-C5	-3.06	118.39	124.37
2	A	602	GTP	C8-N7-C5	3.04	108.78	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	GTP	C3'-C2'-C1'	3.03	105.55	100.98
4	C	603	IMP	O3P-P-O2P	3.03	119.23	107.64
4	A	604	IMP	O6-C6-C5	-3.03	118.46	124.37
4	H	604	IMP	O3P-P-O2P	3.02	119.19	107.64
2	D	601	GTP	C2-N1-C6	-2.98	119.62	125.10
3	E	603	ATP	C3'-C2'-C1'	2.96	105.44	100.98
5	H	605	NAD	C3D-C2D-C1D	2.95	105.43	100.98
2	B	601	GTP	C3'-C2'-C1'	2.95	105.43	100.98
2	D	601	GTP	C2'-C3'-C4'	2.94	108.35	102.64
2	A	602	GTP	PB-O3B-PG	-2.89	122.91	132.83
2	H	601	GTP	PA-O3A-PB	-2.87	122.97	132.83
4	H	604	IMP	O6-C6-C5	-2.87	118.78	124.37
2	D	601	GTP	PA-O3A-PB	-2.86	123.03	132.83
3	H	603	ATP	PA-O3A-PB	-2.85	123.03	132.83
2	H	601	GTP	C2-N1-C6	-2.85	119.86	125.10
5	H	605	NAD	PN-O3-PA	-2.81	123.17	132.83
4	G	603	IMP	O6-C6-C5	-2.80	118.90	124.37
2	D	602	GTP	PA-O3A-PB	-2.79	123.24	132.83
5	G	604	NAD	C3D-C2D-C1D	2.79	105.18	100.98
3	F	603	ATP	PA-O3A-PB	-2.75	123.40	132.83
5	G	604	NAD	C3B-C2B-C1B	2.72	105.08	100.98
2	F	602	GTP	PA-O3A-PB	-2.70	123.57	132.83
3	C	602	ATP	PB-O3B-PG	-2.69	123.59	132.83
2	D	602	GTP	C8-N7-C5	2.69	108.11	102.99
5	A	605	NAD	C3B-C2B-C1B	2.67	105.00	100.98
5	B	605	NAD	C2N-C3N-C4N	2.67	121.28	118.26
2	B	602	GTP	PA-O3A-PB	-2.66	123.68	132.83
2	D	601	GTP	C8-N7-C5	2.66	108.06	102.99
2	F	602	GTP	C8-N7-C5	2.66	108.05	102.99
2	H	602	GTP	C2-N1-C6	-2.66	120.21	125.10
2	H	601	GTP	C8-N7-C5	2.65	108.04	102.99
3	G	602	ATP	PB-O3B-PG	-2.65	123.73	132.83
2	E	601	GTP	C8-N7-C5	2.65	108.03	102.99
2	F	602	GTP	O4'-C1'-C2'	-2.63	103.08	106.93
2	E	602	GTP	PB-O3B-PG	-2.63	123.81	132.83
3	G	602	ATP	PA-O3A-PB	-2.63	123.81	132.83
2	H	602	GTP	C8-N7-C5	2.62	107.98	102.99
2	B	602	GTP	O6-C6-C5	-2.62	119.26	124.37
5	F	605	NAD	C3B-C2B-C1B	2.61	104.91	100.98
5	D	605	NAD	PN-O3-PA	-2.61	123.86	132.83
2	F	601	GTP	C8-N7-C5	2.59	107.92	102.99
2	A	601	GTP	O6-C6-C5	-2.58	119.33	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GTP	C8-N7-C5	2.58	107.90	102.99
2	E	602	GTP	PA-O3A-PB	-2.57	124.00	132.83
3	G	601	ATP	C2'-C3'-C4'	2.56	107.62	102.64
4	G	603	IMP	N1-C2-N3	-2.56	119.18	125.87
2	D	602	GTP	PB-O3B-PG	-2.56	124.06	132.83
3	D	603	ATP	C3'-C2'-C1'	2.55	104.82	100.98
2	F	601	GTP	O6-C6-C5	-2.54	119.40	124.37
4	G	603	IMP	C8-N7-C5	2.54	107.83	102.99
2	D	601	GTP	O6-C6-C5	-2.52	119.46	124.37
2	A	602	GTP	O6-C6-C5	-2.51	119.46	124.37
5	C	604	NAD	C2D-C3D-C4D	2.50	107.50	102.64
4	F	604	IMP	C8-N7-C5	2.50	107.75	102.99
4	B	604	IMP	N1-C2-N3	-2.50	119.36	125.87
4	B	604	IMP	C8-N7-C5	2.50	107.74	102.99
5	H	605	NAD	C3B-C2B-C1B	2.49	104.72	100.98
2	A	602	GTP	O4'-C1'-C2'	-2.47	103.32	106.93
5	E	605	NAD	C3B-C2B-C1B	2.46	104.69	100.98
2	F	602	GTP	O6-C6-C5	-2.46	119.57	124.37
2	B	602	GTP	PB-O3B-PG	-2.45	124.42	132.83
2	H	602	GTP	PB-O3B-PG	-2.45	124.44	132.83
5	D	605	NAD	C3D-C2D-C1D	2.44	104.65	100.98
2	E	601	GTP	O6-C6-C5	-2.44	119.61	124.37
2	H	602	GTP	C2'-C3'-C4'	2.42	107.34	102.64
4	E	604	IMP	C8-N7-C5	2.42	107.59	102.99
2	B	601	GTP	C8-N7-C5	2.41	107.59	102.99
5	D	605	NAD	C3B-C2B-C1B	2.41	104.61	100.98
4	C	603	IMP	C8-N7-C5	2.40	107.57	102.99
3	D	603	ATP	PA-O3A-PB	-2.39	124.62	132.83
2	H	602	GTP	PA-O3A-PB	-2.37	124.69	132.83
5	F	605	NAD	C2N-C3N-C4N	2.36	120.93	118.26
2	B	602	GTP	C8-N7-C5	2.35	107.47	102.99
2	A	602	GTP	PA-O3A-PB	-2.34	124.79	132.83
2	F	602	GTP	C3'-C2'-C1'	2.34	104.50	100.98
4	D	604	IMP	C8-N7-C5	2.33	107.44	102.99
4	H	604	IMP	C8-N7-C5	2.33	107.44	102.99
5	B	605	NAD	C3B-C2B-C1B	2.31	104.46	100.98
3	C	602	ATP	PA-O3A-PB	-2.29	124.98	132.83
2	B	601	GTP	O6-C6-C5	-2.28	119.91	124.37
5	F	605	NAD	C2D-C3D-C4D	2.28	107.06	102.64
5	A	605	NAD	C2N-C3N-C4N	2.27	120.83	118.26
5	D	605	NAD	O4B-C1B-C2B	-2.26	103.62	106.93
5	D	605	NAD	C2N-C3N-C4N	2.24	120.80	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	NAD	O4D-C1D-C2D	-2.24	103.66	106.93
2	F	601	GTP	PA-O3A-PB	-2.23	125.19	132.83
4	G	603	IMP	O2P-P-O1P	2.22	119.38	110.68
5	H	605	NAD	C2N-C3N-C4N	2.21	120.77	118.26
4	A	604	IMP	C8-N7-C5	2.20	107.18	102.99
3	G	601	ATP	PA-O3A-PB	-2.18	125.35	132.83
2	F	602	GTP	PB-O3B-PG	-2.17	125.37	132.83
3	C	601	ATP	PA-O3A-PB	-2.16	125.43	132.83
2	D	602	GTP	O6-C6-C5	-2.16	120.16	124.37
2	H	601	GTP	O6-C6-C5	-2.15	120.16	124.37
3	B	603	ATP	C3'-C2'-C1'	2.14	104.21	100.98
2	D	601	GTP	O2G-PG-O3B	2.14	111.81	104.64
4	F	604	IMP	O2P-P-O1P	2.11	118.95	110.68
5	E	605	NAD	C2N-C3N-C4N	2.09	120.63	118.26
4	A	604	IMP	O2P-P-O1P	2.09	118.85	110.68
5	G	604	NAD	C2B-C3B-C4B	2.08	106.69	102.64
4	E	604	IMP	O2P-P-O1P	2.08	118.83	110.68
5	E	605	NAD	C2D-C3D-C4D	2.07	106.66	102.64
4	C	603	IMP	N1-C2-N3	-2.06	120.50	125.87
2	H	602	GTP	O6-C6-C5	-2.04	120.38	124.37
4	D	604	IMP	N1-C2-N3	-2.03	120.57	125.87
2	E	602	GTP	O6-C6-C5	-2.03	120.41	124.37
5	G	604	NAD	C2D-C3D-C4D	2.03	106.58	102.64
2	B	602	GTP	O4'-C1'-C2'	-2.02	103.97	106.93
2	F	602	GTP	C2'-C3'-C4'	2.02	106.56	102.64
4	F	604	IMP	N1-C2-N3	-2.00	120.64	125.87
5	G	604	NAD	O4B-C1B-C2B	-2.00	104.00	106.93

There are no chirality outliers.

All (199) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GTP	PB-O3B-PG-O2G
2	A	601	GTP	PB-O3B-PG-O3G
2	D	601	GTP	PB-O3B-PG-O2G
2	D	601	GTP	PB-O3B-PG-O3G
2	D	601	GTP	C5'-O5'-PA-O1A
2	D	601	GTP	O4'-C4'-C5'-O5'
2	D	602	GTP	PB-O3B-PG-O3G
2	E	601	GTP	C5'-O5'-PA-O3A
2	E	602	GTP	PB-O3B-PG-O3G
2	E	602	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	F	601	GTP	PB-O3B-PG-O2G
2	F	601	GTP	C5'-O5'-PA-O1A
2	F	601	GTP	O4'-C4'-C5'-O5'
2	F	602	GTP	PB-O3A-PA-O5'
2	H	601	GTP	C5'-O5'-PA-O1A
2	H	601	GTP	C5'-O5'-PA-O2A
3	A	603	ATP	C5'-O5'-PA-O2A
3	A	603	ATP	C5'-O5'-PA-O3A
3	B	603	ATP	C5'-O5'-PA-O1A
3	B	603	ATP	C5'-O5'-PA-O2A
3	B	603	ATP	C5'-O5'-PA-O3A
3	B	603	ATP	O4'-C4'-C5'-O5'
3	B	603	ATP	C3'-C4'-C5'-O5'
3	D	603	ATP	PB-O3B-PG-O3G
3	D	603	ATP	C5'-O5'-PA-O3A
3	D	603	ATP	O4'-C4'-C5'-O5'
3	E	603	ATP	C5'-O5'-PA-O3A
3	E	603	ATP	O4'-C4'-C5'-O5'
3	E	603	ATP	C3'-C4'-C5'-O5'
3	G	601	ATP	C5'-O5'-PA-O2A
3	G	601	ATP	O4'-C4'-C5'-O5'
3	G	602	ATP	C5'-O5'-PA-O1A
4	B	604	IMP	C5'-O5'-P-O2P
4	C	603	IMP	C5'-O5'-P-O1P
4	C	603	IMP	C5'-O5'-P-O2P
4	C	603	IMP	C5'-O5'-P-O3P
4	C	603	IMP	C3'-C4'-C5'-O5'
4	E	604	IMP	C5'-O5'-P-O1P
4	E	604	IMP	C5'-O5'-P-O2P
4	E	604	IMP	C5'-O5'-P-O3P
4	G	603	IMP	C5'-O5'-P-O2P
4	G	603	IMP	C5'-O5'-P-O3P
5	A	605	NAD	C5D-O5D-PN-O3
5	A	605	NAD	C5D-O5D-PN-O1N
5	A	605	NAD	C5D-O5D-PN-O2N
5	B	605	NAD	C5B-O5B-PA-O3
5	B	605	NAD	C5D-O5D-PN-O3
5	B	605	NAD	O4D-C4D-C5D-O5D
5	B	605	NAD	C3D-C4D-C5D-O5D
5	C	604	NAD	C5D-O5D-PN-O3
5	C	604	NAD	C5D-O5D-PN-O2N
5	D	605	NAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	D	605	NAD	C5B-O5B-PA-O3
5	D	605	NAD	C5D-O5D-PN-O3
5	E	605	NAD	C5B-O5B-PA-O1A
5	E	605	NAD	C5B-O5B-PA-O2A
5	E	605	NAD	C5D-O5D-PN-O3
5	E	605	NAD	C5D-O5D-PN-O2N
5	E	605	NAD	O4D-C1D-N1N-C2N
5	E	605	NAD	O4D-C1D-N1N-C6N
5	F	605	NAD	C5B-O5B-PA-O1A
5	F	605	NAD	C2N-C3N-C7N-O7N
5	F	605	NAD	C2N-C3N-C7N-N7N
5	G	604	NAD	O4B-C4B-C5B-O5B
5	G	604	NAD	C5D-O5D-PN-O3
5	G	604	NAD	C5D-O5D-PN-O1N
5	G	604	NAD	C5D-O5D-PN-O2N
5	H	605	NAD	C5B-O5B-PA-O1A
5	H	605	NAD	C5D-O5D-PN-O3
5	H	605	NAD	C5D-O5D-PN-O1N
5	F	605	NAD	C4N-C3N-C7N-O7N
5	F	605	NAD	C4N-C3N-C7N-N7N
2	A	601	GTP	O4'-C4'-C5'-O5'
2	A	601	GTP	C3'-C4'-C5'-O5'
2	A	602	GTP	O4'-C4'-C5'-O5'
2	B	601	GTP	C3'-C4'-C5'-O5'
2	D	602	GTP	O4'-C4'-C5'-O5'
2	D	602	GTP	C3'-C4'-C5'-O5'
3	C	601	ATP	C3'-C4'-C5'-O5'
3	D	603	ATP	C3'-C4'-C5'-O5'
3	G	601	ATP	C3'-C4'-C5'-O5'
4	G	603	IMP	C3'-C4'-C5'-O5'
5	B	605	NAD	O4B-C4B-C5B-O5B
5	D	605	NAD	O4B-C4B-C5B-O5B
5	E	605	NAD	O4B-C4B-C5B-O5B
5	F	605	NAD	O4B-C4B-C5B-O5B
5	G	604	NAD	C3B-C4B-C5B-O5B
2	D	601	GTP	C3'-C4'-C5'-O5'
2	E	601	GTP	O4'-C4'-C5'-O5'
2	E	601	GTP	C3'-C4'-C5'-O5'
2	F	601	GTP	C3'-C4'-C5'-O5'
4	C	603	IMP	O4'-C4'-C5'-O5'
5	D	605	NAD	C3B-C4B-C5B-O5B
5	H	605	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
5	H	605	NAD	O4D-C4D-C5D-O5D
3	C	601	ATP	O4'-C4'-C5'-O5'
2	B	601	GTP	O4'-C4'-C5'-O5'
4	E	604	IMP	C3'-C4'-C5'-O5'
5	H	605	NAD	C3B-C4B-C5B-O5B
5	B	605	NAD	C2N-C3N-C7N-O7N
4	G	603	IMP	O4'-C4'-C5'-O5'
5	C	604	NAD	O4D-C4D-C5D-O5D
5	B	605	NAD	C2N-C3N-C7N-N7N
2	H	601	GTP	PB-O3B-PG-O1G
4	B	604	IMP	C5'-O5'-P-O1P
4	F	604	IMP	C5'-O5'-P-O1P
4	G	603	IMP	C5'-O5'-P-O1P
2	E	601	GTP	PG-O3B-PB-O1B
5	C	604	NAD	C3D-C4D-C5D-O5D
5	B	605	NAD	C4N-C3N-C7N-N7N
5	B	605	NAD	C4N-C3N-C7N-O7N
5	B	605	NAD	C3B-C4B-C5B-O5B
5	C	604	NAD	O4B-C4B-C5B-O5B
5	E	605	NAD	C3B-C4B-C5B-O5B
5	B	605	NAD	PN-O3-PA-O5B
5	C	604	NAD	PN-O3-PA-O5B
5	E	605	NAD	PN-O3-PA-O5B
5	F	605	NAD	PN-O3-PA-O5B
5	A	605	NAD	O4B-C4B-C5B-O5B
5	H	605	NAD	C3D-C4D-C5D-O5D
4	F	604	IMP	C5'-O5'-P-O3P
2	D	602	GTP	C4'-C5'-O5'-PA
2	D	602	GTP	PB-O3B-PG-O2G
2	H	601	GTP	PB-O3B-PG-O2G
2	A	602	GTP	C5'-O5'-PA-O3A
2	H	601	GTP	C5'-O5'-PA-O3A
3	C	602	ATP	C5'-O5'-PA-O3A
3	G	601	ATP	C5'-O5'-PA-O3A
3	G	602	ATP	C5'-O5'-PA-O3A
5	H	605	NAD	C5B-O5B-PA-O3
2	H	602	GTP	O4'-C4'-C5'-O5'
4	E	604	IMP	O4'-C4'-C5'-O5'
5	C	604	NAD	C3B-C4B-C5B-O5B
2	A	601	GTP	PB-O3A-PA-O2A
2	E	602	GTP	PA-O3A-PB-O1B
3	B	603	ATP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	G	602	ATP	PG-O3B-PB-O1B
5	B	605	NAD	PA-O3-PN-O2N
2	E	601	GTP	C5'-O5'-PA-O1A
2	E	601	GTP	C5'-O5'-PA-O2A
2	E	602	GTP	C5'-O5'-PA-O2A
3	A	603	ATP	C5'-O5'-PA-O1A
3	C	602	ATP	C5'-O5'-PA-O2A
3	D	603	ATP	C5'-O5'-PA-O1A
3	D	603	ATP	C5'-O5'-PA-O2A
3	E	603	ATP	C5'-O5'-PA-O1A
3	E	603	ATP	C5'-O5'-PA-O2A
3	G	601	ATP	C5'-O5'-PA-O1A
3	G	602	ATP	C5'-O5'-PA-O2A
5	B	605	NAD	C5B-O5B-PA-O1A
5	B	605	NAD	C5D-O5D-PN-O2N
5	C	604	NAD	C5D-O5D-PN-O1N
5	D	605	NAD	C5D-O5D-PN-O1N
5	D	605	NAD	C5D-O5D-PN-O2N
5	E	605	NAD	C5D-O5D-PN-O1N
2	H	602	GTP	C3'-C4'-C5'-O5'
3	G	602	ATP	O4'-C4'-C5'-O5'
3	C	602	ATP	PG-O3B-PB-O2B
3	D	603	ATP	PA-O3A-PB-O2B
2	E	602	GTP	O4'-C4'-C5'-O5'
2	F	602	GTP	O4'-C4'-C5'-O5'
4	F	604	IMP	C3'-C4'-C5'-O5'
5	G	604	NAD	C2N-C3N-C7N-N7N
2	B	601	GTP	PA-O3A-PB-O2B
2	B	602	GTP	PA-O3A-PB-O1B
3	G	602	ATP	PA-O3A-PB-O1B
3	A	603	ATP	O4'-C4'-C5'-O5'
4	A	604	IMP	C3'-C4'-C5'-O5'
2	D	602	GTP	PB-O3B-PG-O1G
3	D	603	ATP	PB-O3B-PG-O1G
5	G	604	NAD	C2N-C3N-C7N-O7N
2	A	602	GTP	C4'-C5'-O5'-PA
3	F	603	ATP	O4'-C4'-C5'-O5'
2	E	602	GTP	PB-O3B-PG-O2G
2	F	601	GTP	PB-O3B-PG-O3G
3	D	603	ATP	PB-O3B-PG-O2G
2	B	601	GTP	C5'-O5'-PA-O3A
5	E	605	NAD	C5B-O5B-PA-O3

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
5	F	605	NAD	C5B-O5B-PA-O3
5	D	605	NAD	C4B-C5B-O5B-PA
2	B	602	GTP	O4'-C4'-C5'-O5'
2	E	602	GTP	C3'-C4'-C5'-O5'
2	A	601	GTP	PB-O3A-PA-O1A
2	A	602	GTP	PB-O3A-PA-O2A
2	E	601	GTP	PA-O3A-PB-O2B
2	H	602	GTP	PA-O3A-PB-O2B
3	A	603	ATP	PG-O3B-PB-O2B
3	C	602	ATP	PG-O3B-PB-O1B
3	D	603	ATP	PA-O3A-PB-O1B
3	F	603	ATP	PG-O3B-PB-O2B
3	G	602	ATP	PG-O3B-PB-O2B
5	D	605	NAD	PN-O3-PA-O2A
2	B	601	GTP	C5'-O5'-PA-O1A
2	E	602	GTP	C5'-O5'-PA-O1A
3	C	601	ATP	C5'-O5'-PA-O1A
5	B	605	NAD	C5D-O5D-PN-O1N
2	E	602	GTP	PB-O3B-PG-O1G
5	H	605	NAD	C4B-C5B-O5B-PA
5	H	605	NAD	C2N-C3N-C7N-N7N

There are no ring outliers.

25 monomers are involved in 43 short contacts:

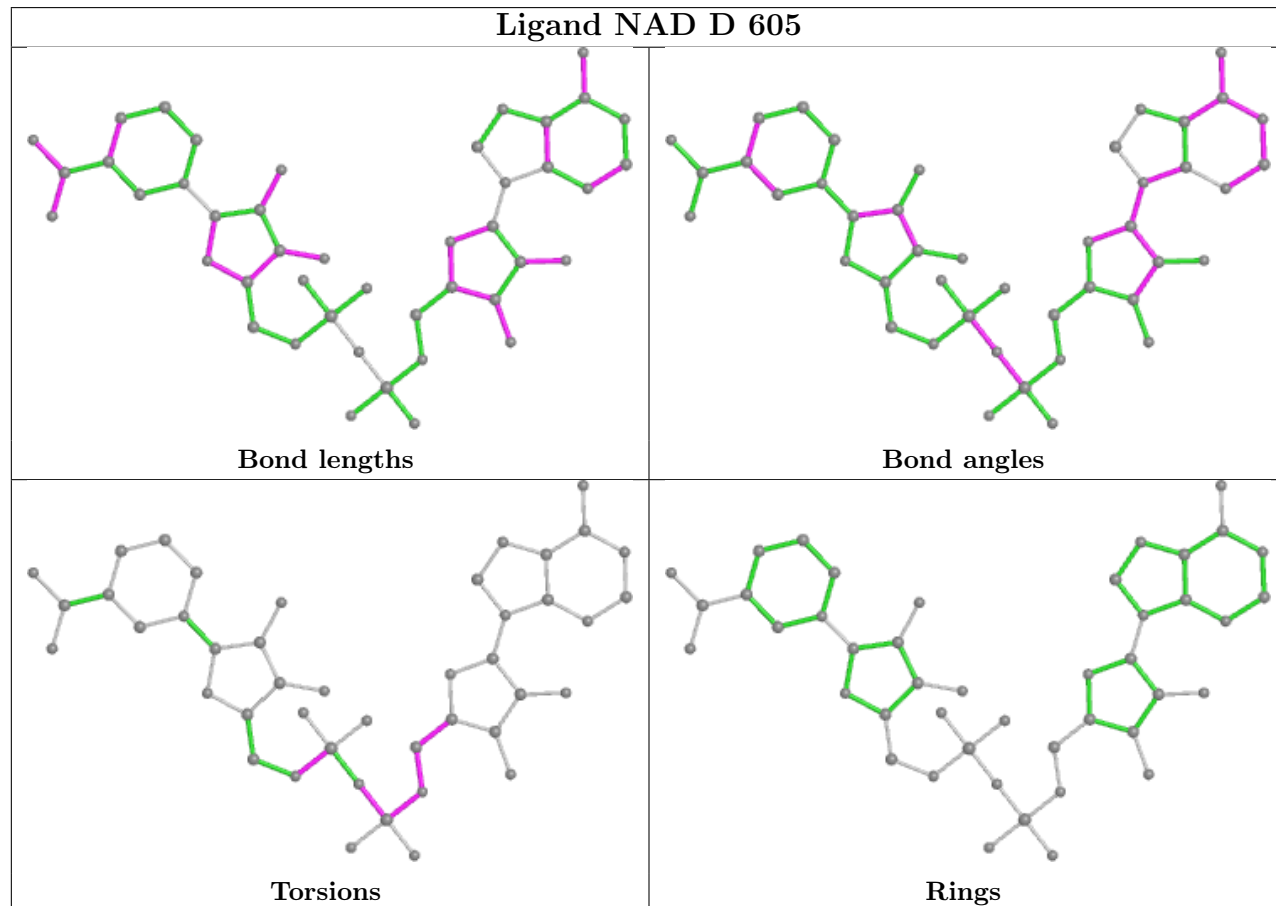
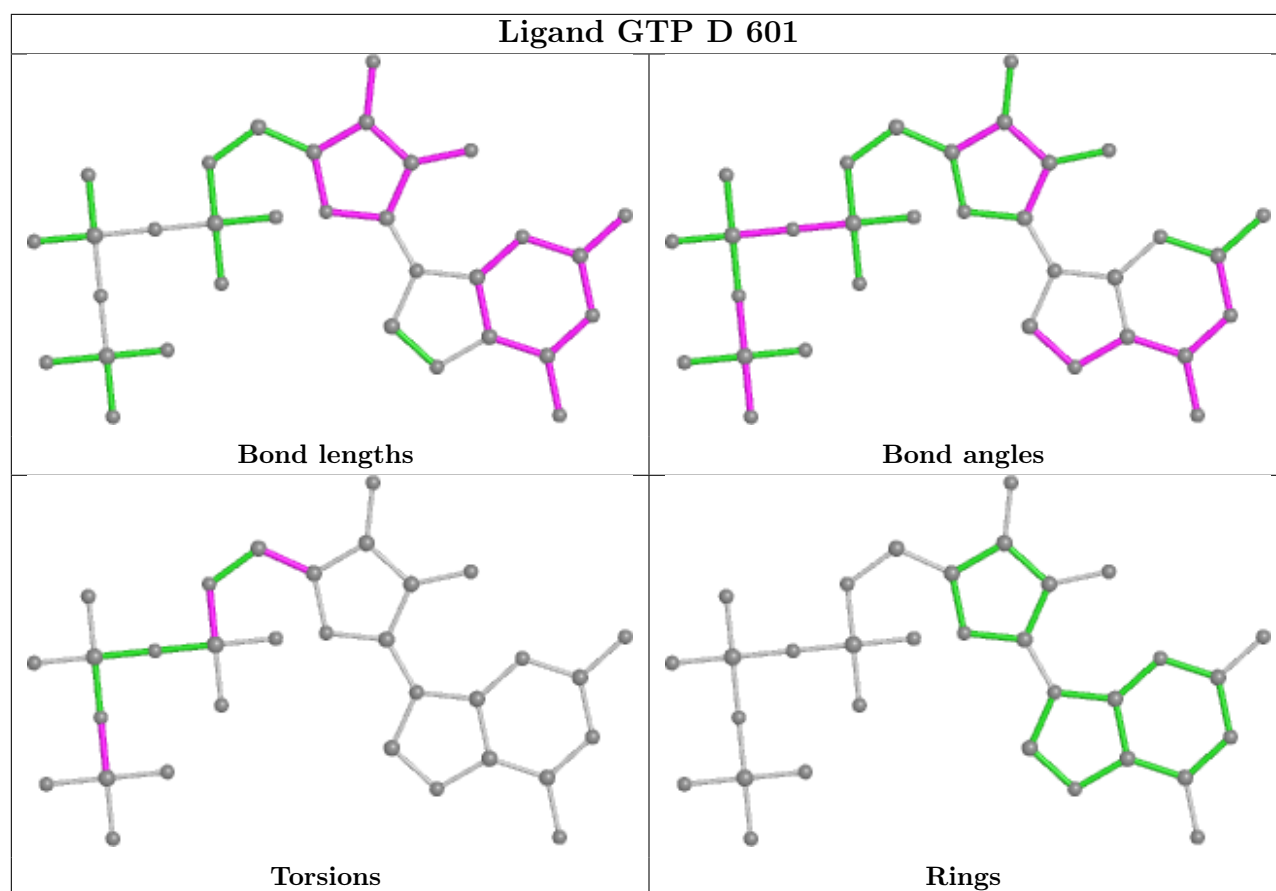
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	605	NAD	1	0
2	E	601	GTP	1	0
4	A	604	IMP	1	0
3	F	603	ATP	3	0
5	B	605	NAD	4	0
2	E	602	GTP	2	0
5	C	604	NAD	1	0
3	C	601	ATP	1	0
4	G	603	IMP	2	0
4	B	604	IMP	2	0
4	C	603	IMP	1	0
4	E	604	IMP	1	0
2	H	602	GTP	1	0
5	G	604	NAD	2	0
2	D	602	GTP	1	0
3	B	603	ATP	2	0

*Continued on next page...*

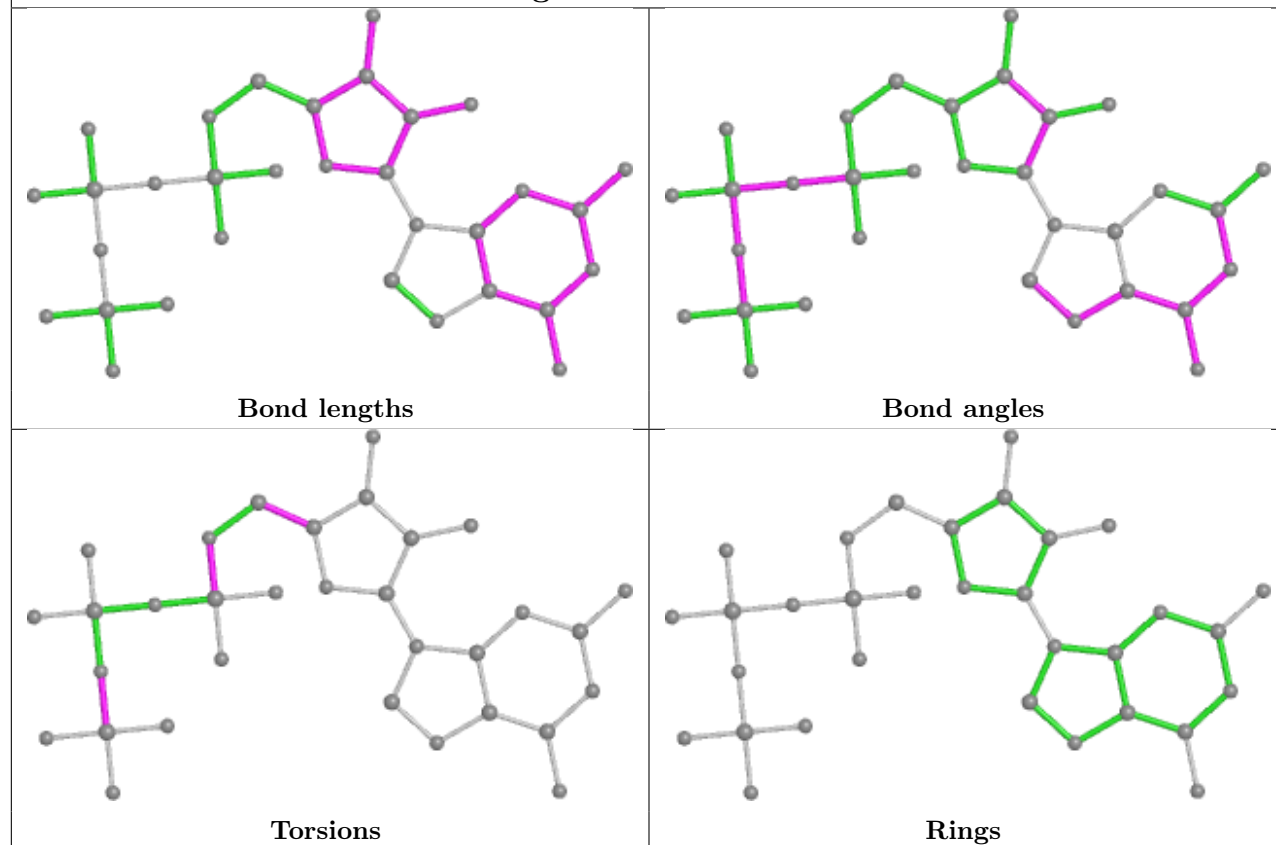
*Continued from previous page...*

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

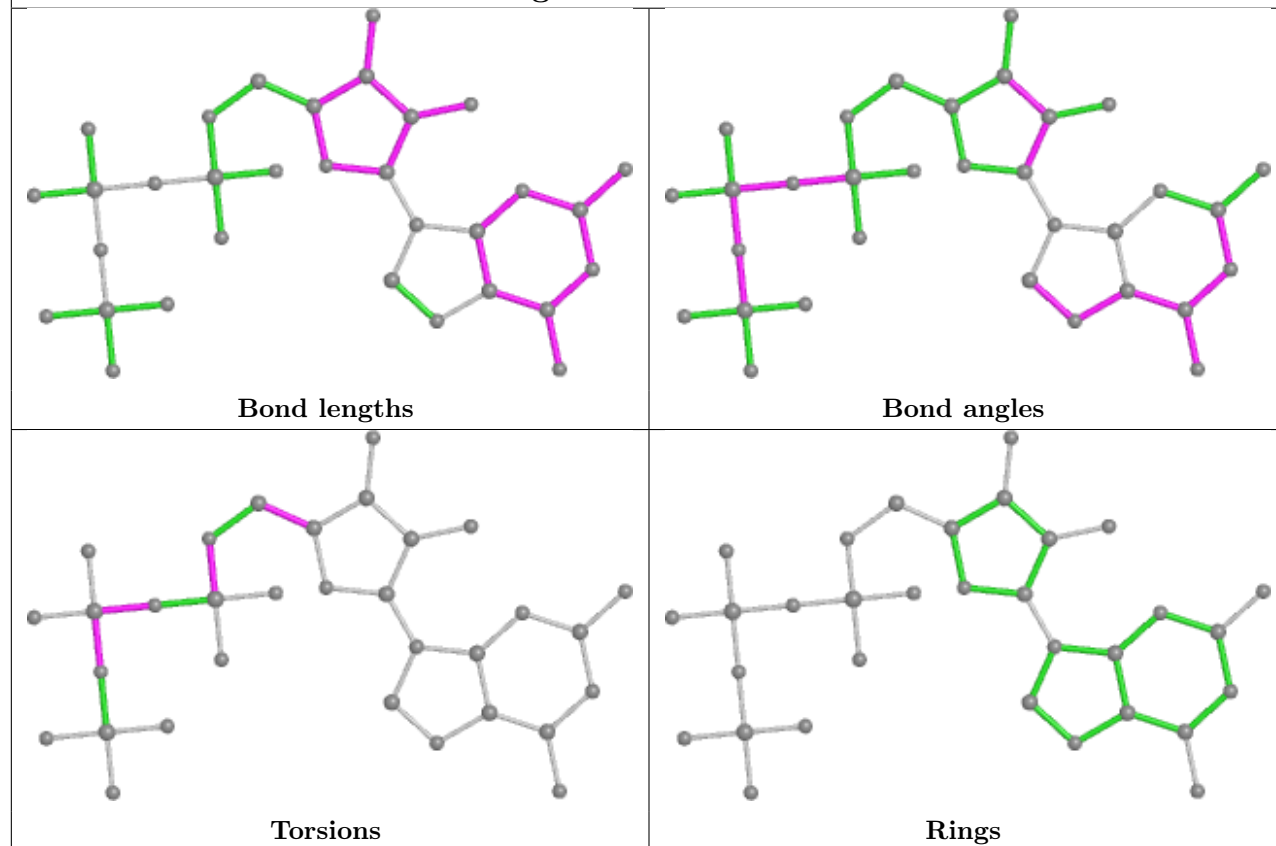
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



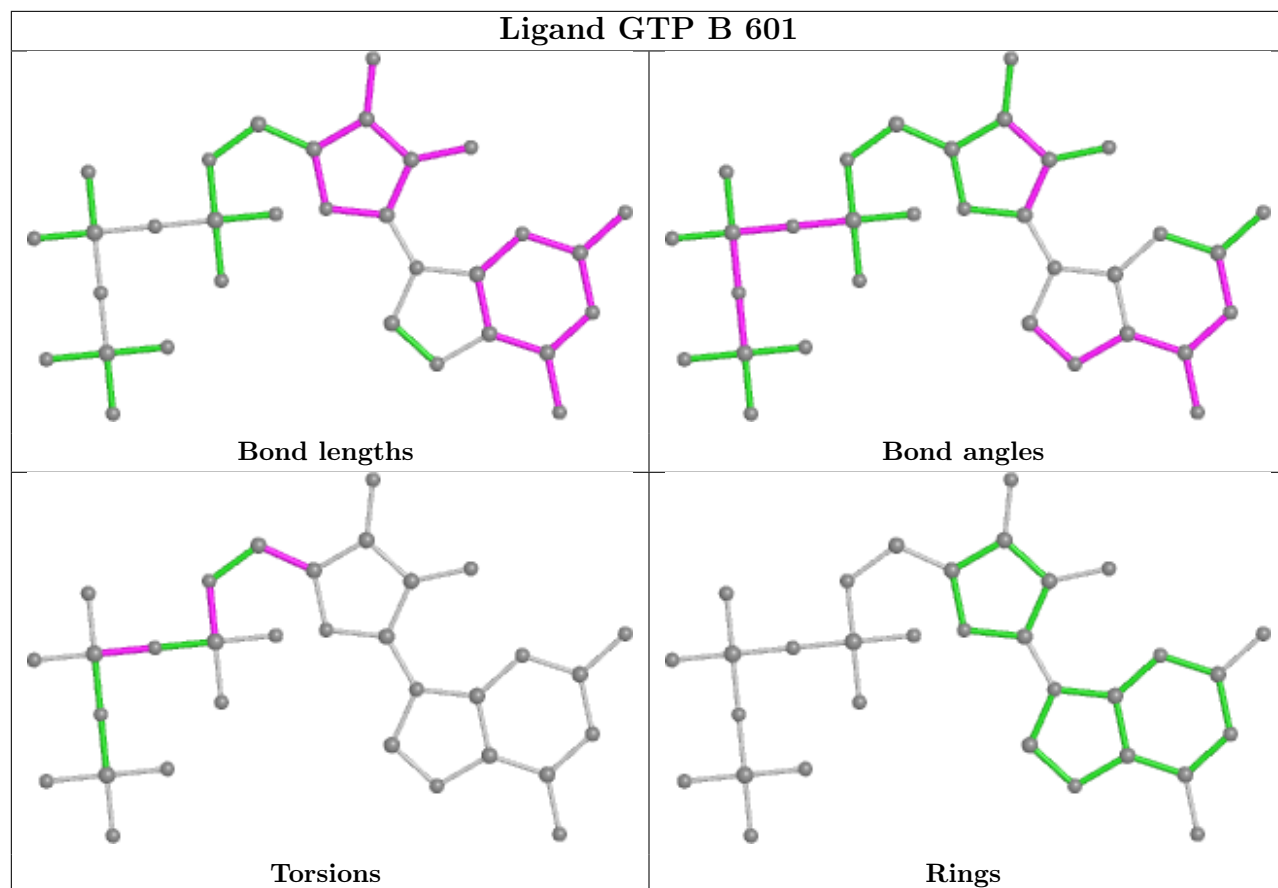
## Ligand GTP F 601



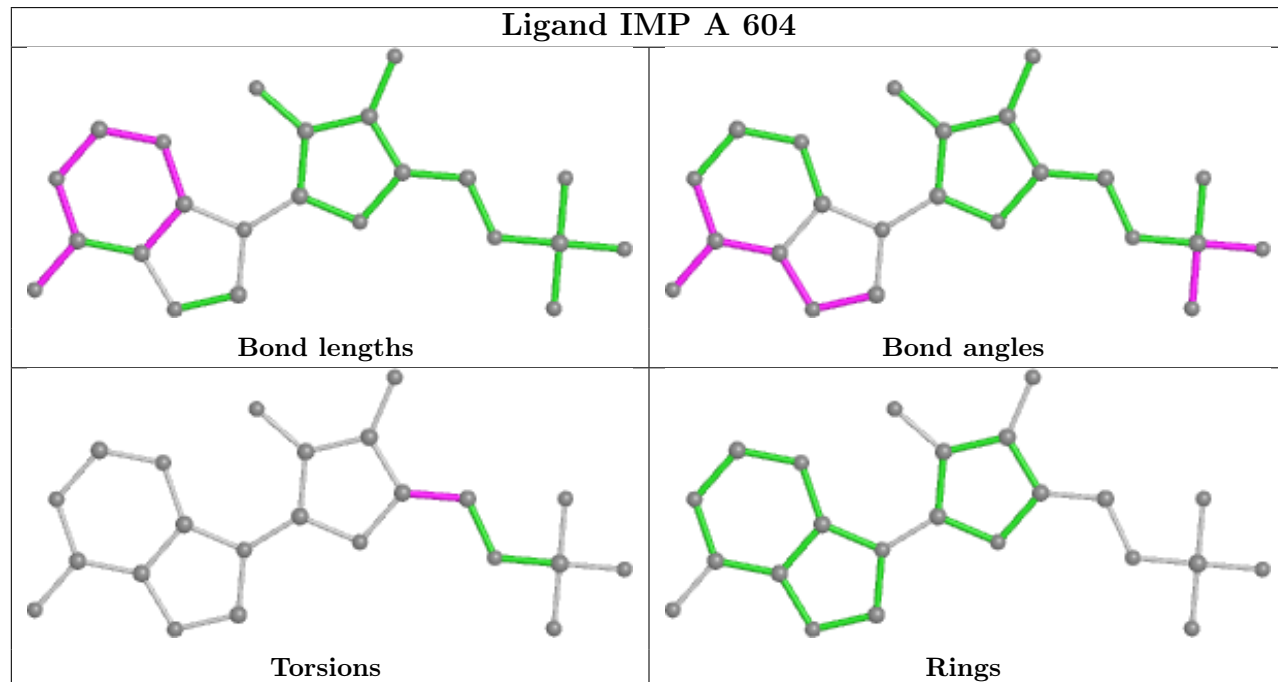
## Ligand GTP E 601

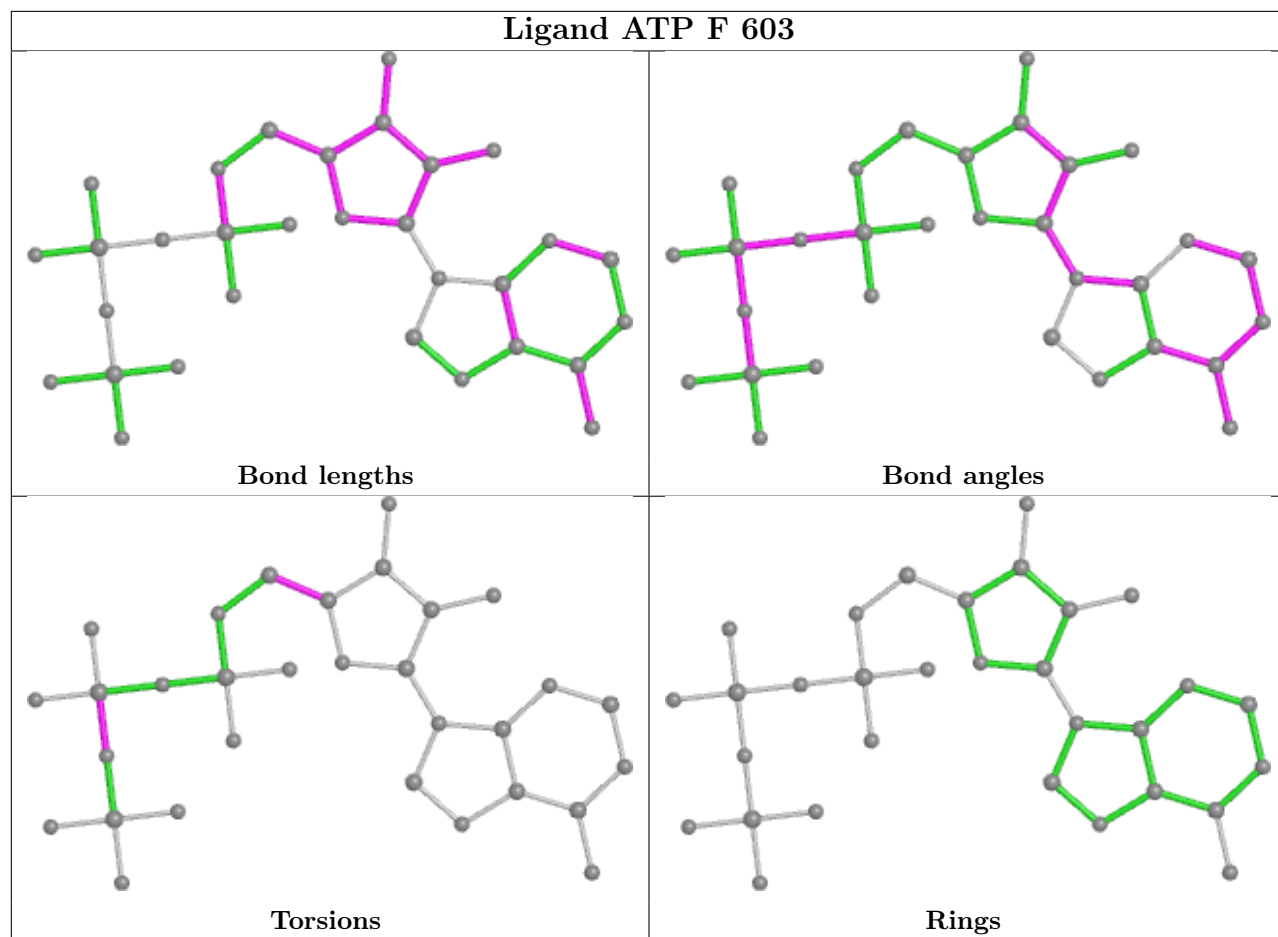


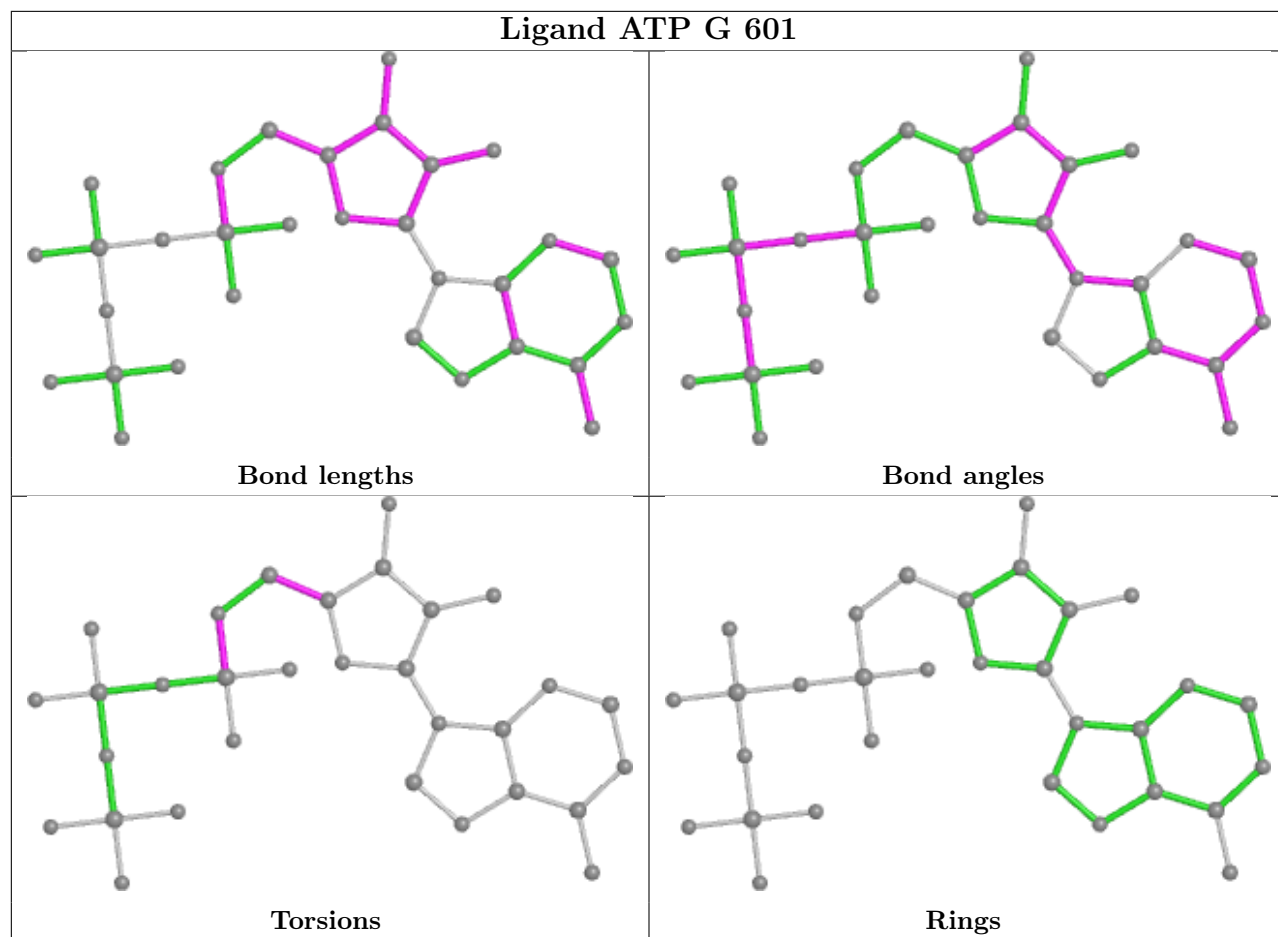
## Ligand GTP B 601

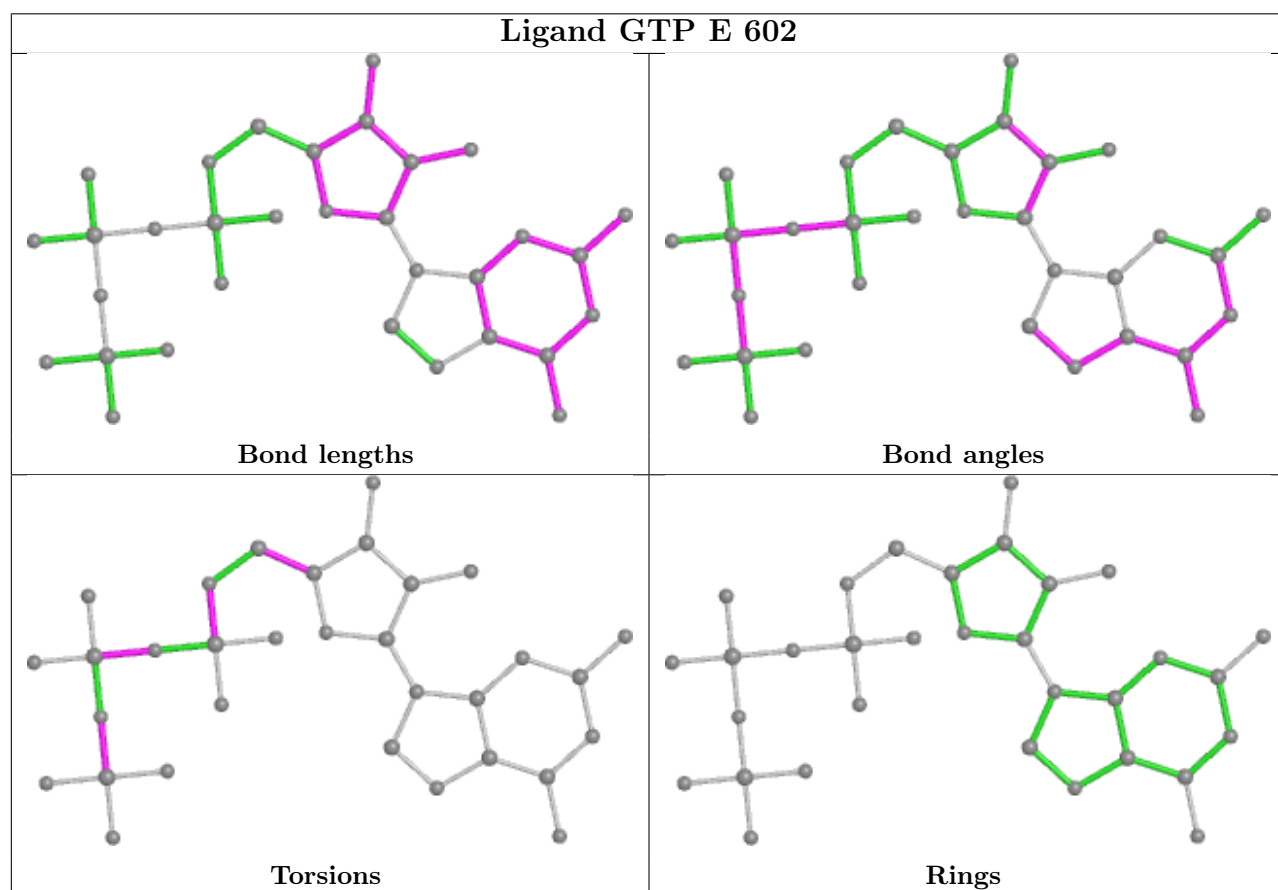
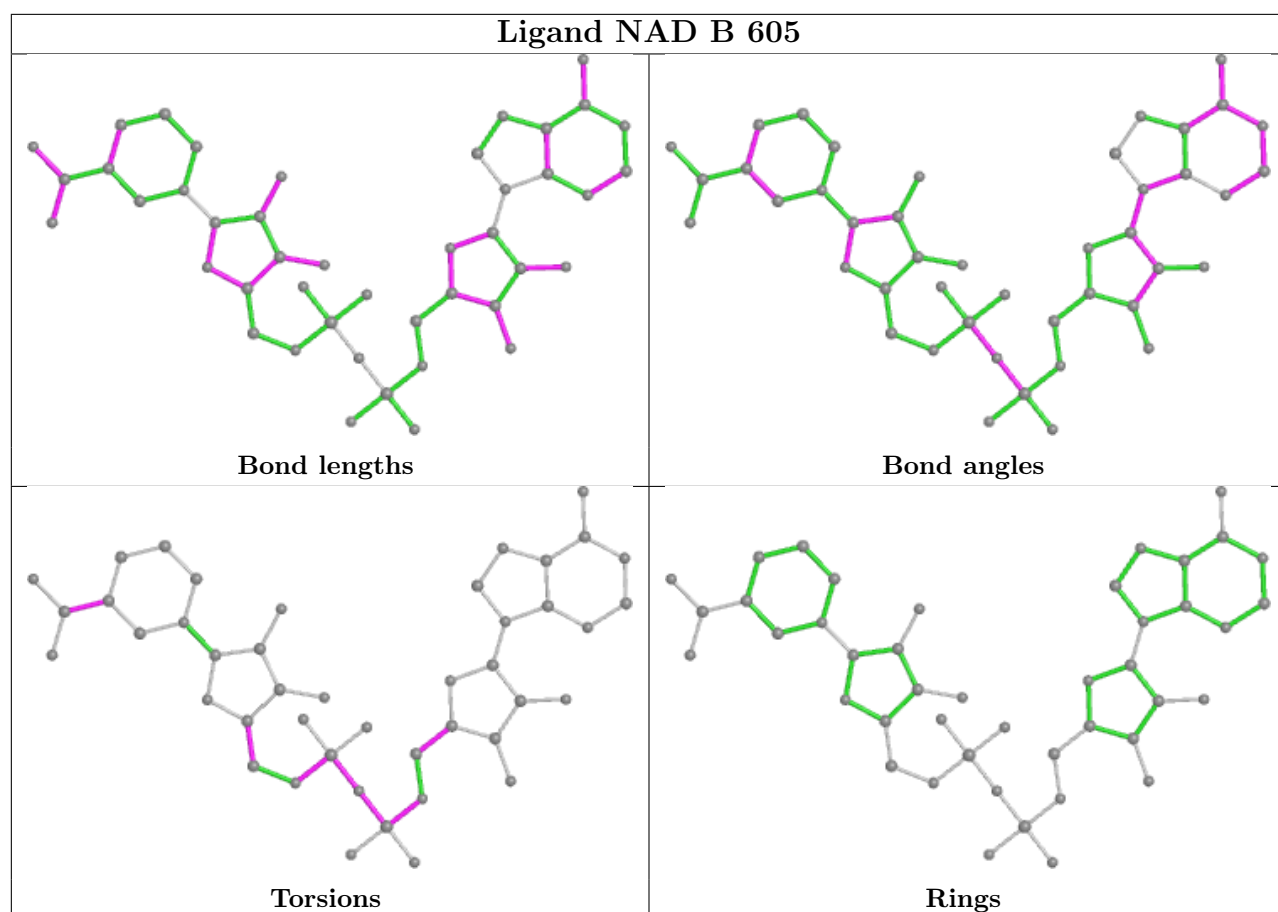


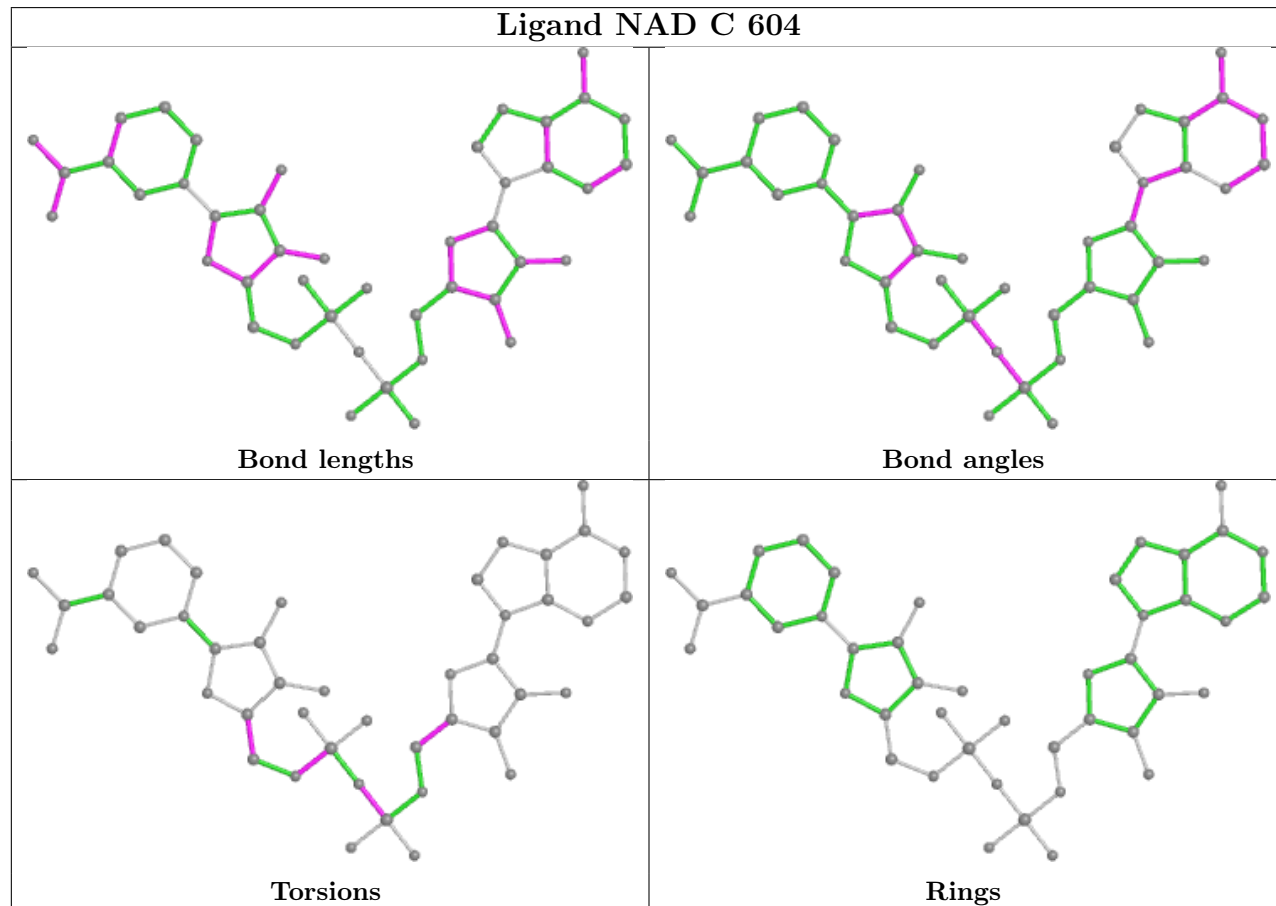
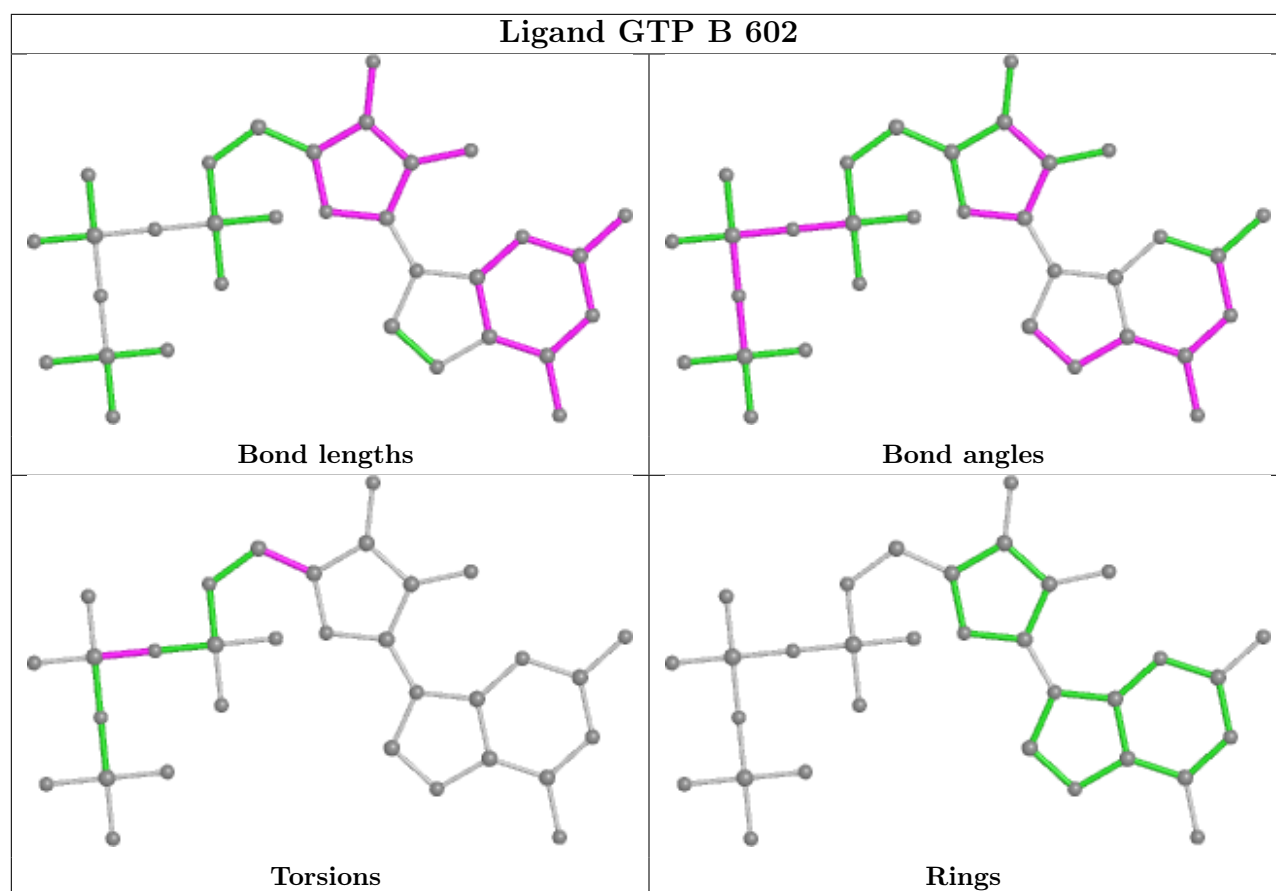
## Ligand IMP A 604



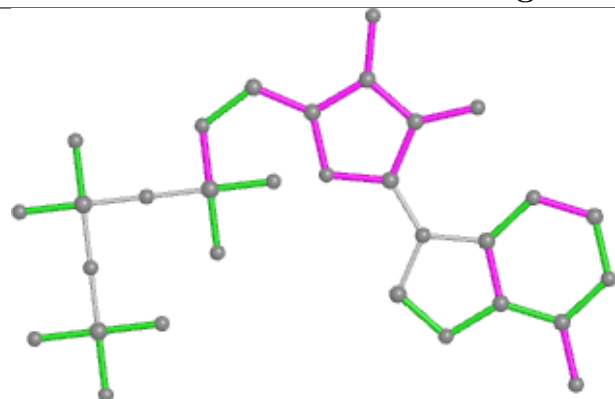




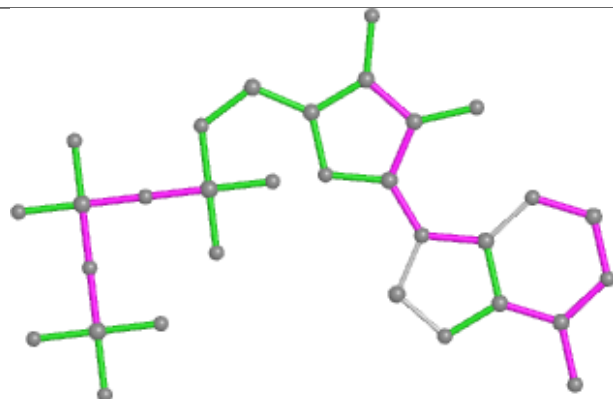




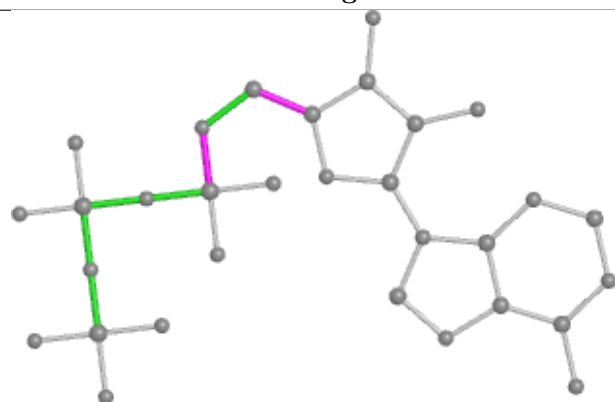
## Ligand ATP C 601



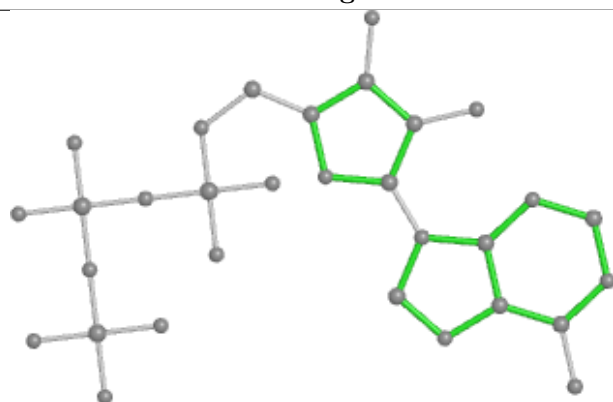
Bond lengths



Bond angles

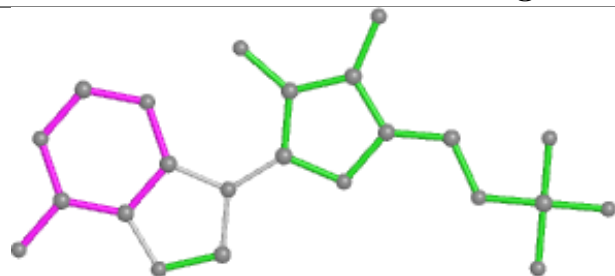


Torsions

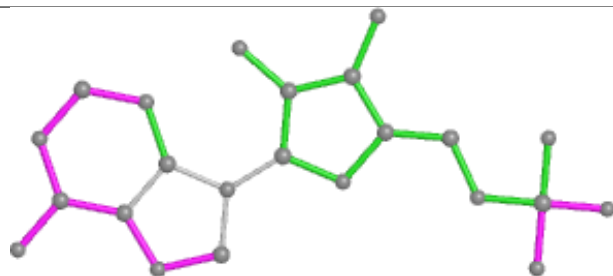


Rings

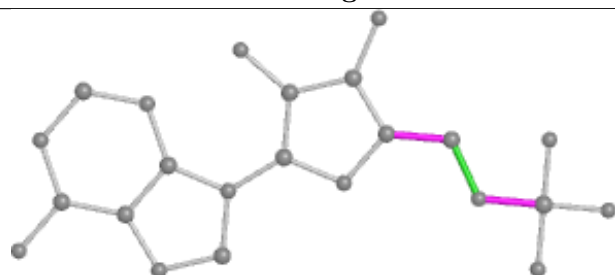
## Ligand IMP G 603



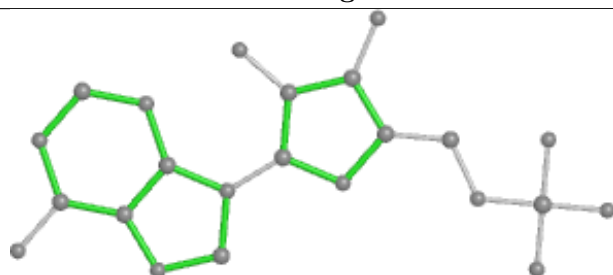
Bond lengths



Bond angles

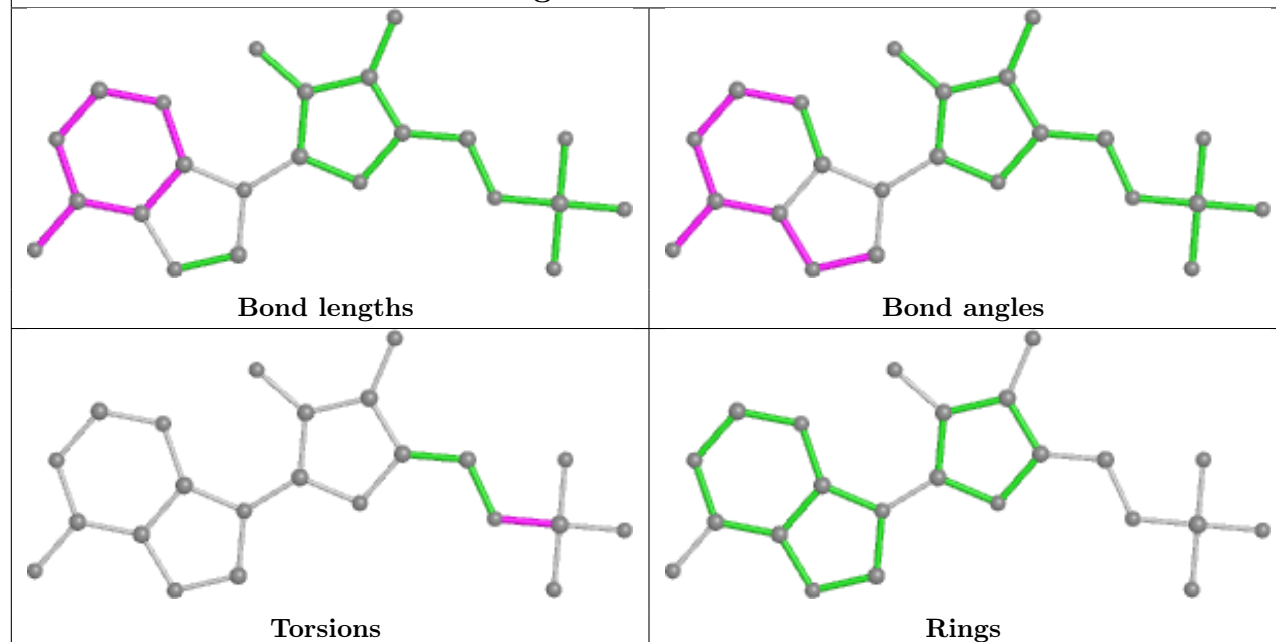


Torsions

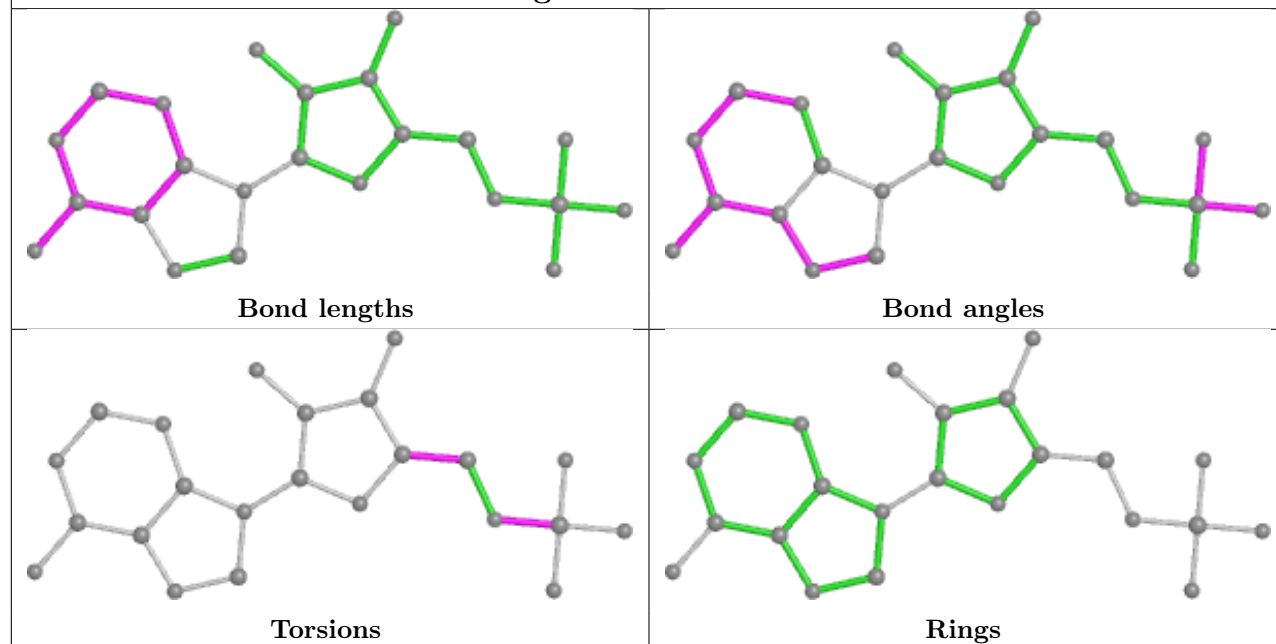


Rings

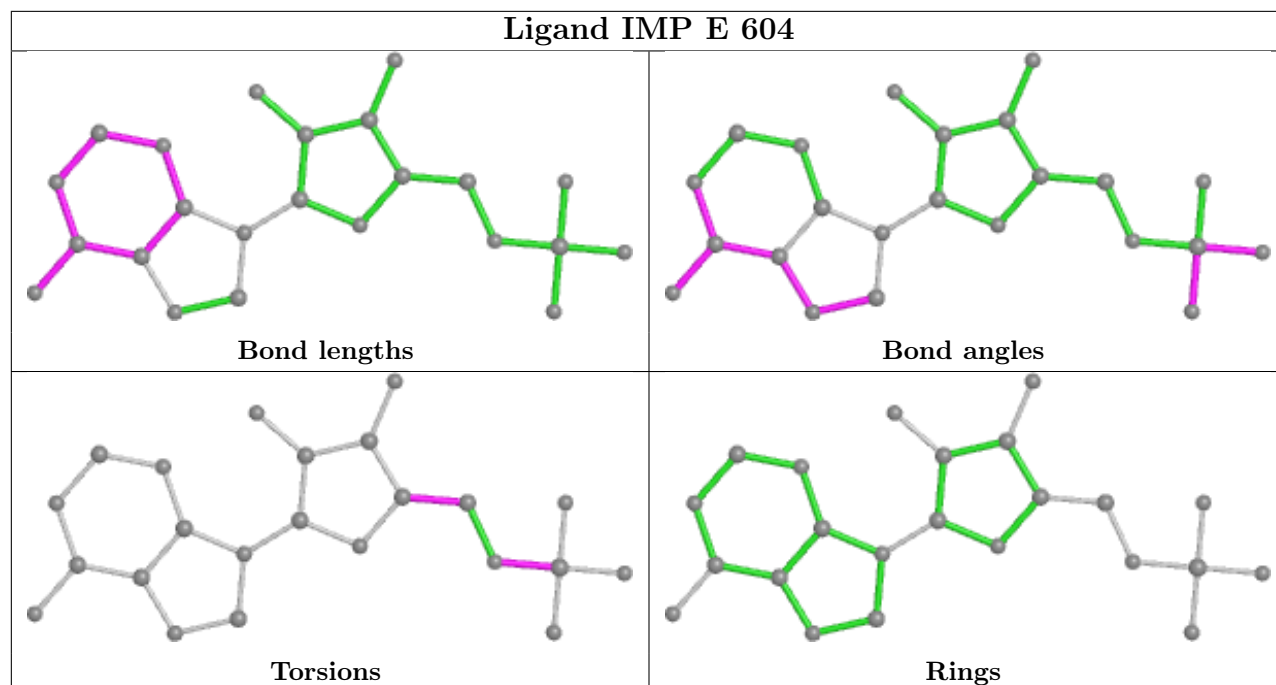
## Ligand IMP B 604



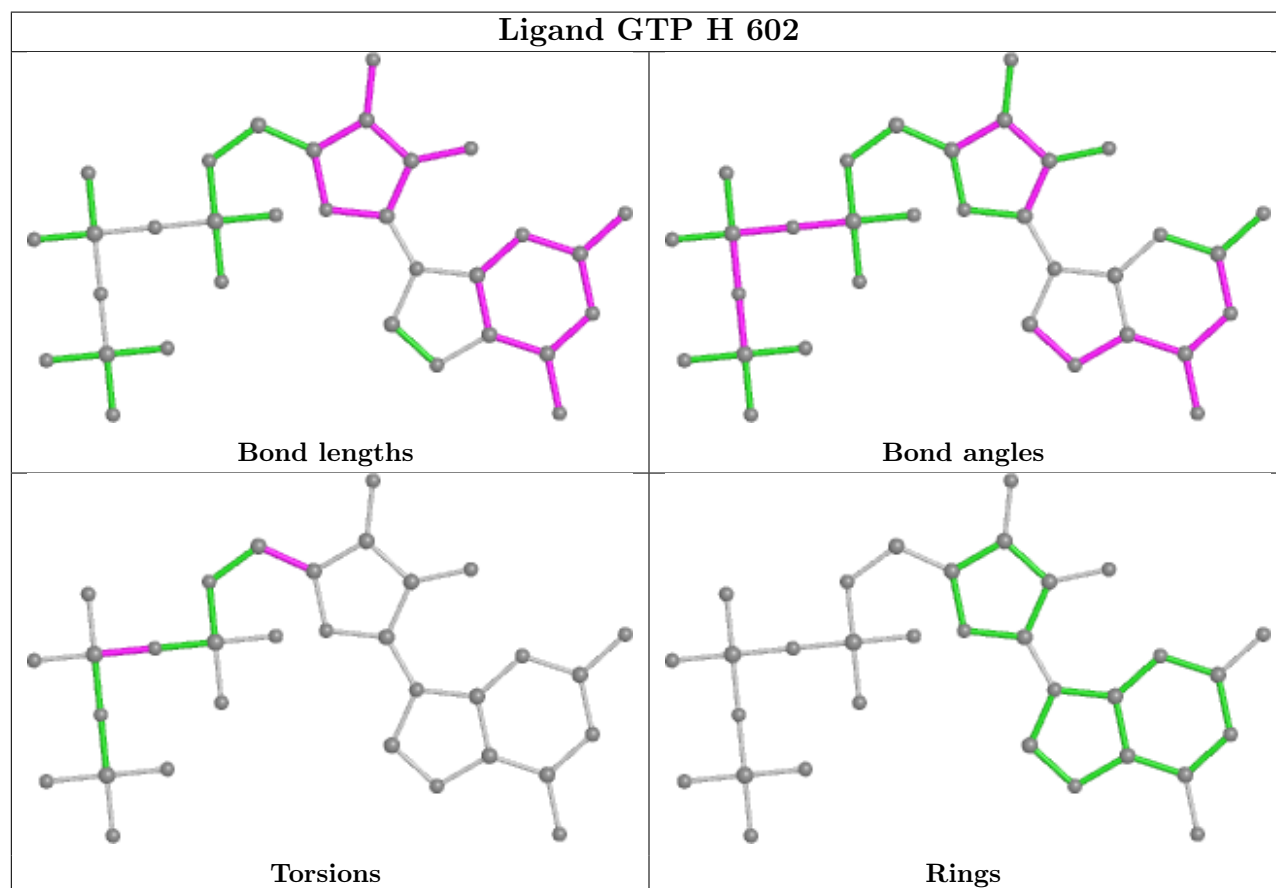
## Ligand IMP C 603

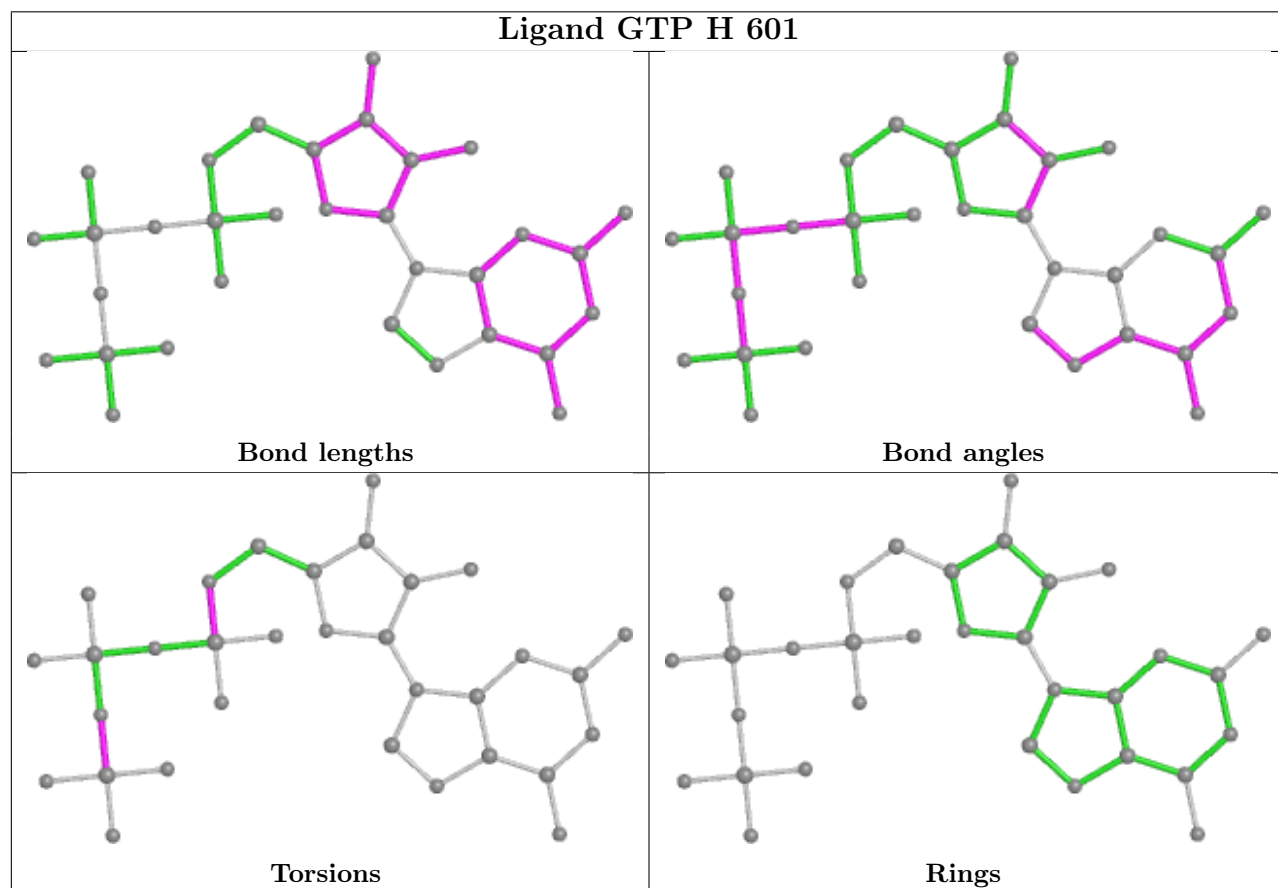
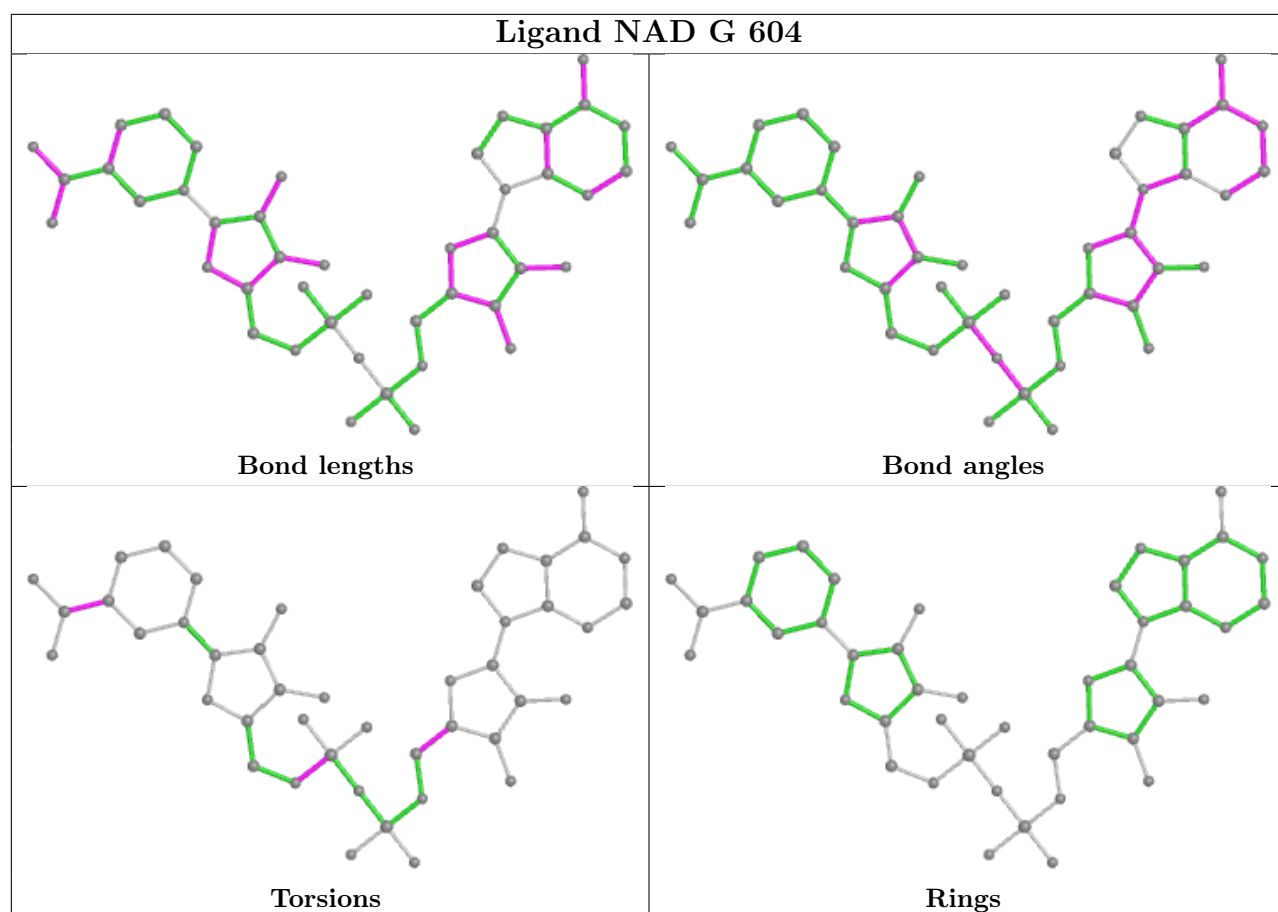


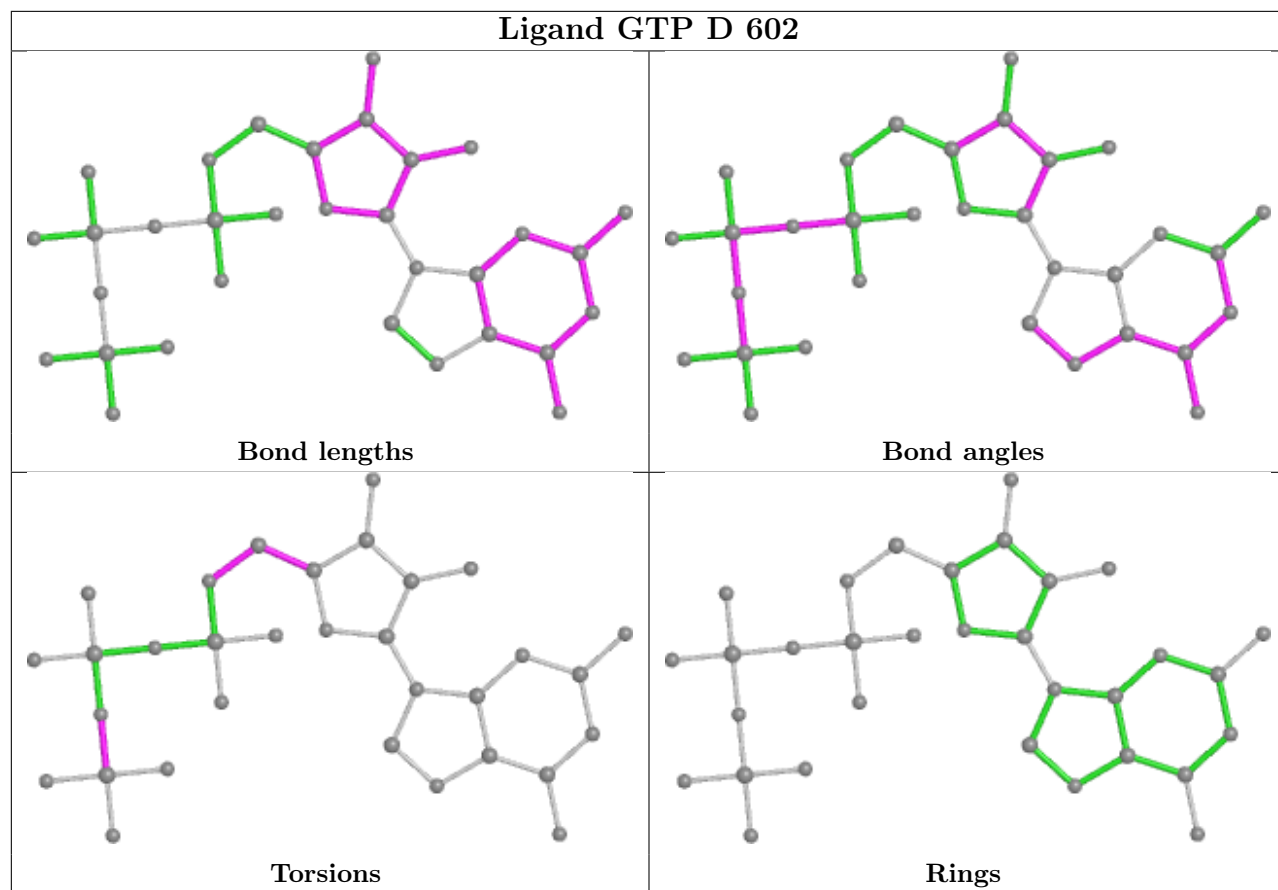
## Ligand IMP E 604

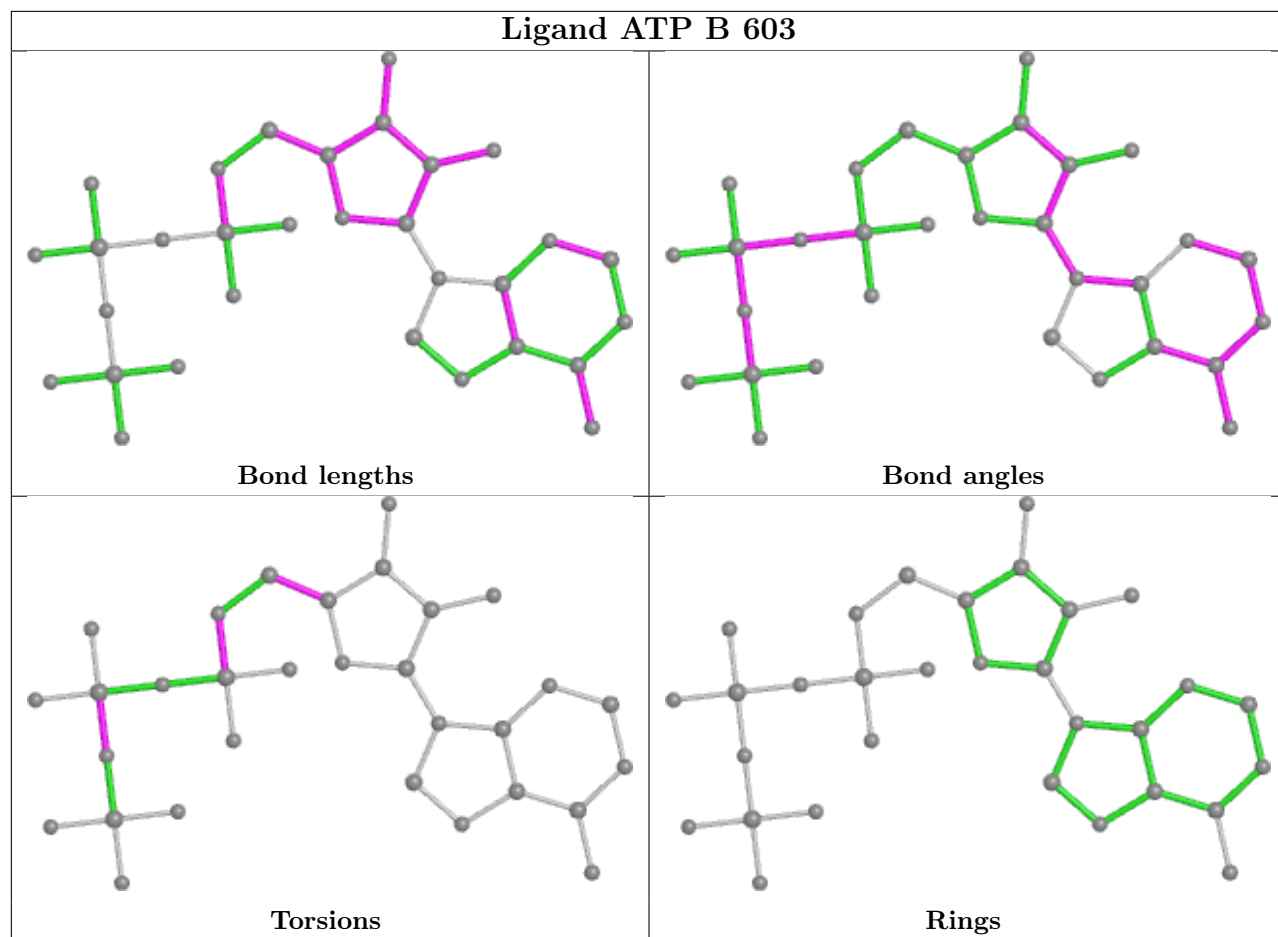


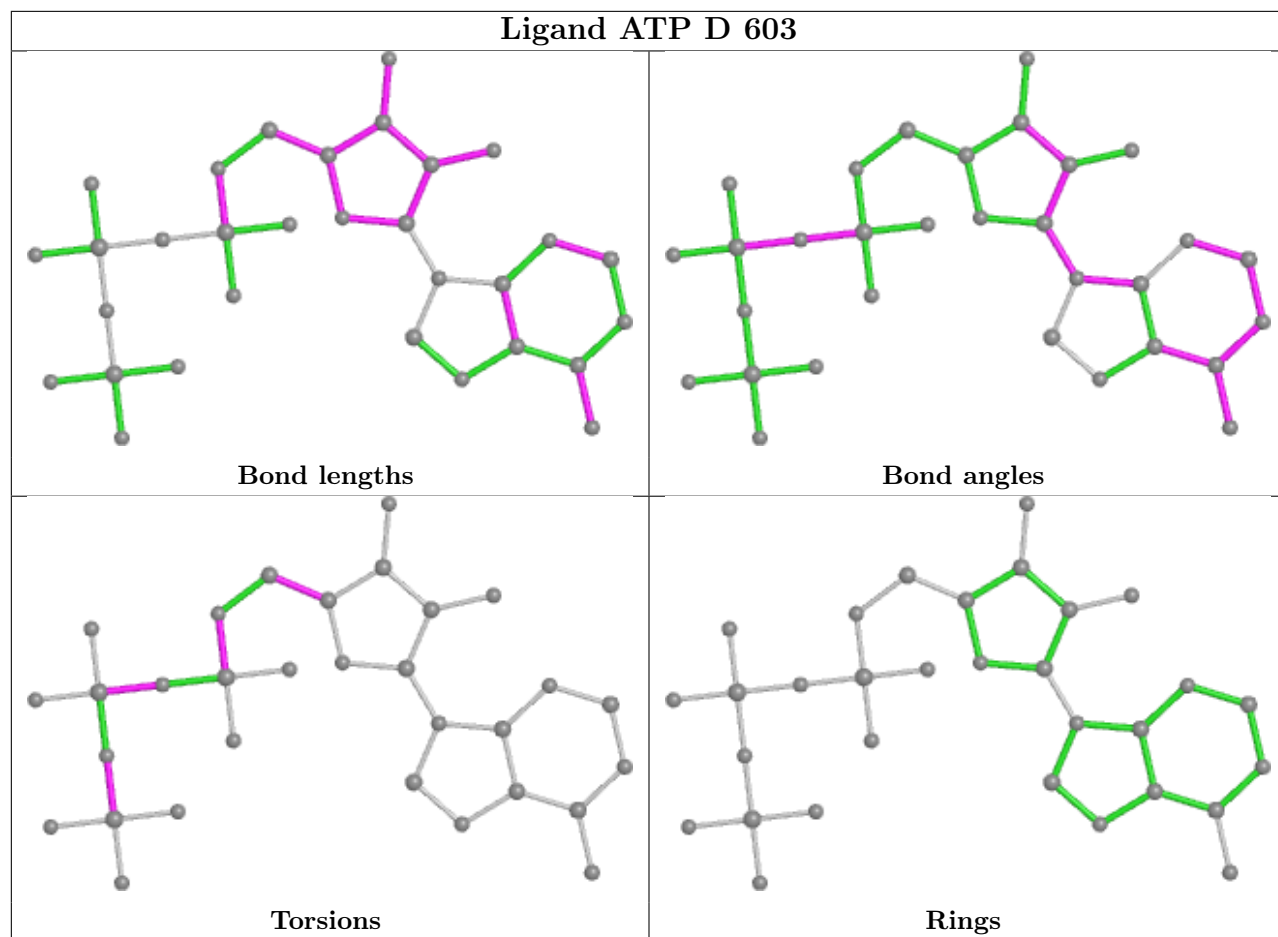
## Ligand GTP H 602

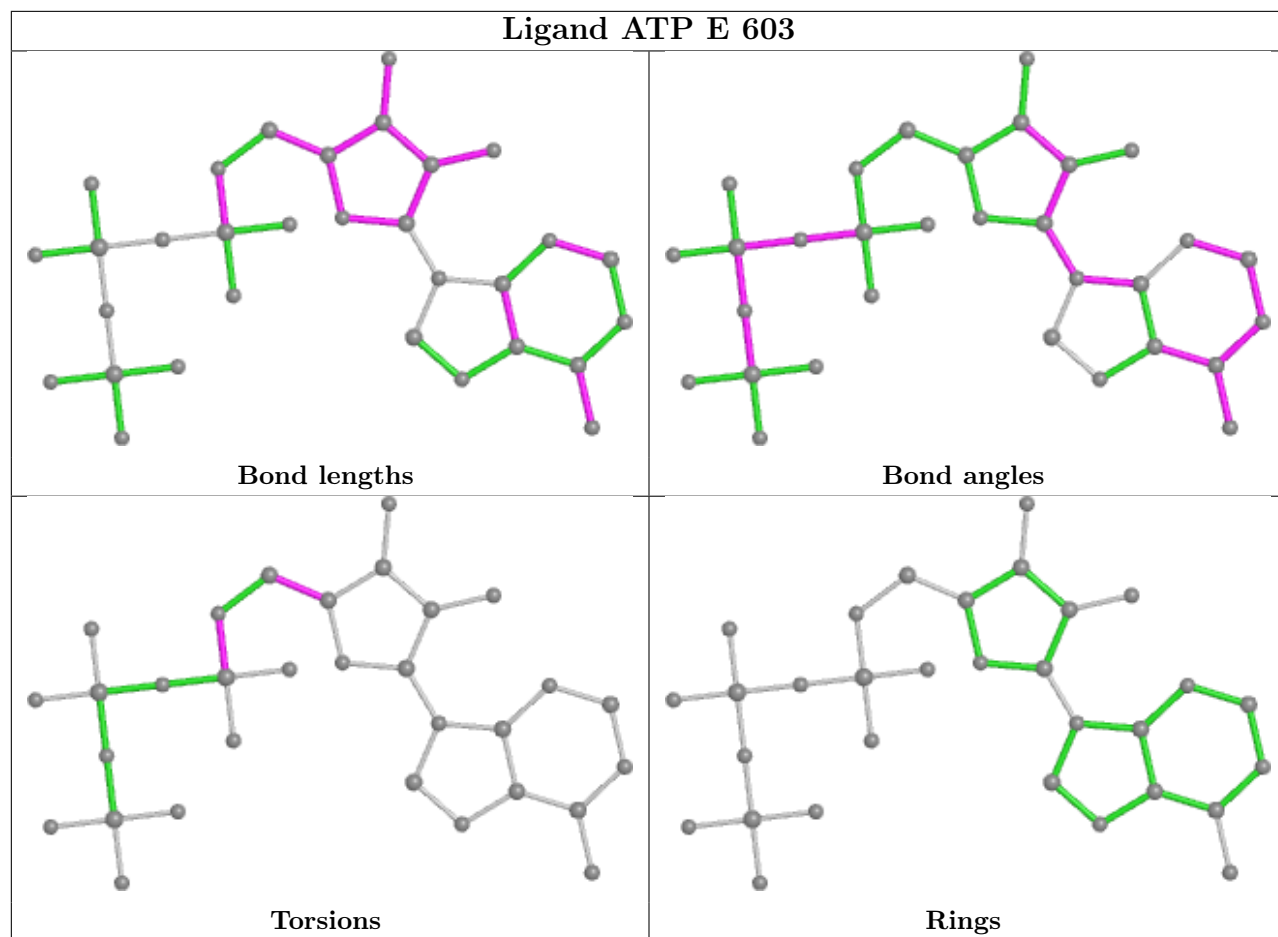


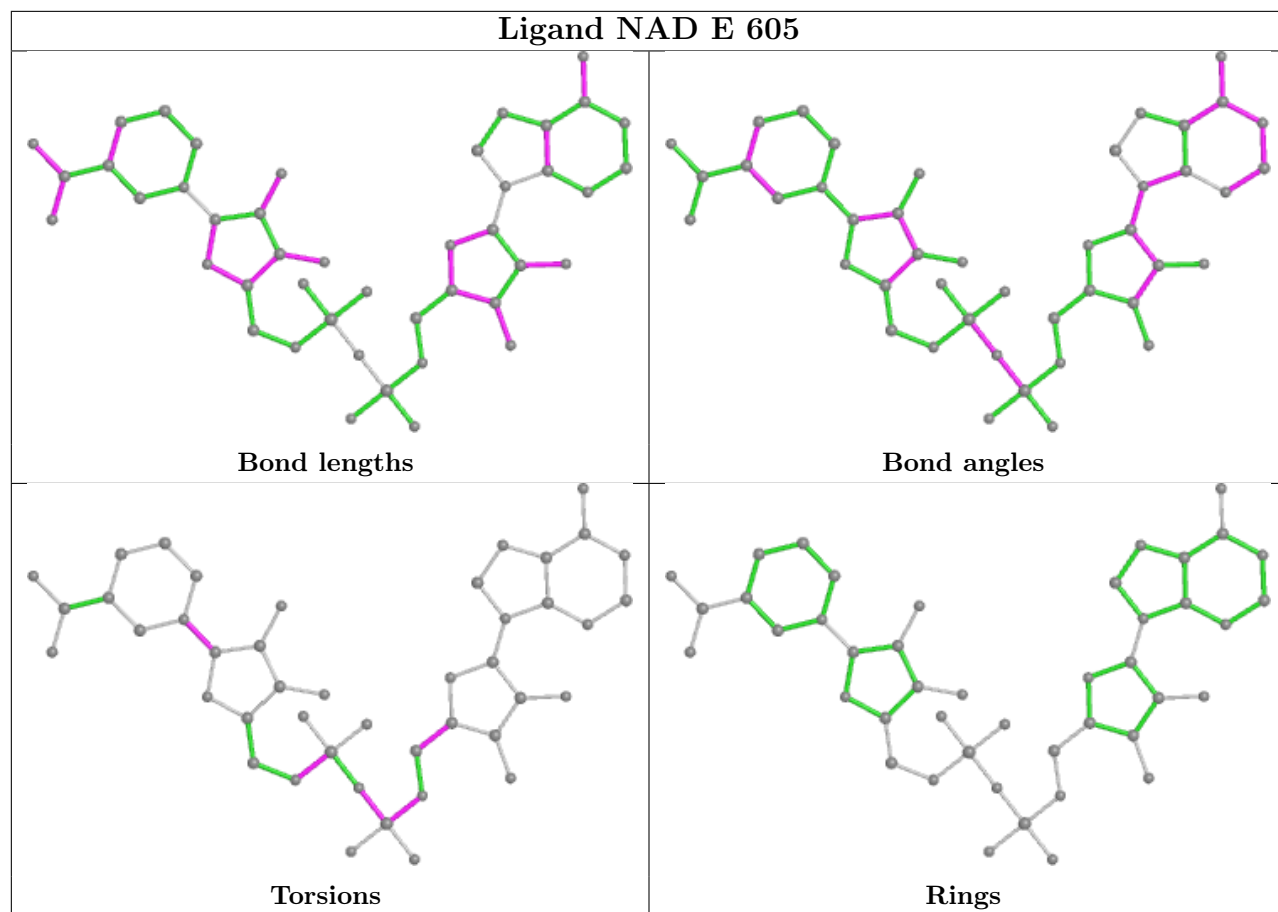


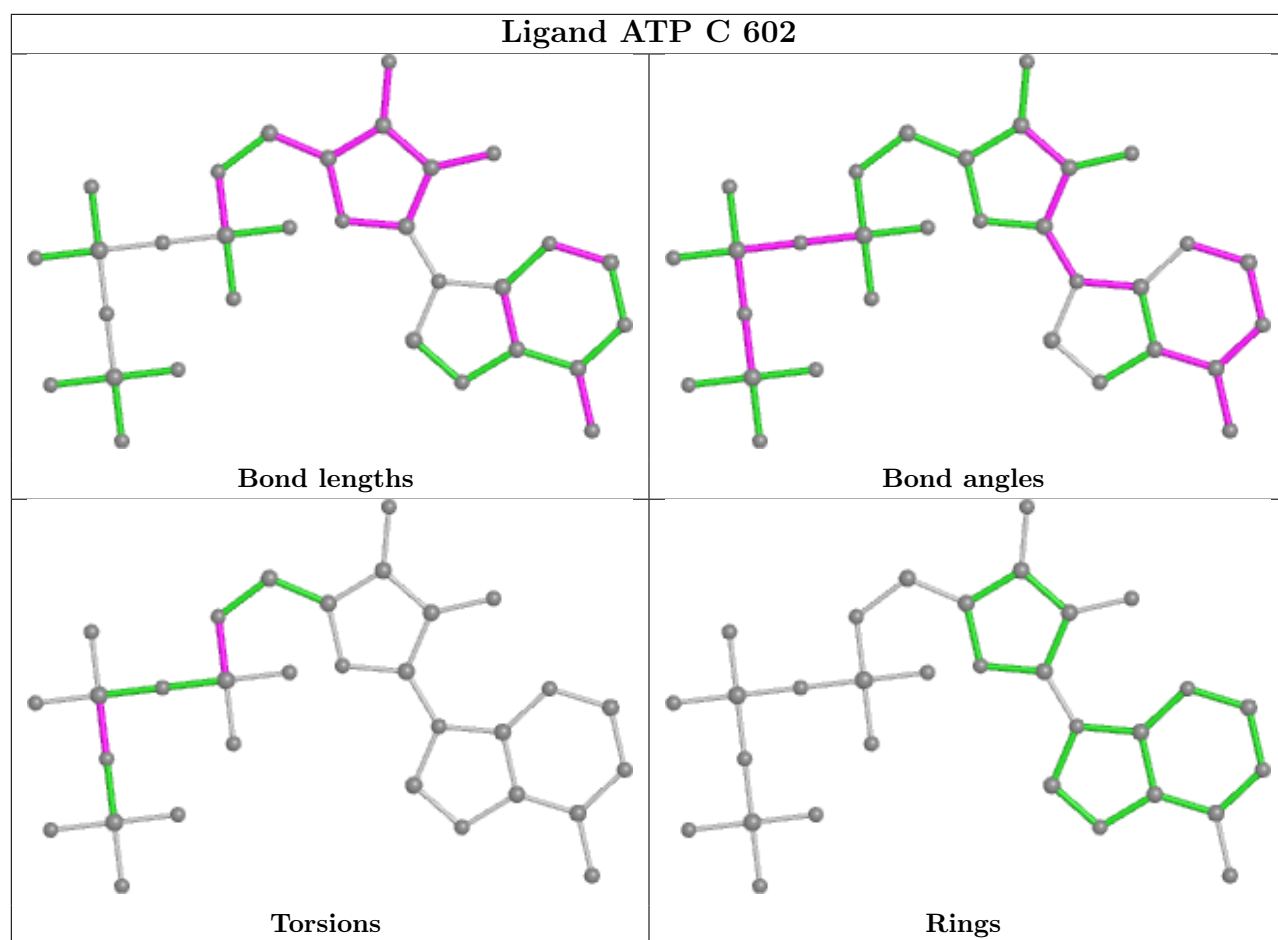


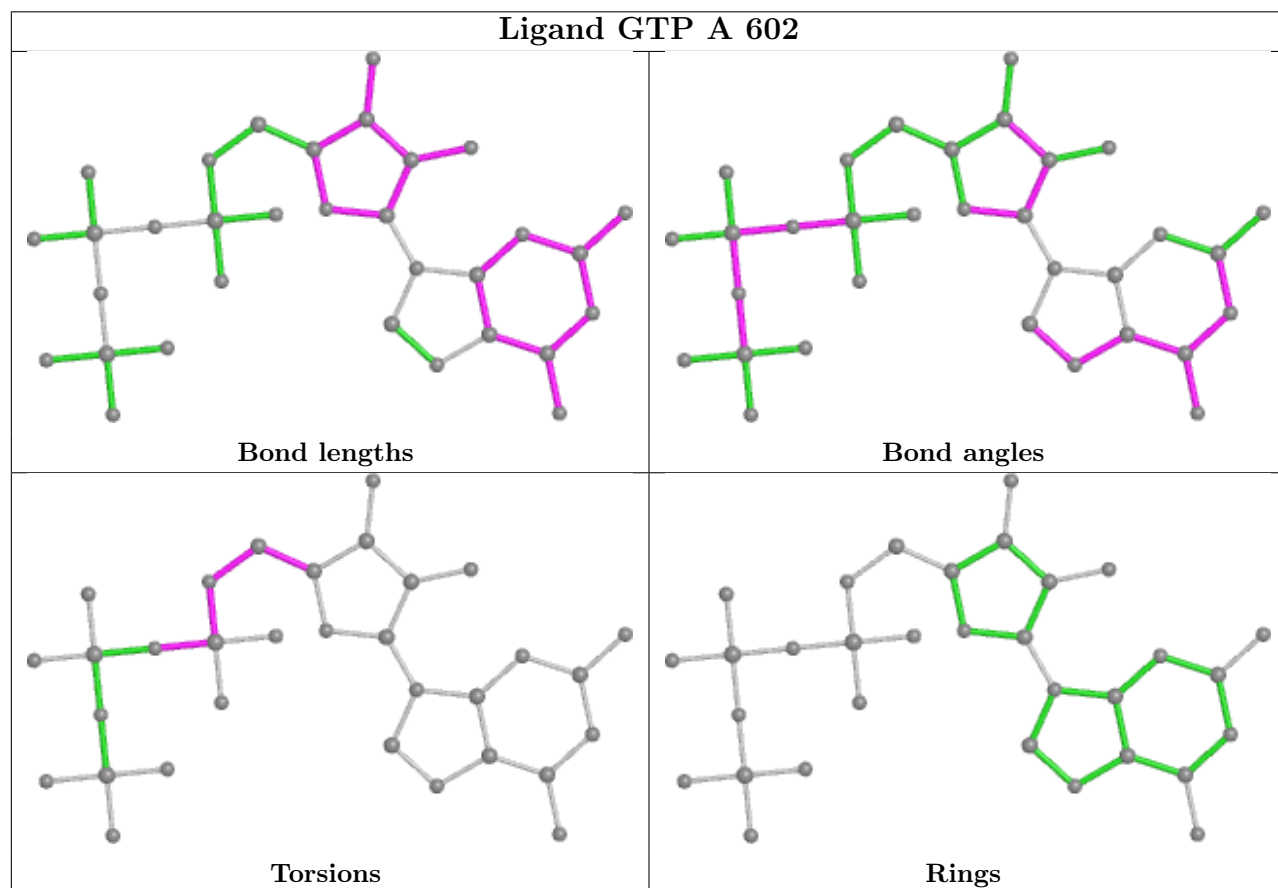
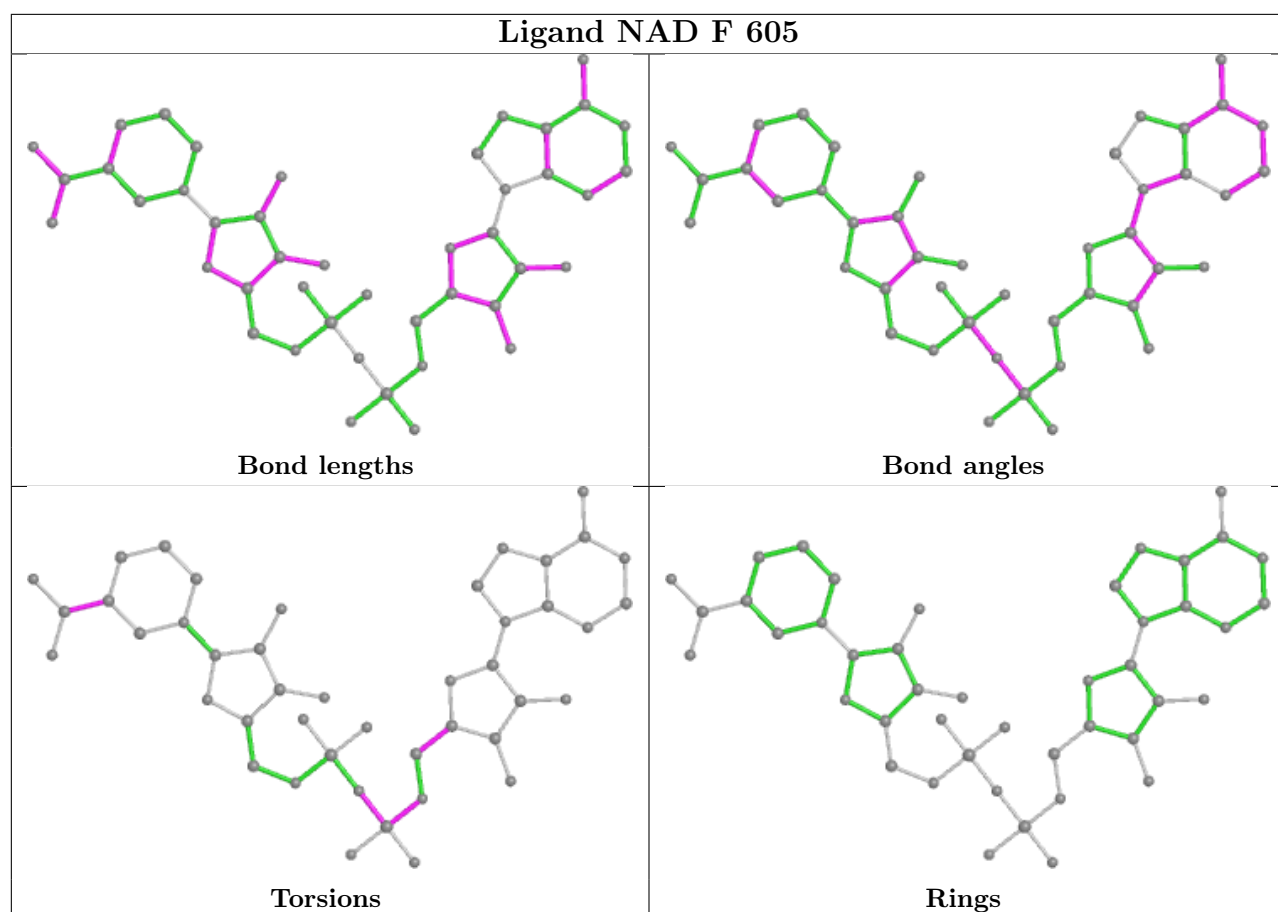


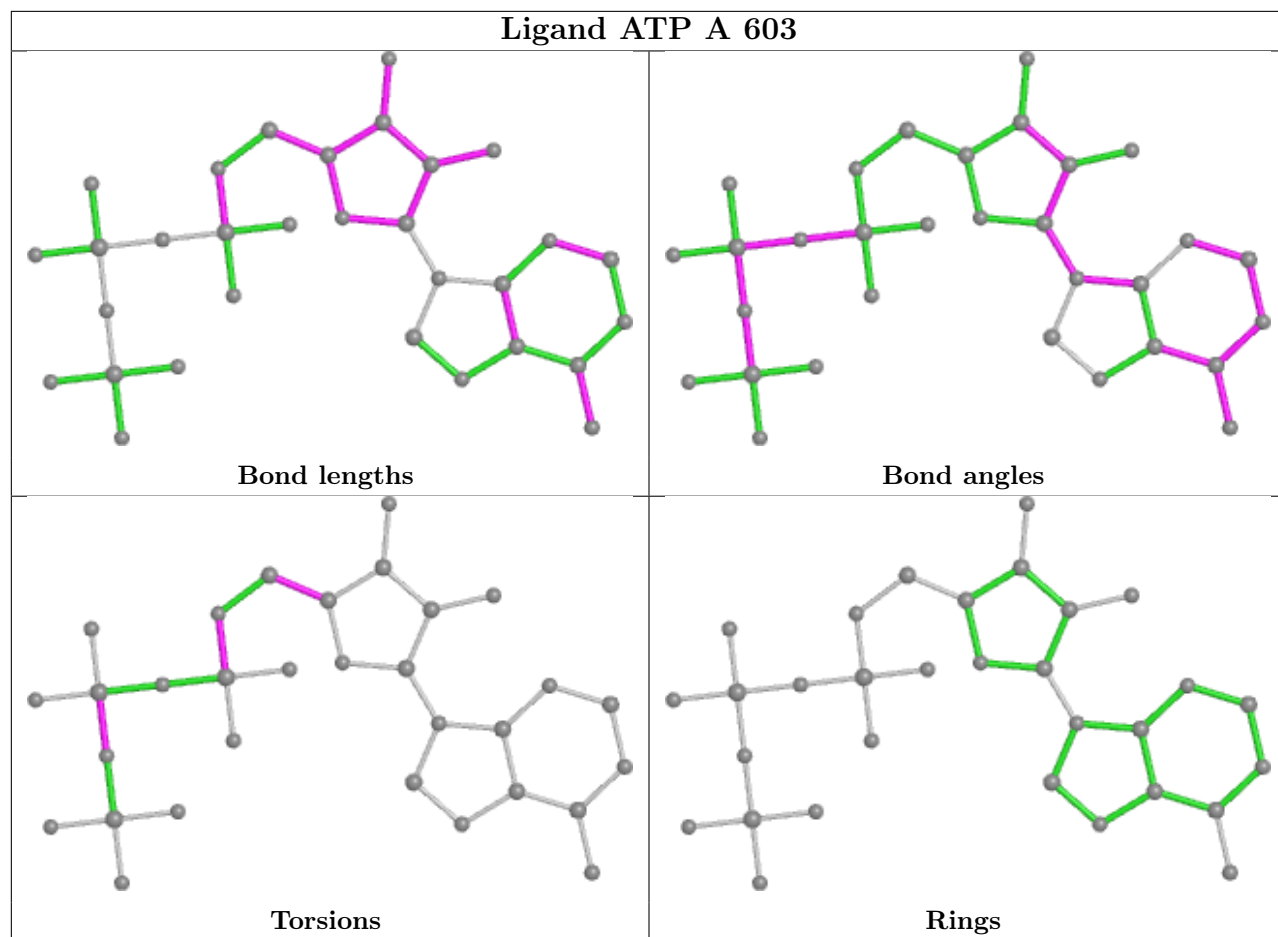




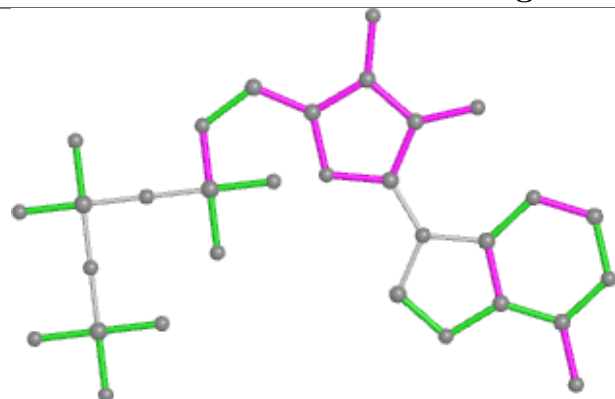




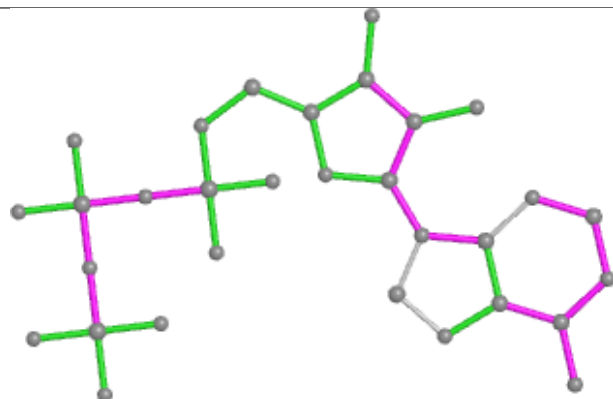




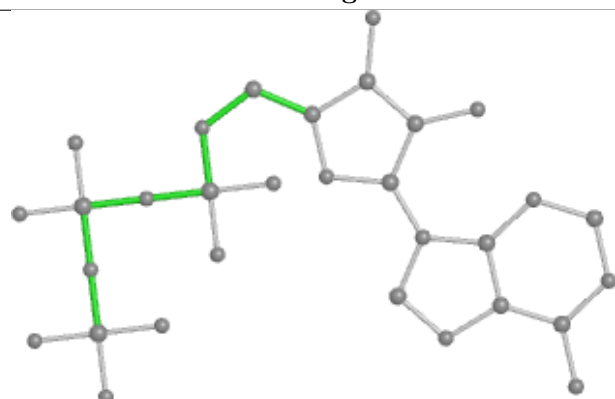
## Ligand ATP H 603



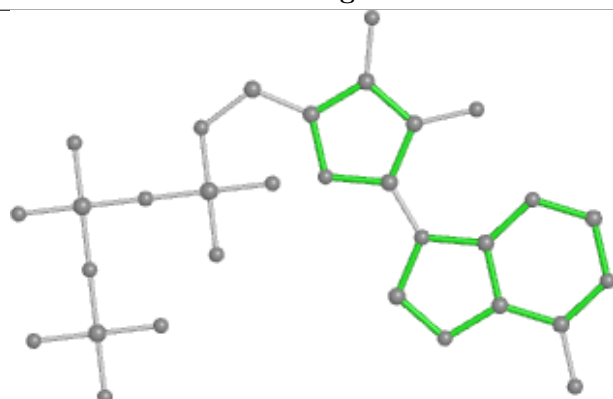
Bond lengths



Bond angles

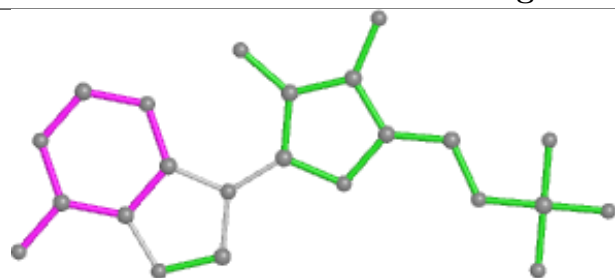


Torsions

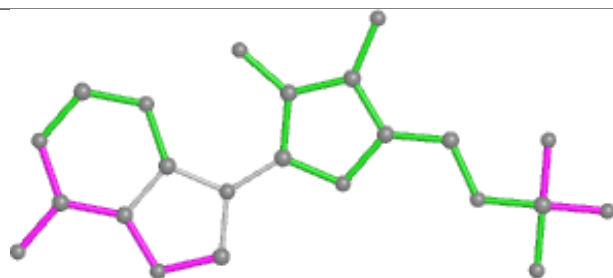


Rings

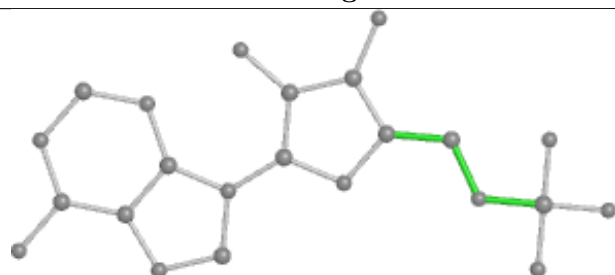
## Ligand IMP H 604



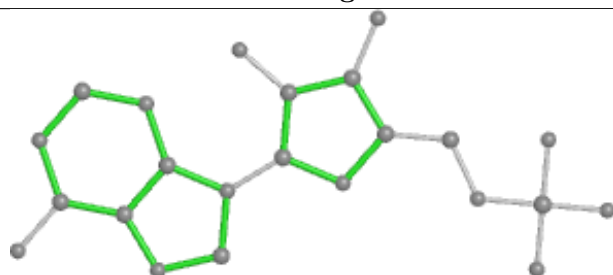
Bond lengths



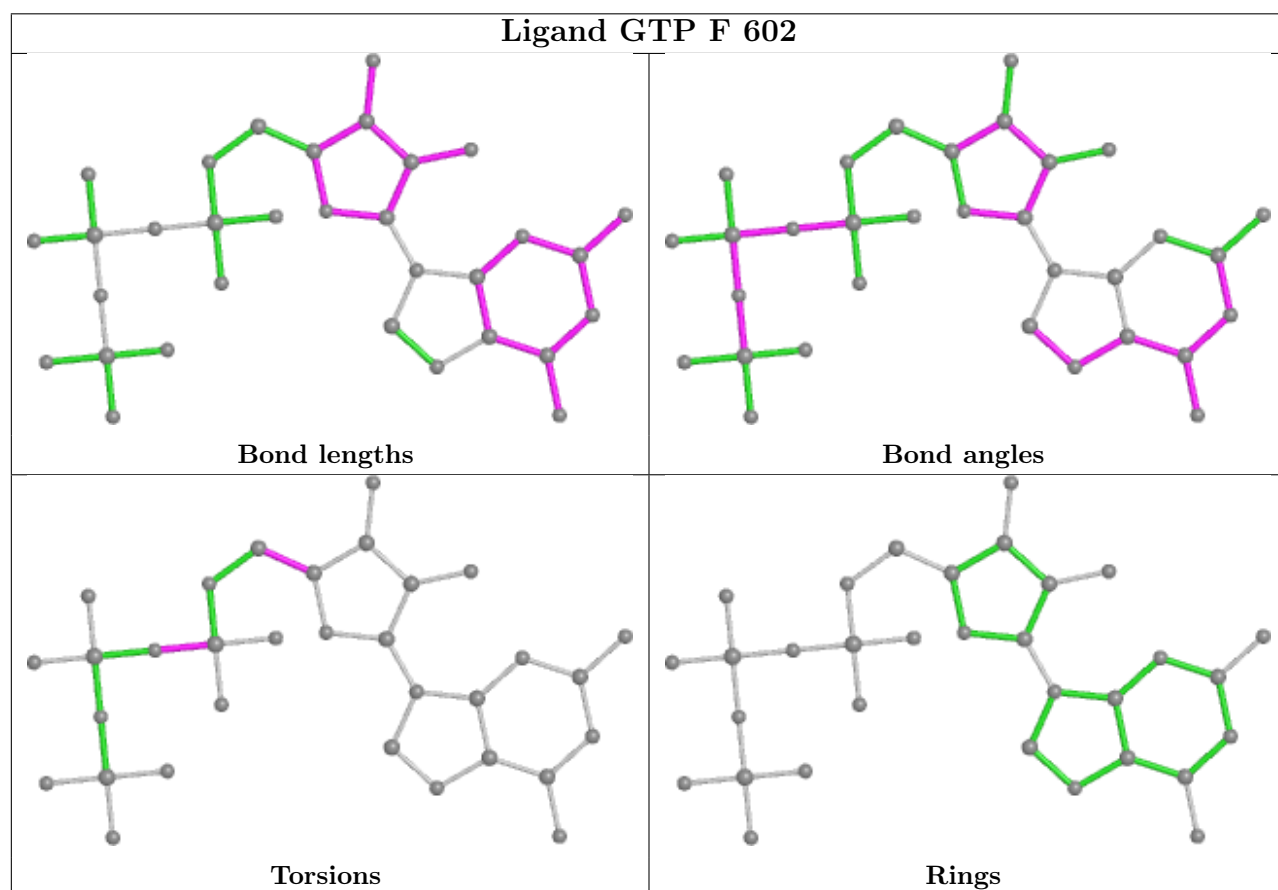
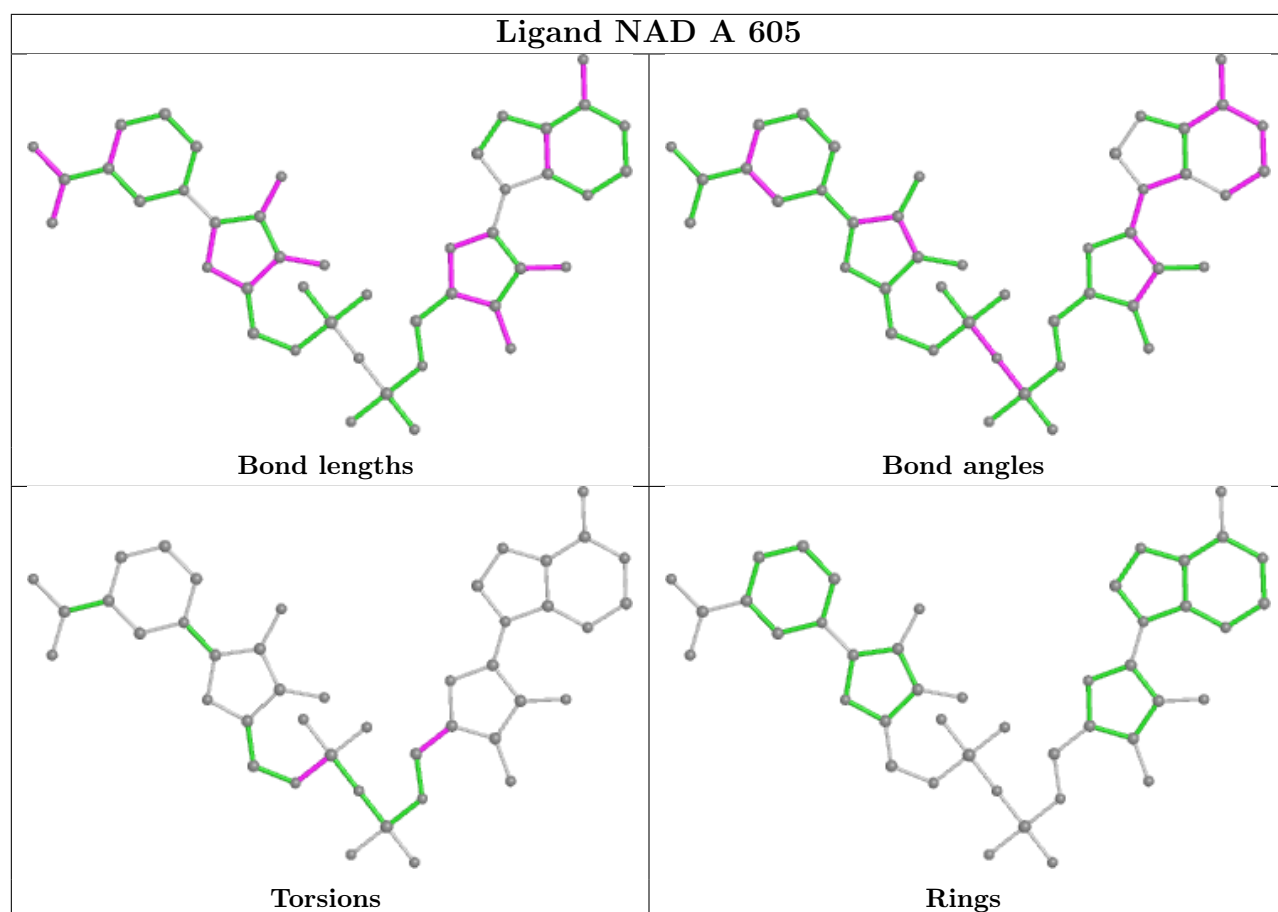
Bond angles



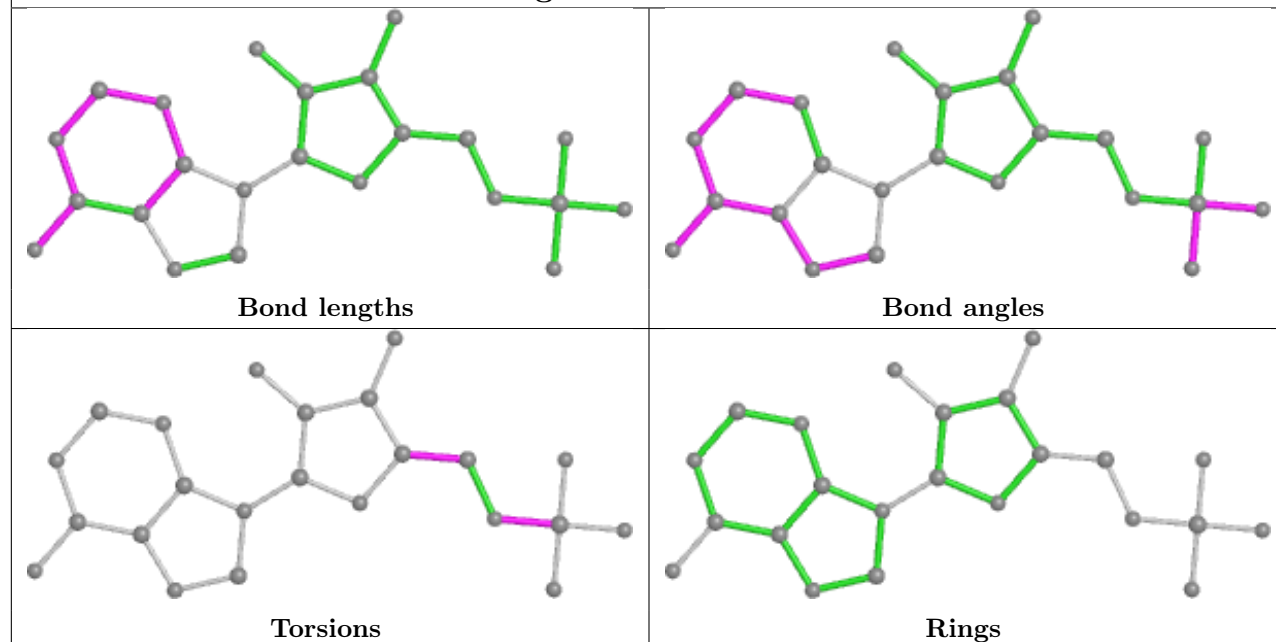
Torsions



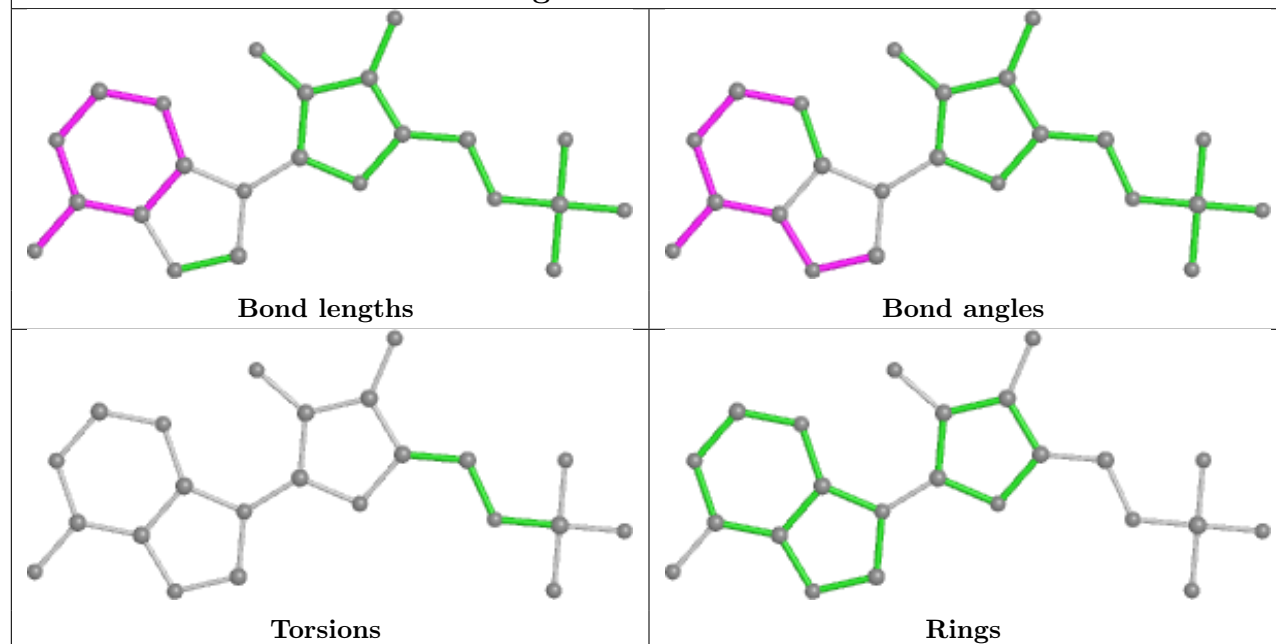
Rings

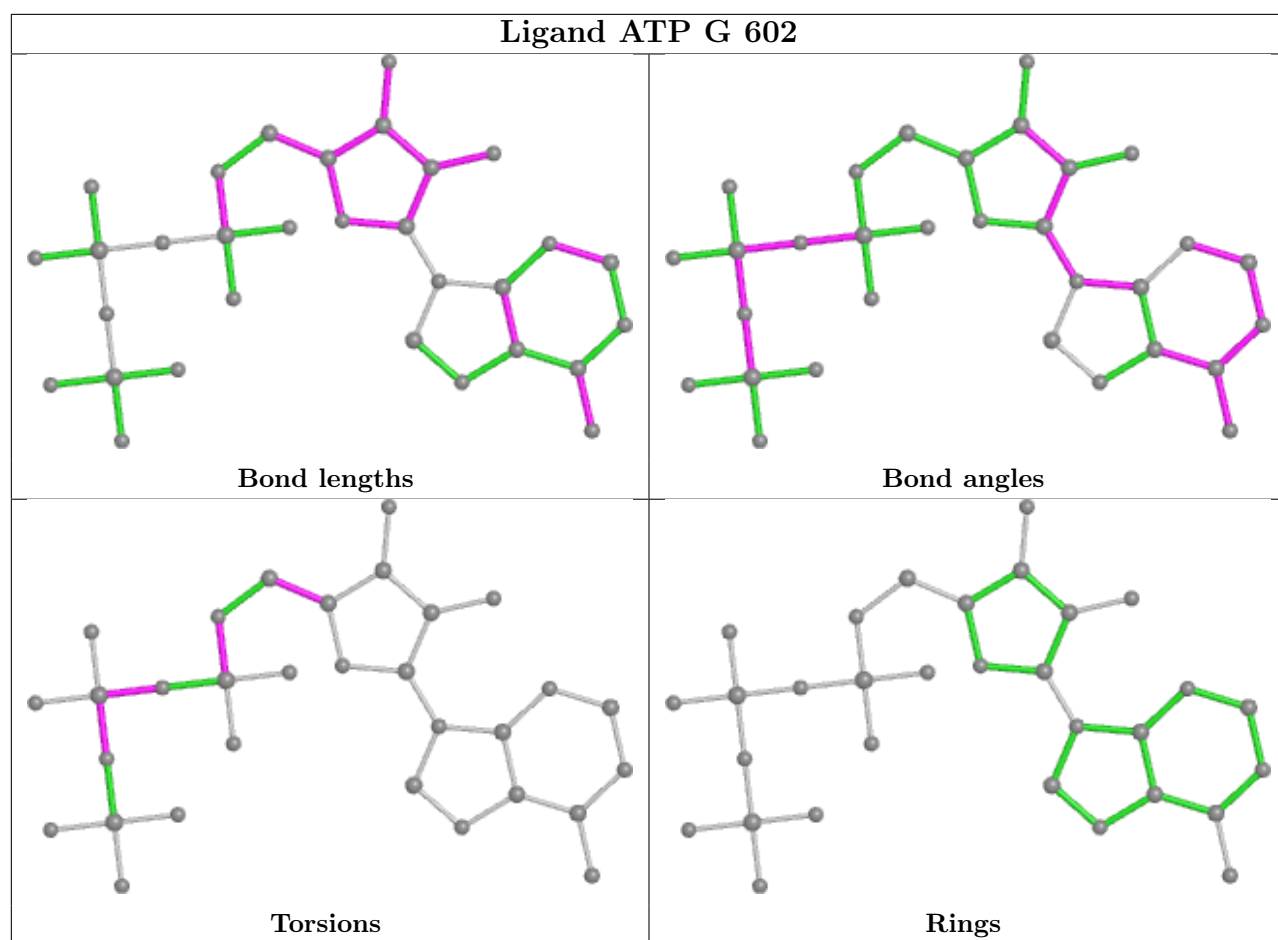


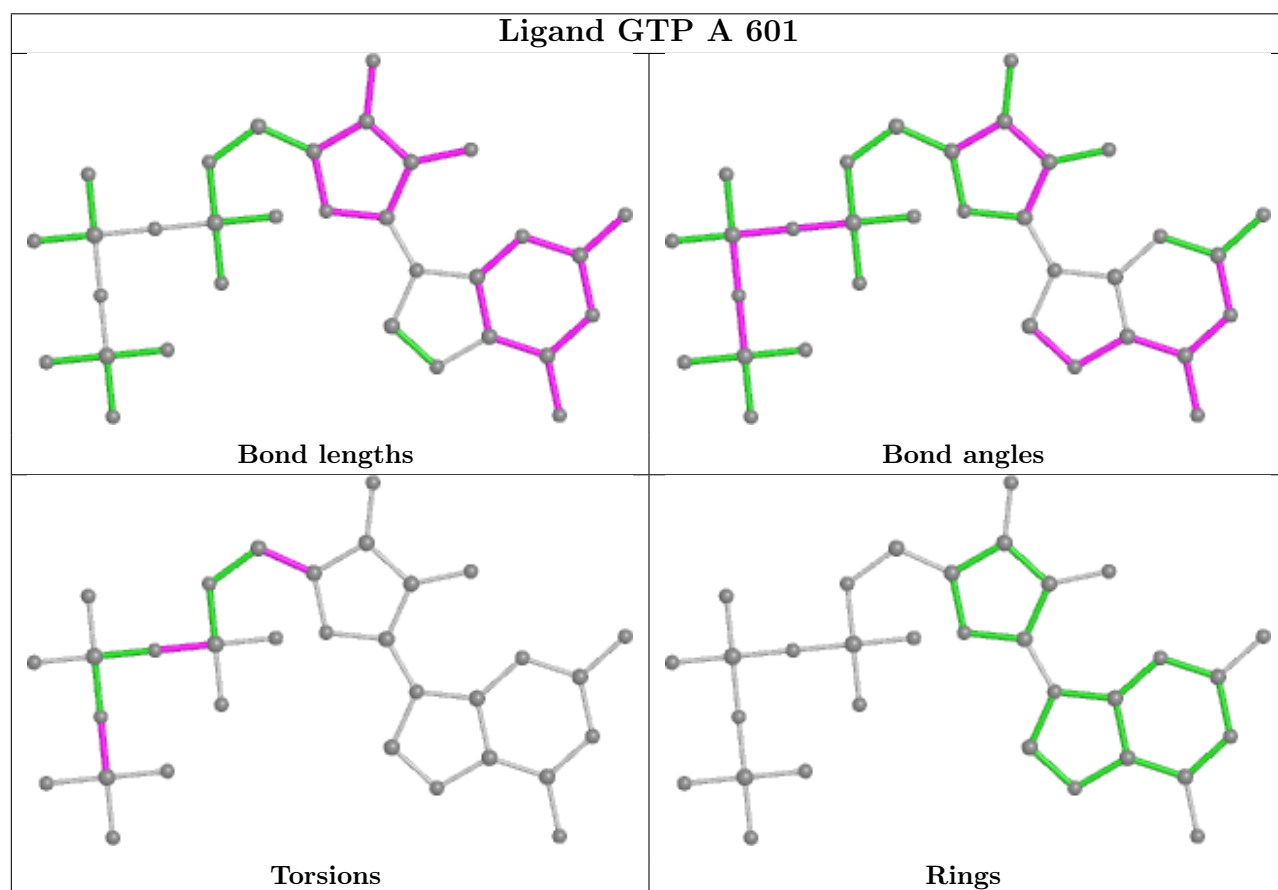
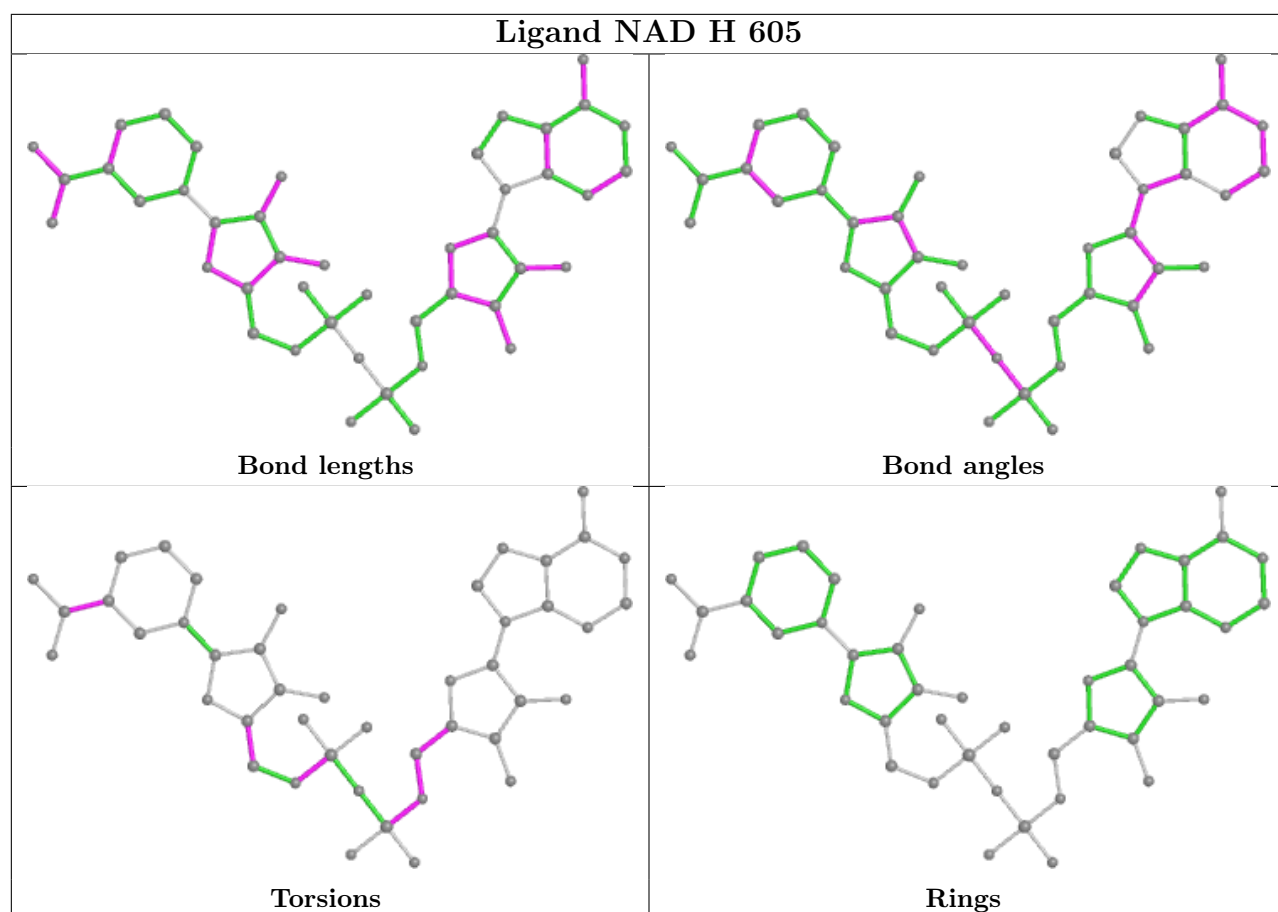
## Ligand IMP F 604



## Ligand IMP D 604







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

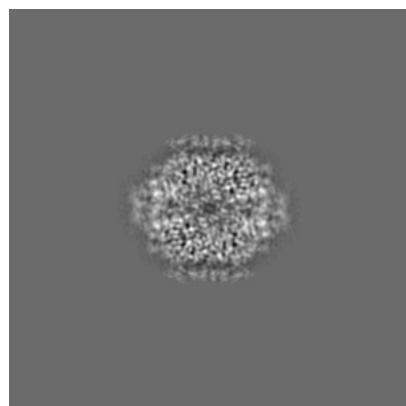
## 6 Map visualisation [i](#)

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

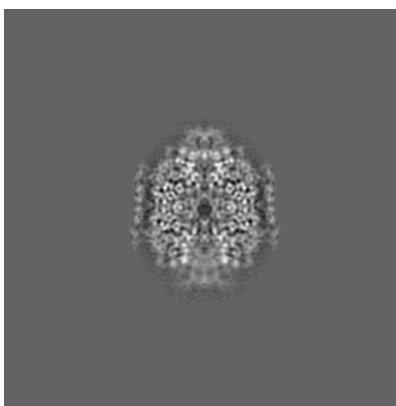
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

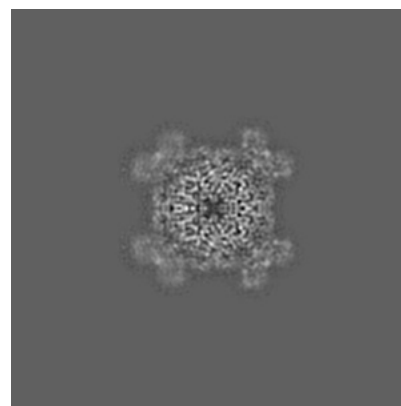
#### 6.1.1 Primary map



X

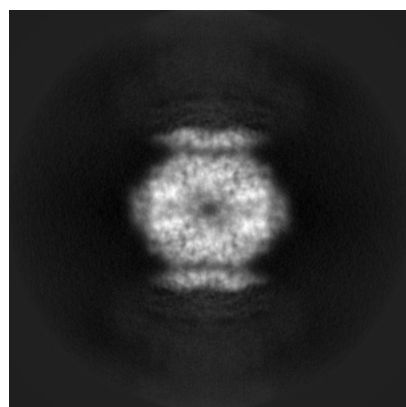


Y

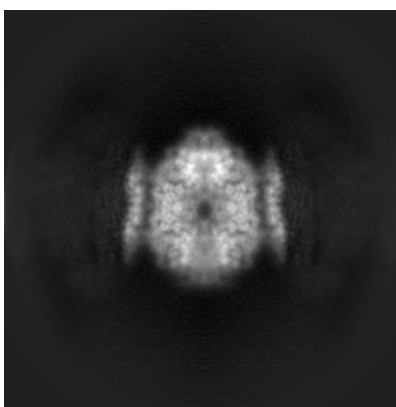


Z

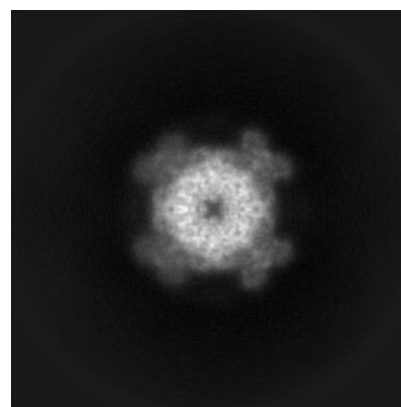
#### 6.1.2 Raw map



X



Y

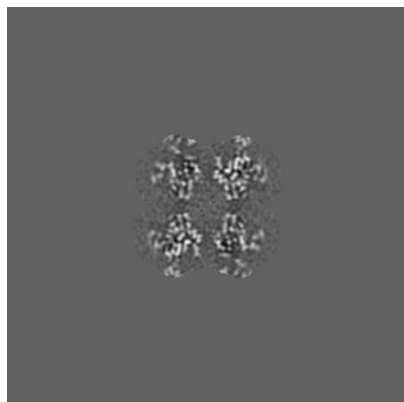


Z

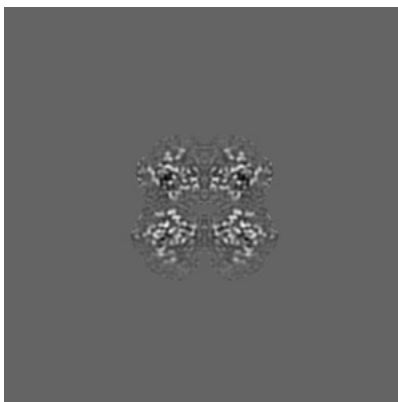
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

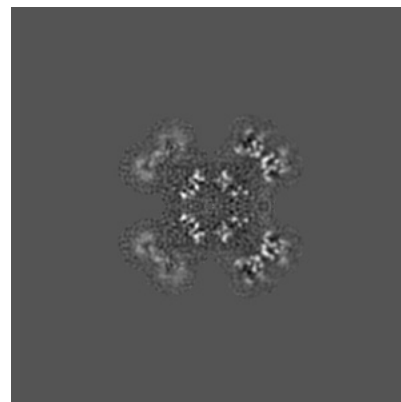
### 6.2.1 Primary map



X Index: 160

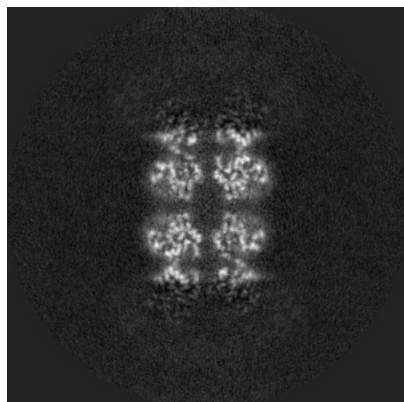


Y Index: 160

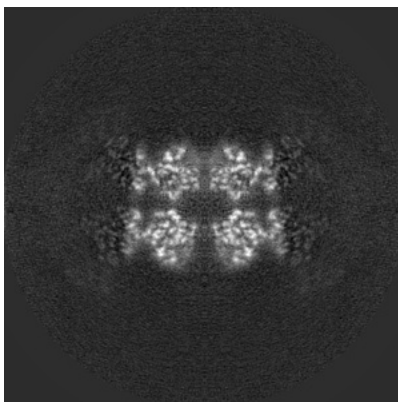


Z Index: 160

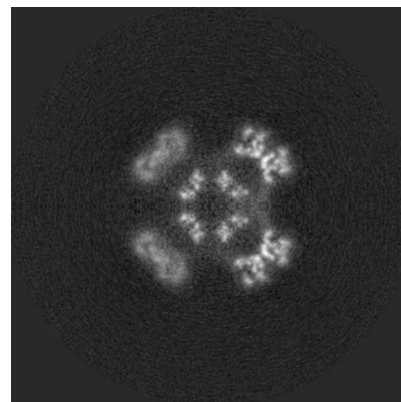
### 6.2.2 Raw map



X Index: 160



Y Index: 160

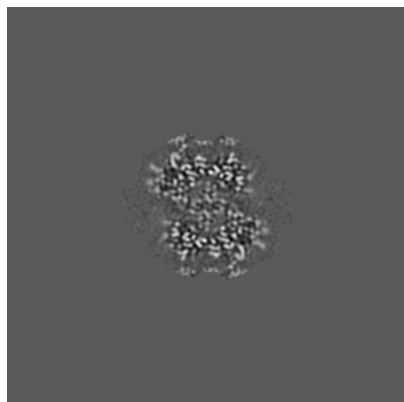


Z Index: 160

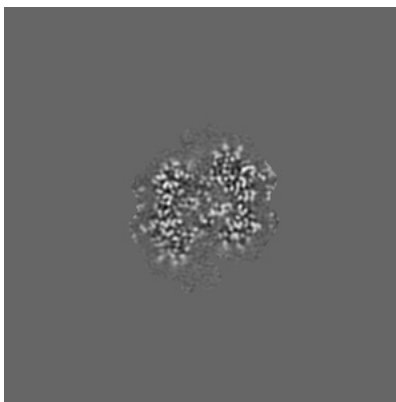
The images above show central slices of the map in three orthogonal directions.

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

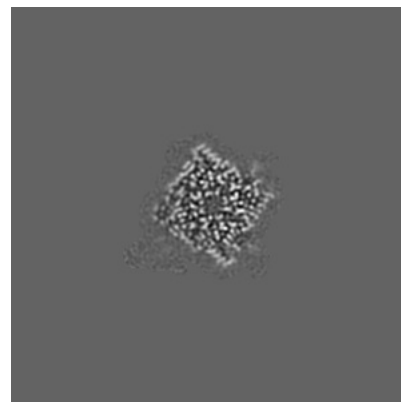
### 6.3.1 Primary map



X Index: 176

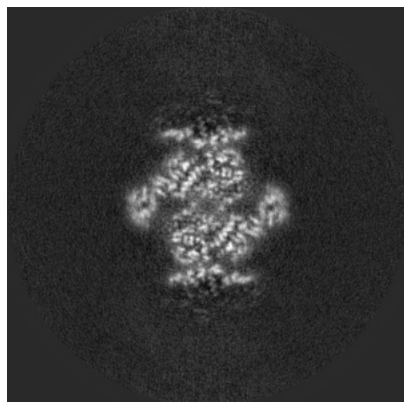


Y Index: 175

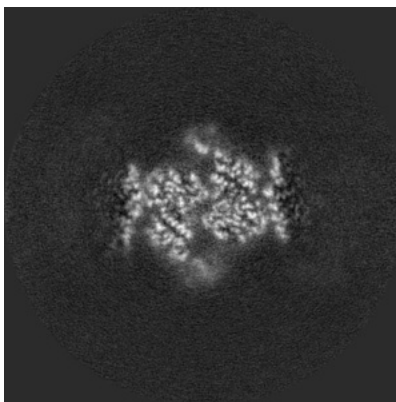


Z Index: 191

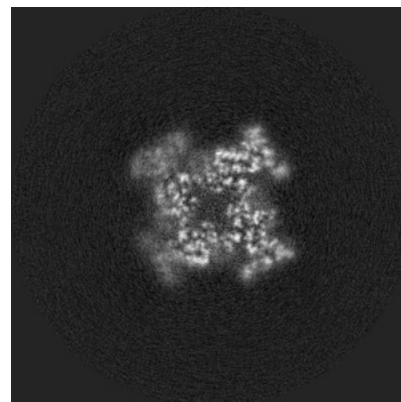
### 6.3.2 Raw map



X Index: 186



Y Index: 183

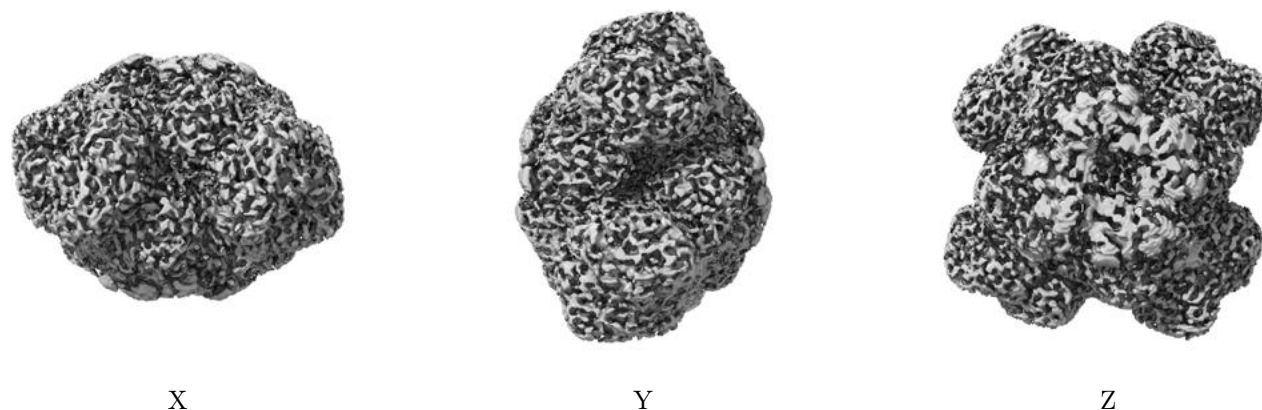


Z Index: 147

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

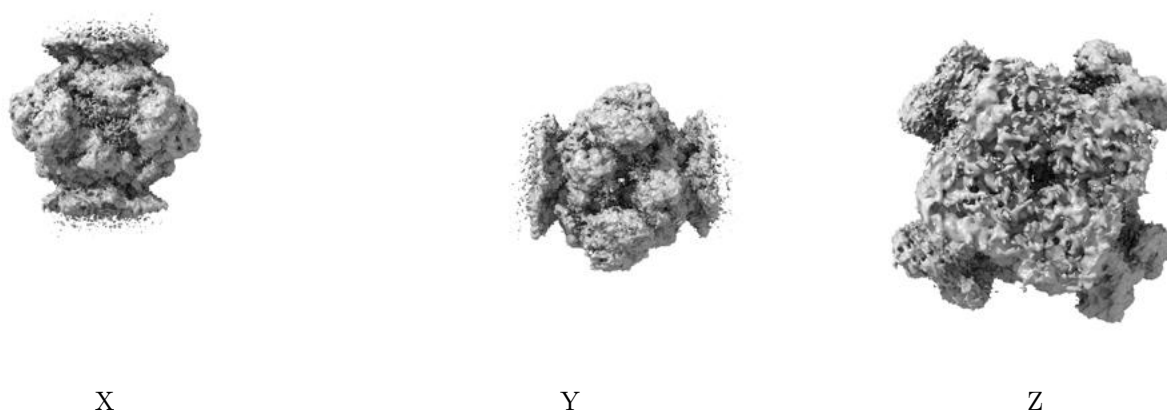
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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

### 6.4.2 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.

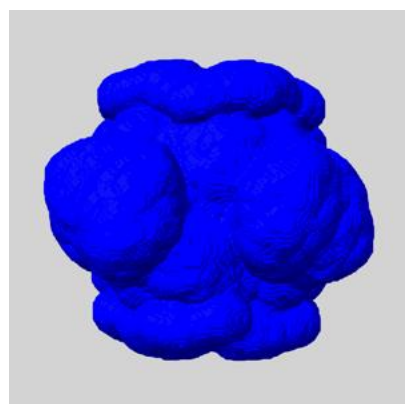
## 6.5 Mask visualisation [i](#)

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

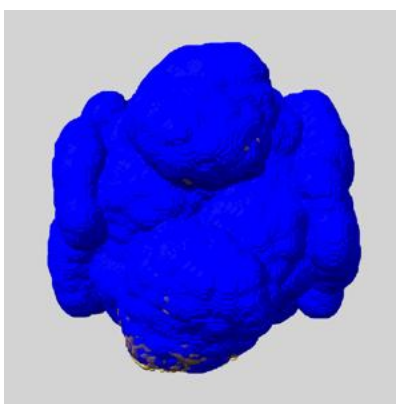
A mask typically either:

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

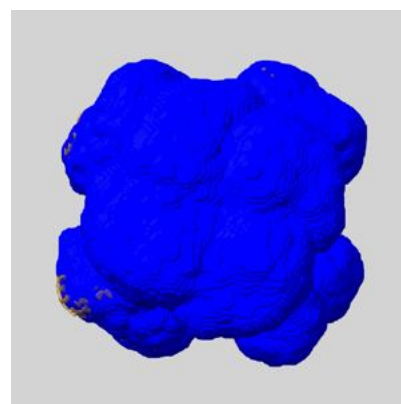
### 6.5.1 emd\_20705\_msk\_1.map [i](#)



X



Y

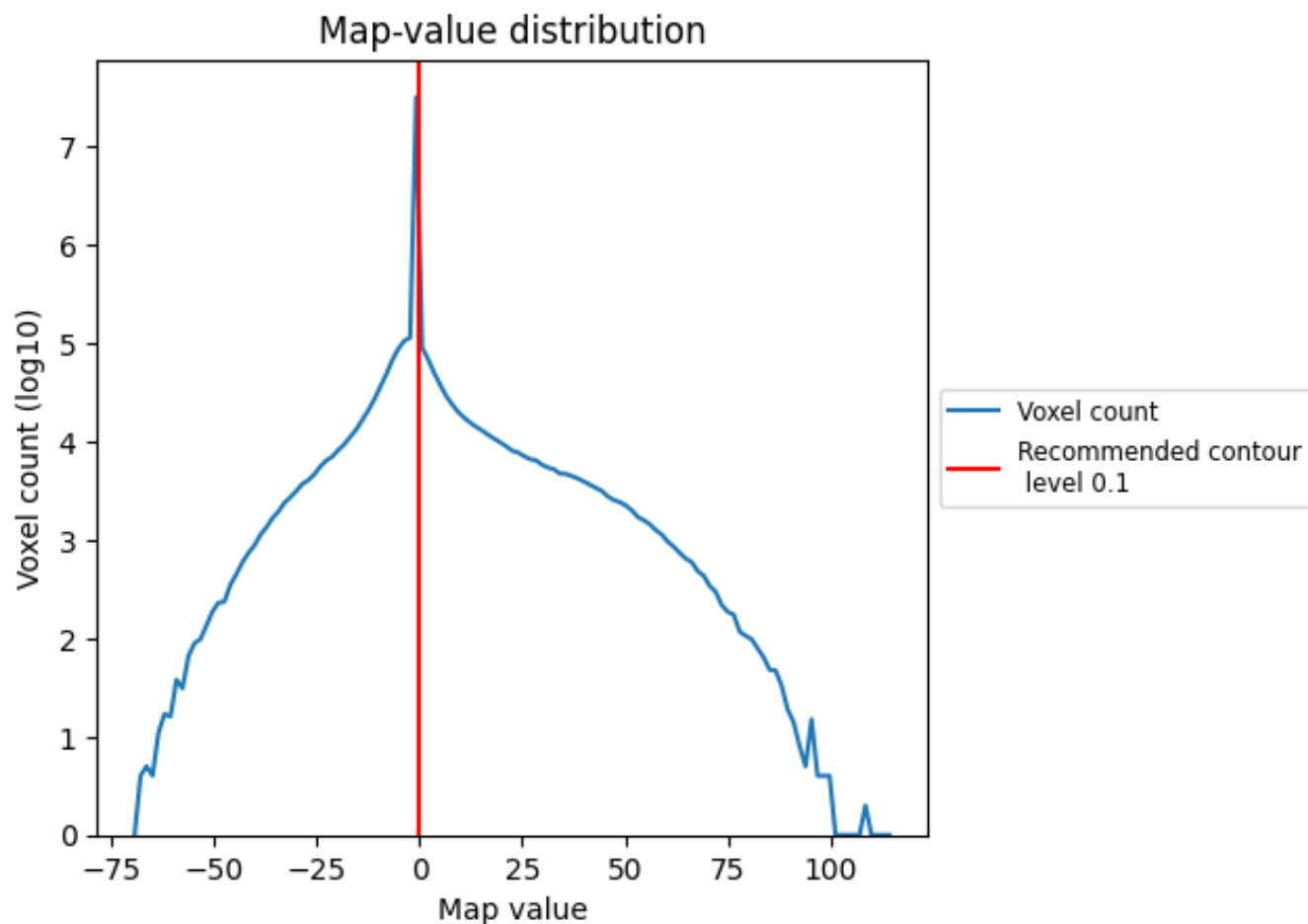


Z

## 7 Map analysis [i](#)

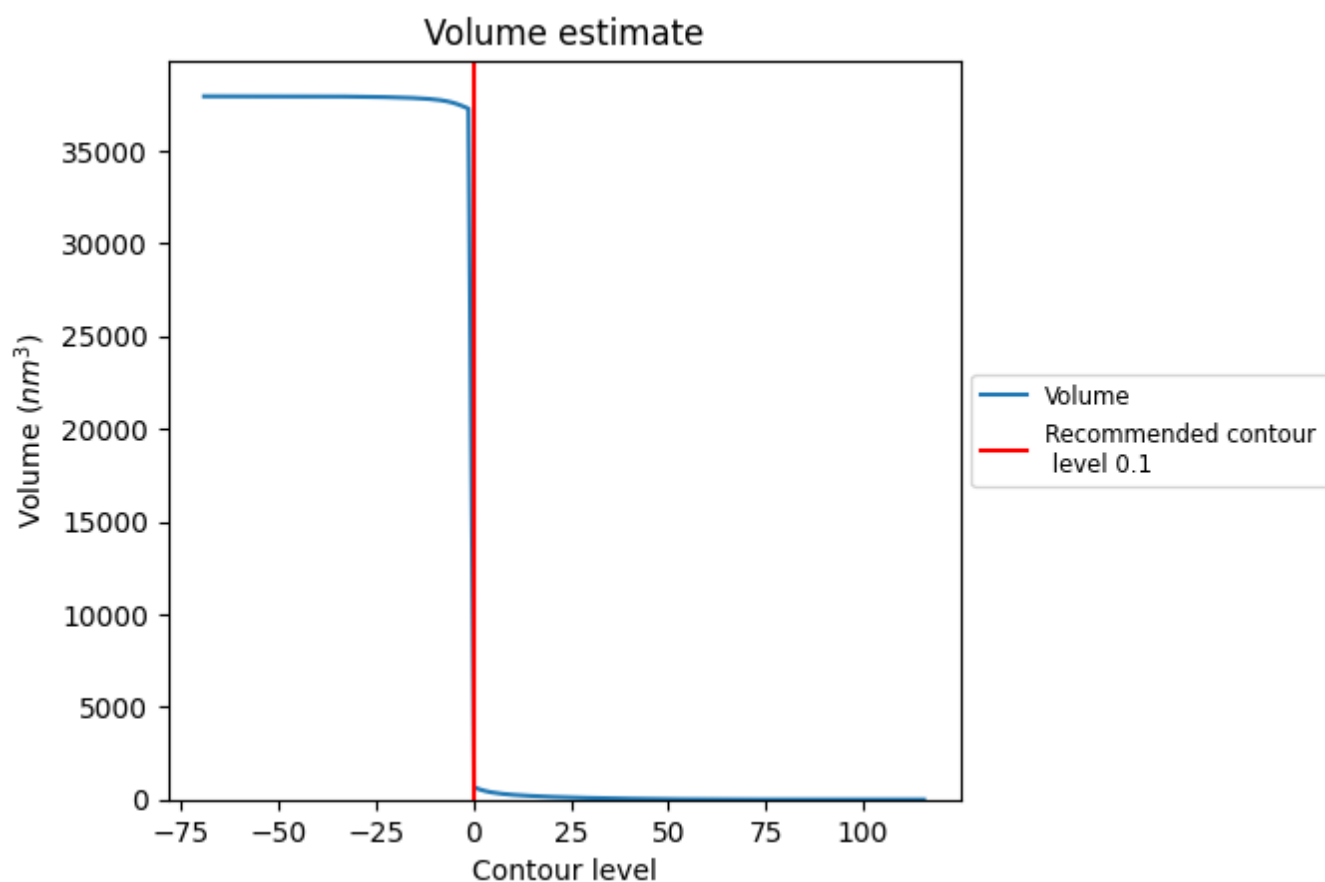
This section contains the results of statistical analysis of the map.

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



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

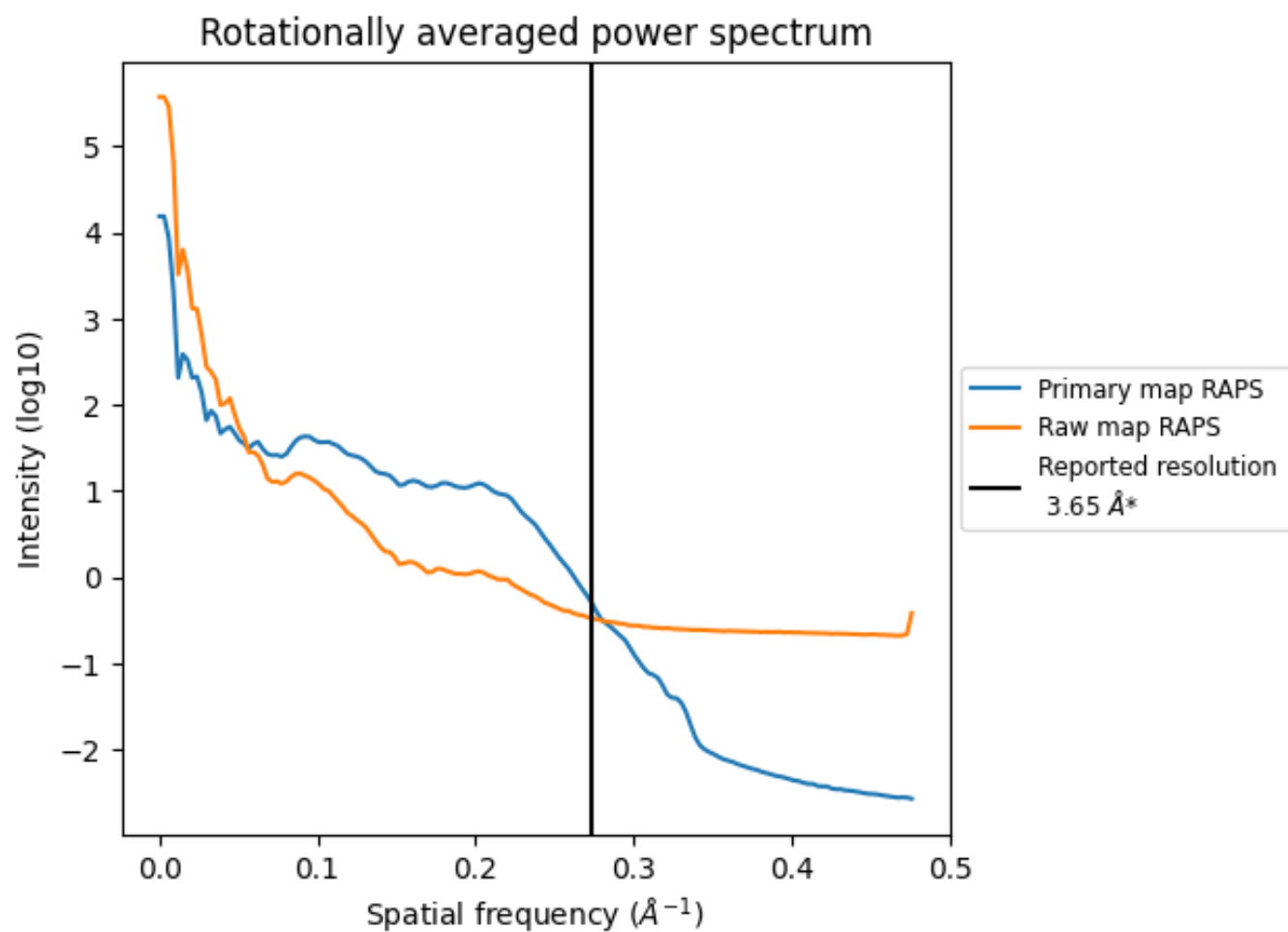
## 7.2 Volume estimate [i](#)



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

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

### 7.3 Rotationally averaged power spectrum ⓘ

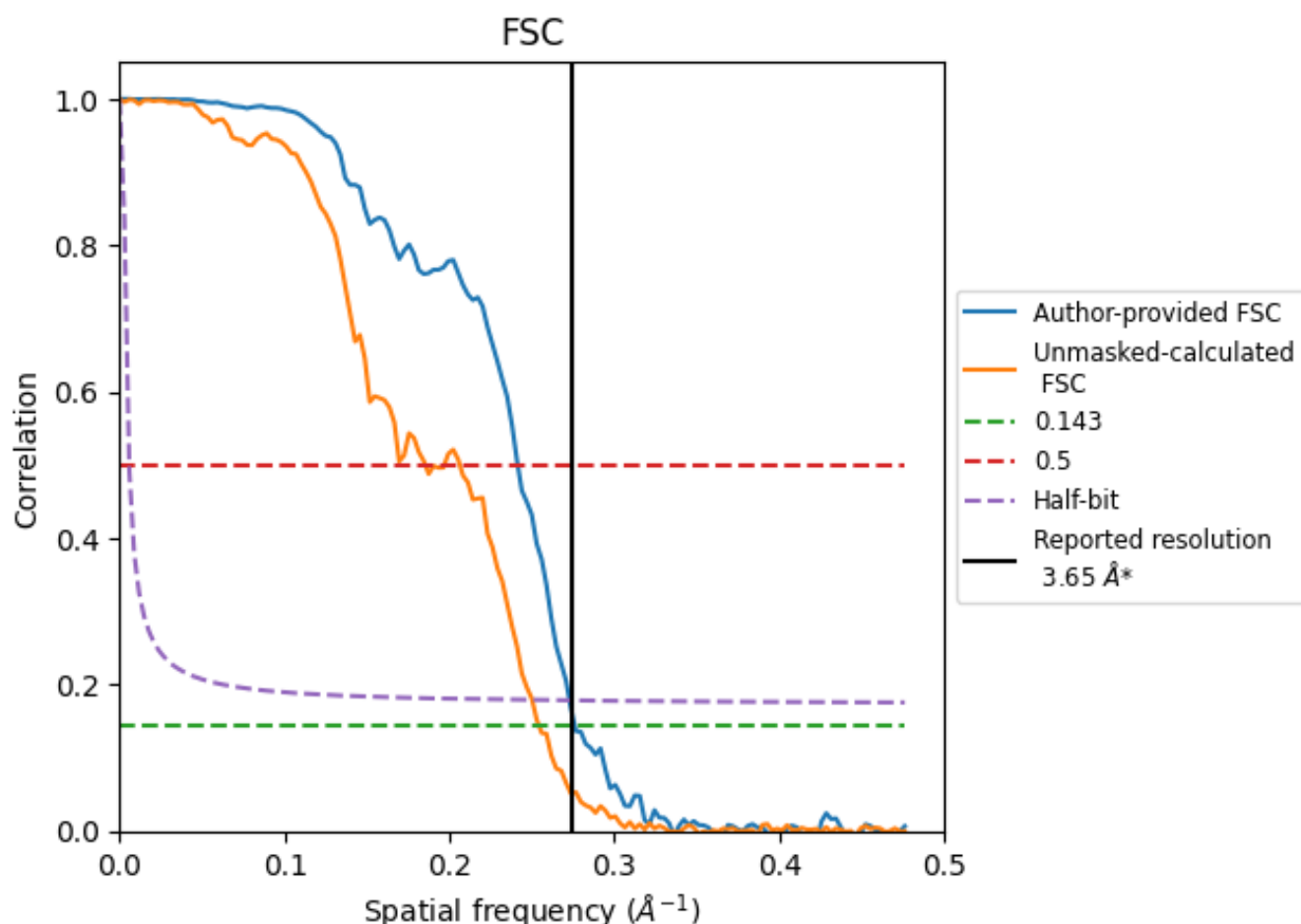


\*Reported resolution corresponds to spatial frequency of 0.274 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.274 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

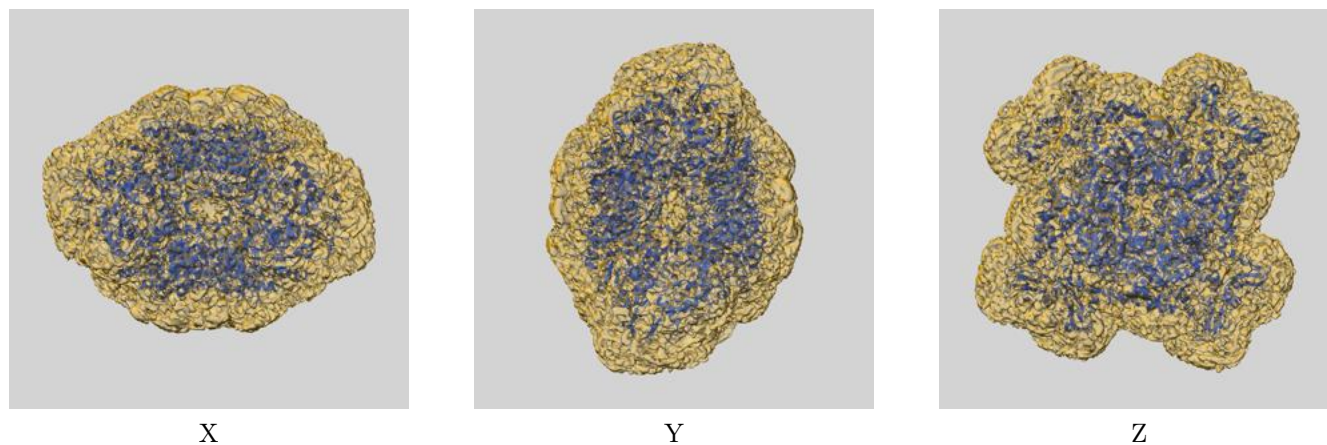
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.62	4.14	3.66
Unmasked-calculated*	3.93	5.39	4.00

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

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

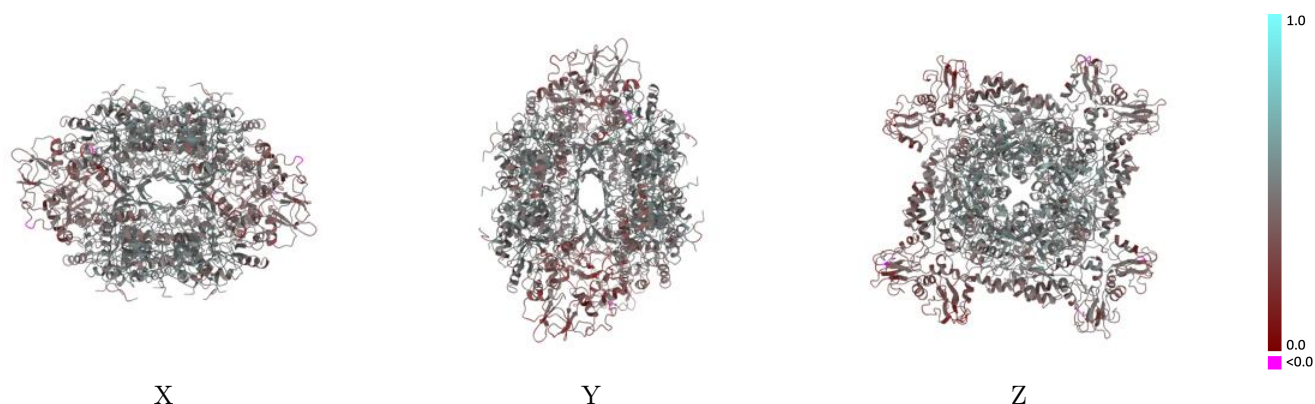
This section contains information regarding the fit between EMDB map EMD-20705 and PDB model 6UA4. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

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



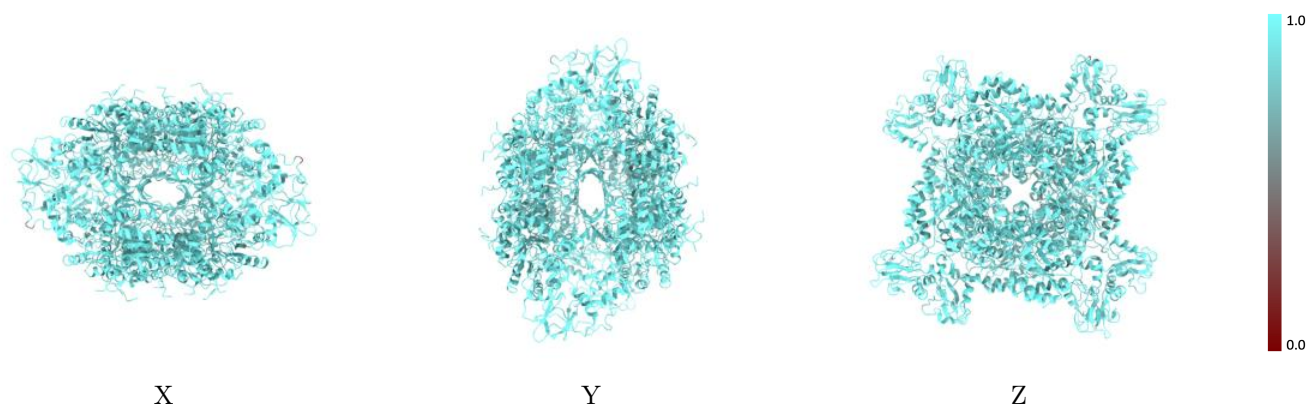
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



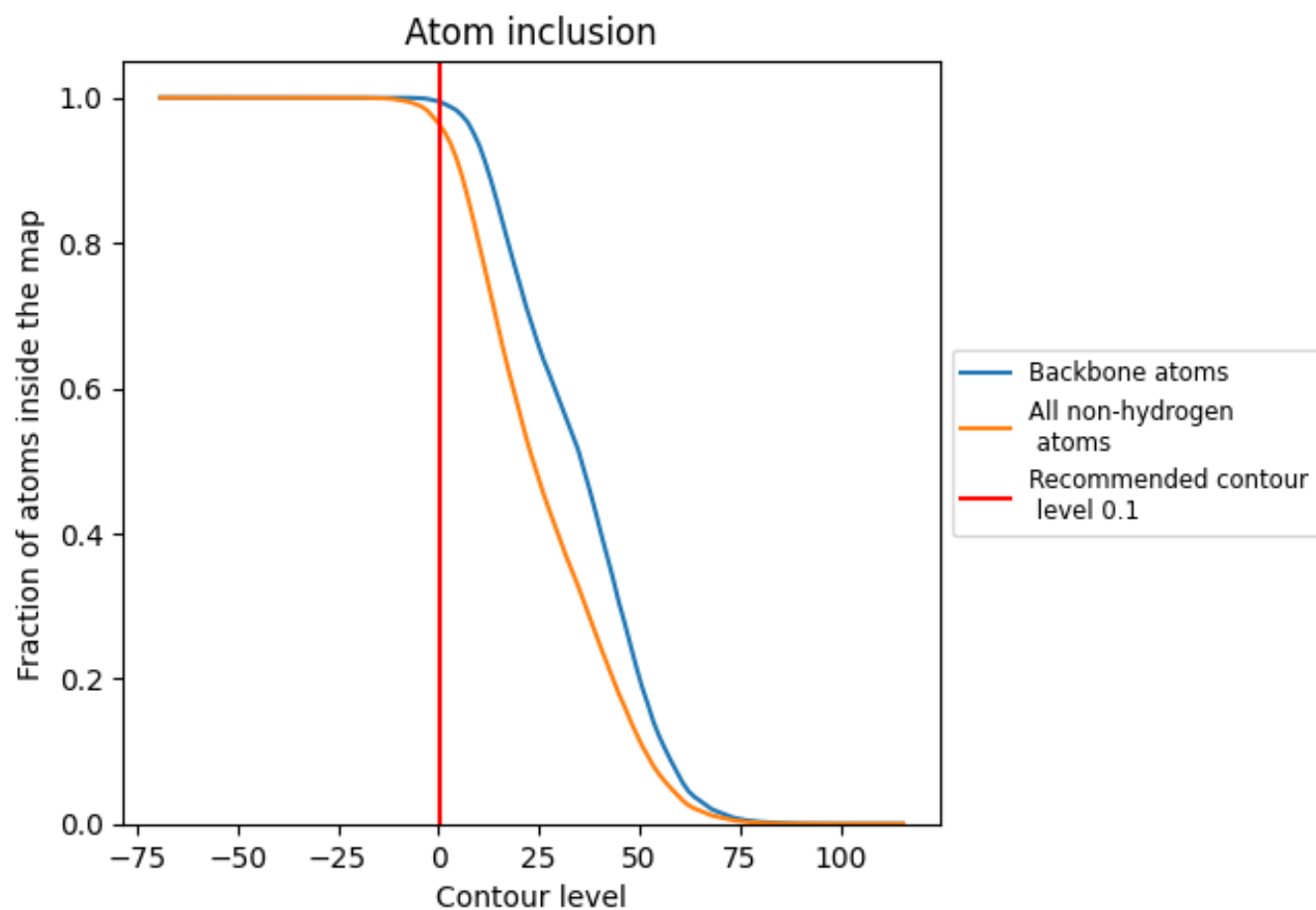
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.9645	 0.4380
A	 0.9644	 0.4480
B	 0.9633	 0.4570
C	 0.9659	 0.4190
D	 0.9675	 0.4320
E	 0.9636	 0.4500
F	 0.9628	 0.4560
G	 0.9662	 0.4180
H	 0.9662	 0.4290
I	 0.9300	 0.4350
J	 0.9600	 0.4310
K	 0.9600	 0.4270
L	 0.9400	 0.4180
M	 0.9400	 0.4410
N	 0.9600	 0.4300
O	 0.9500	 0.4260
P	 0.9300	 0.4270

