



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:12 AM UTC

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

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

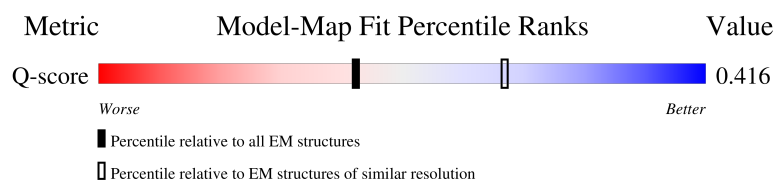
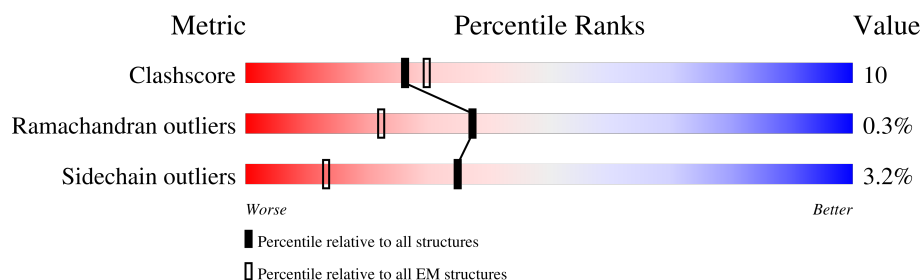
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.91 Å.

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



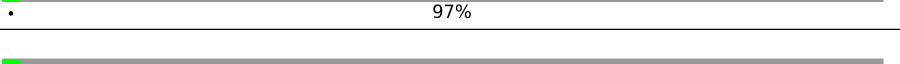
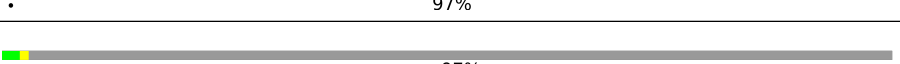
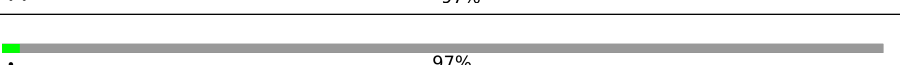
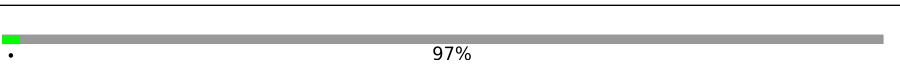
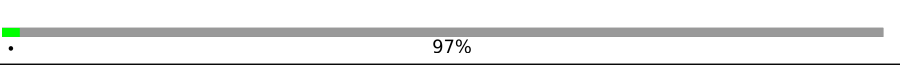
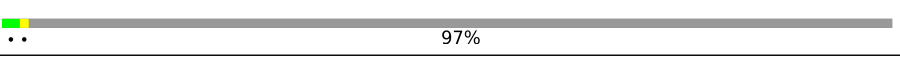
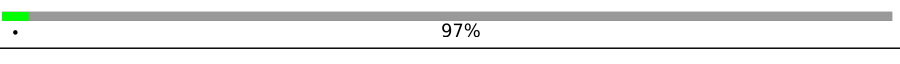
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7920 (3.41 - 4.41)

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

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

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

2 Entry composition [i](#)

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

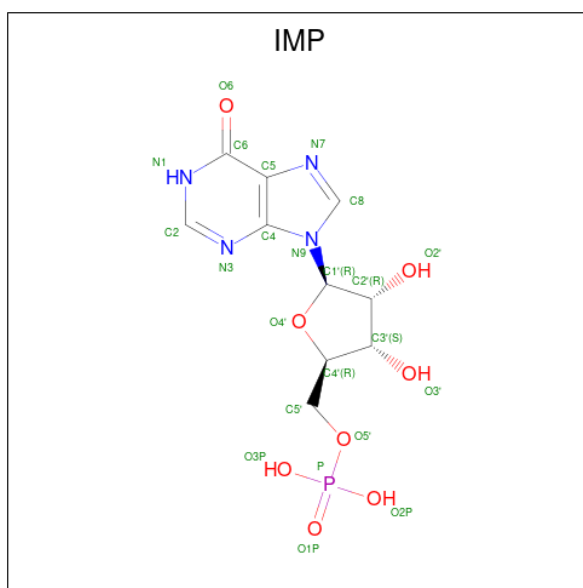
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

of Interest" by depositor).



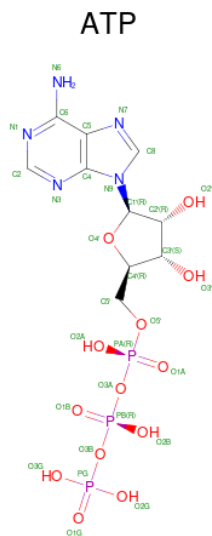
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	B	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	C	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	D	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	E	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	F	1	Total	C	N	O	P	0
			23	10	4	8	1	
2	G	1	Total	C	N	O	P	0
			23	10	4	8	1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

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



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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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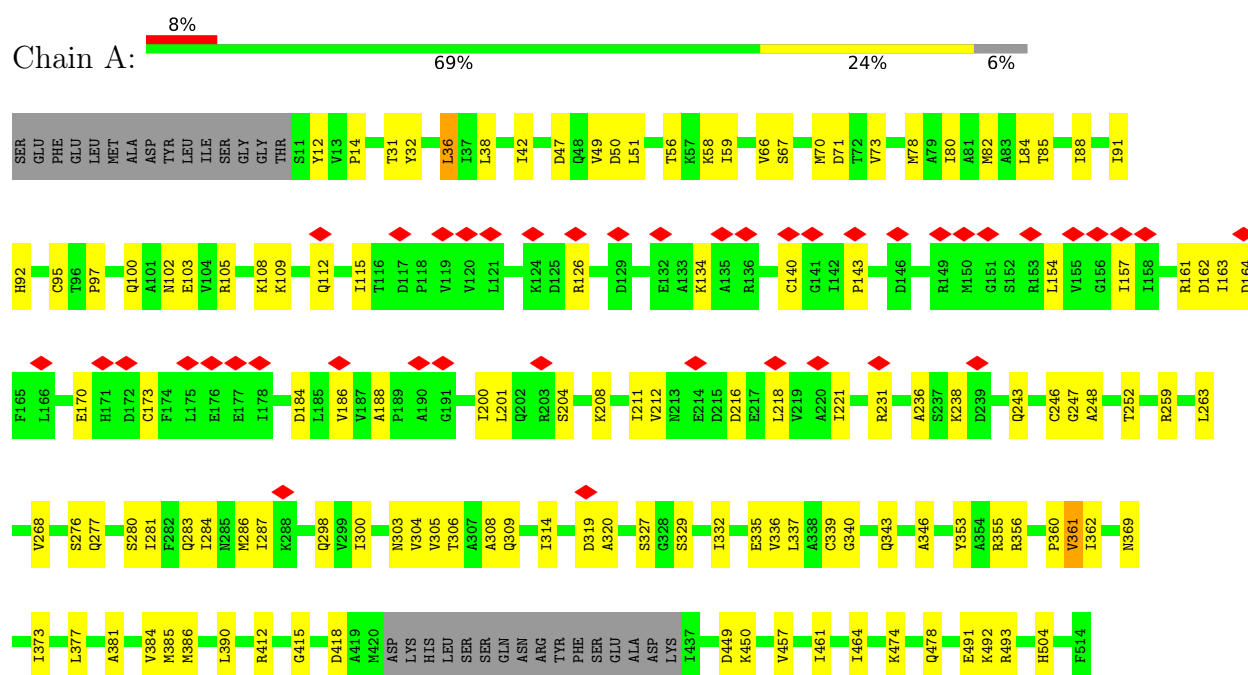
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Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

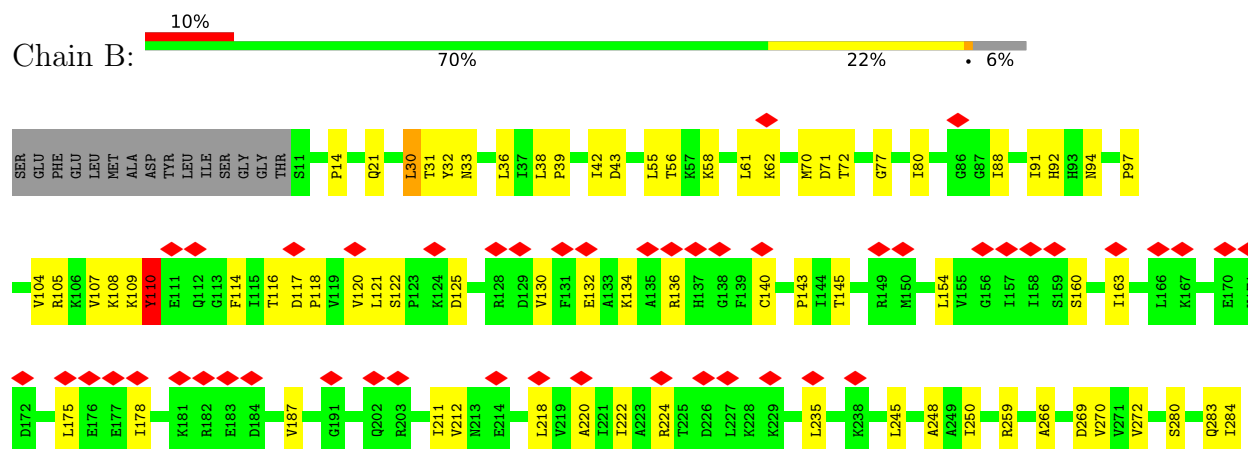
3 Residue-property plots

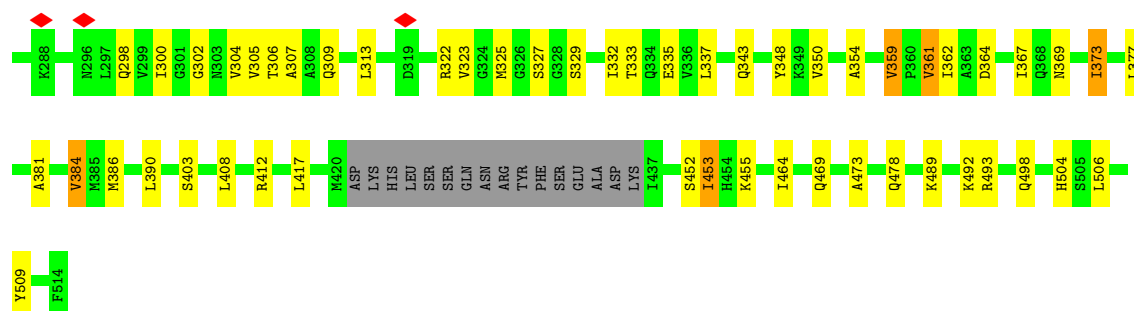
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

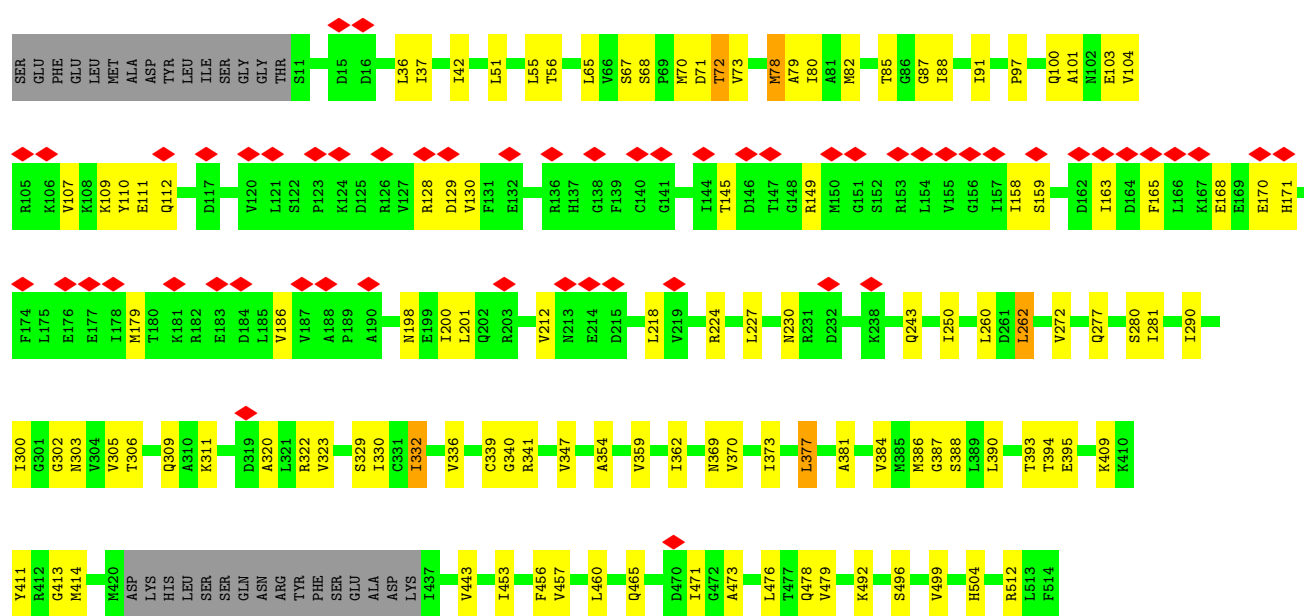


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

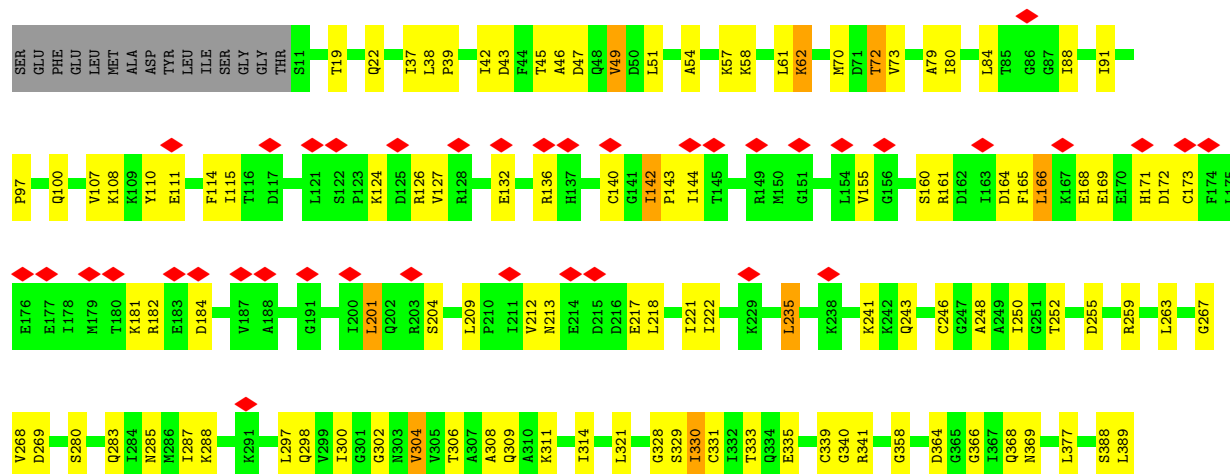


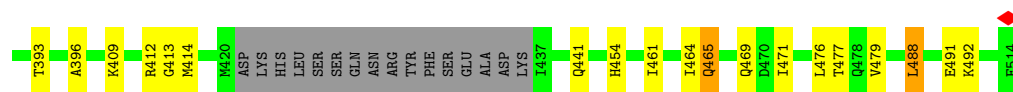


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

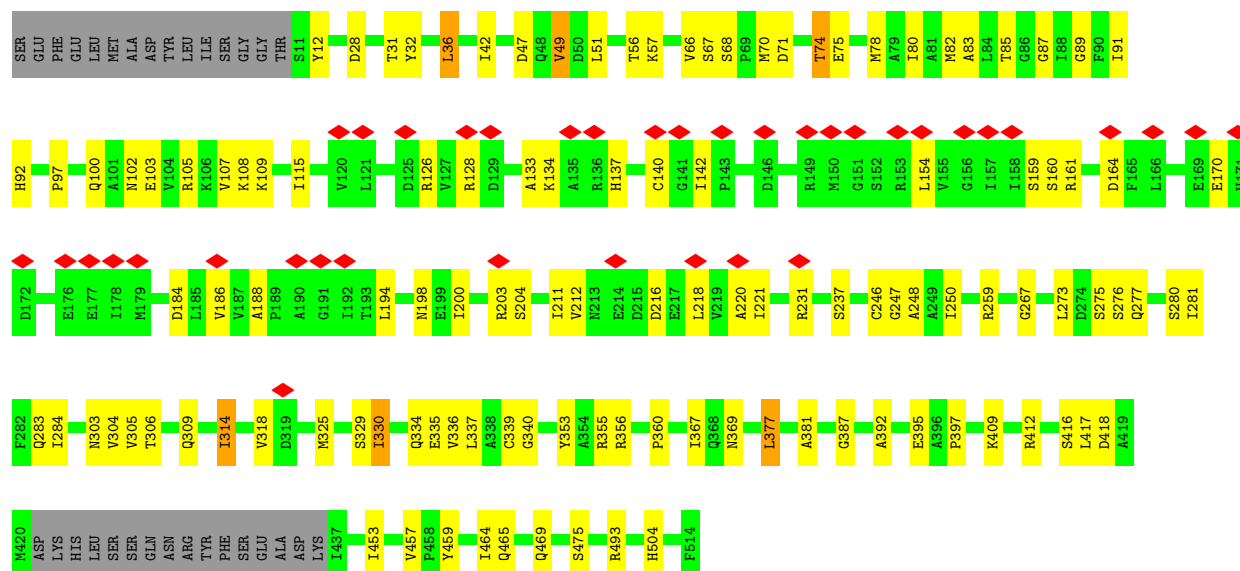


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

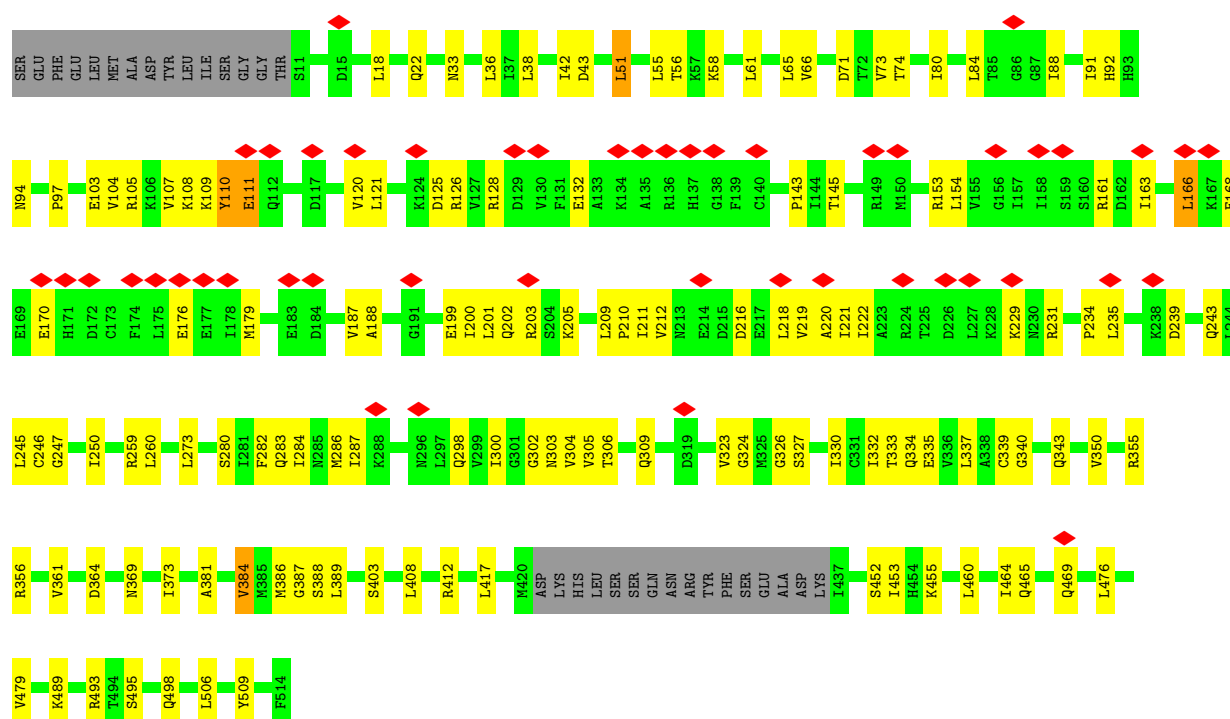




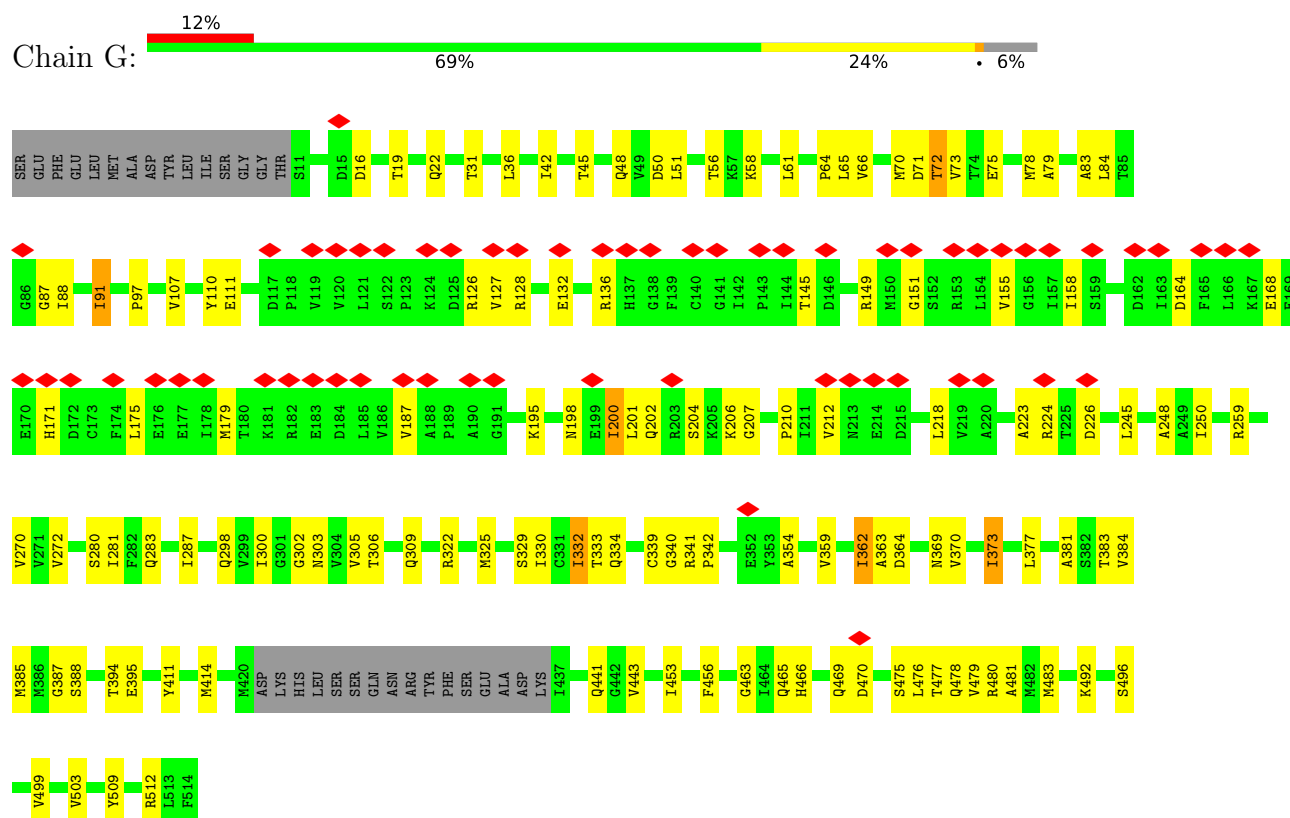
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



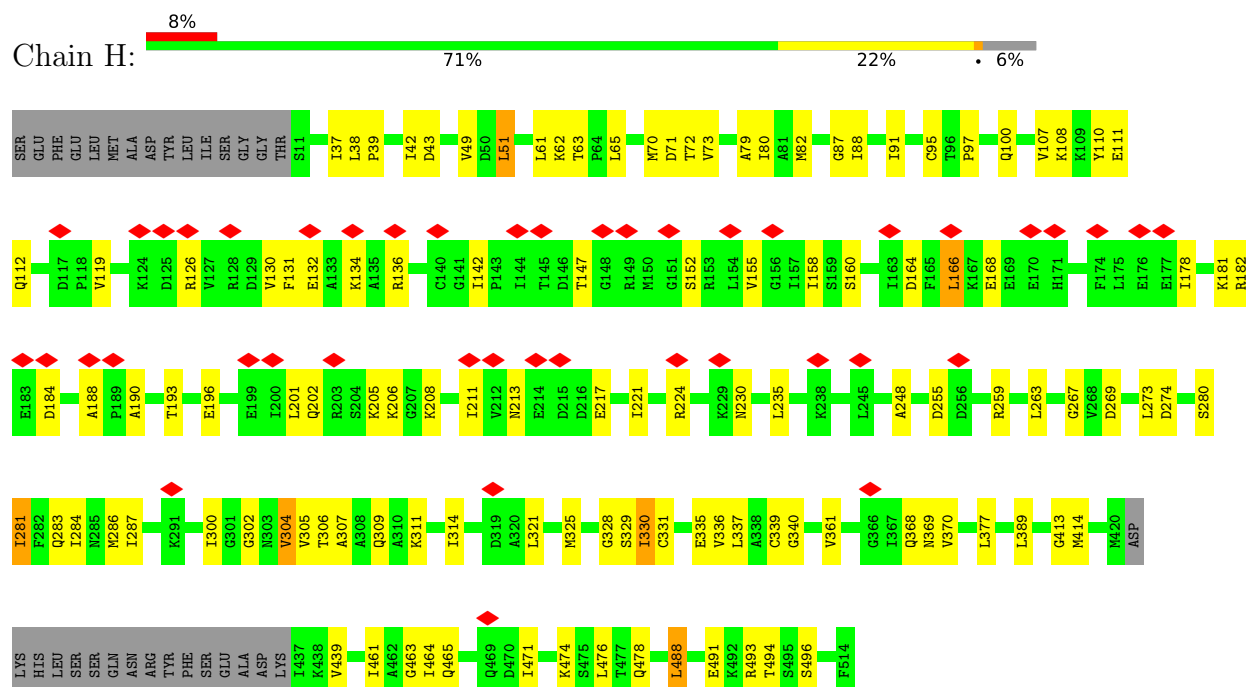
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2



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



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



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





Chain 0: 97%

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

Chain P: 97%

[illegible]

[illegible]

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

Chain K: .. 97%

[illegible]

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

Chain L: 97%

[illegible]

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

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of particles used	16819	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	115.597	Depositor
Minimum map value	-89.660	Depositor
Average map value	0.084	Depositor
Map value standard deviation	3.293	Depositor
Recommended contour level	17	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

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

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

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

All (1) bond length outliers are listed below:

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

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	THR	CA-C-N	-6.23	116.62	122.66
1	D	72	THR	C-N-CA	-6.23	116.62	122.66
1	B	453	ILE	N-CA-C	-5.94	106.47	113.42
1	F	330	ILE	N-CA-C	-5.79	107.86	113.53
1	C	332	ILE	CG1-CB-CG2	-5.72	93.54	110.70
1	G	330	ILE	N-CA-C	-5.60	108.04	113.53
1	H	72	THR	CA-C-N	-5.45	117.39	123.16
1	H	72	THR	C-N-CA	-5.45	117.39	123.16
1	G	477	THR	CA-C-N	-5.40	113.62	122.54
1	G	477	THR	C-N-CA	-5.40	113.62	122.54
1	H	51	LEU	CA-CB-CG	5.28	134.76	116.30
1	G	75	GLU	N-CA-C	-5.27	100.80	108.07
1	G	332	ILE	CG1-CB-CG2	-5.22	95.03	110.70
1	C	311	LYS	CA-C-N	-5.12	113.12	122.38
1	C	311	LYS	C-N-CA	-5.12	113.12	122.38
1	B	110	TYR	CA-C-N	5.07	131.22	121.54
1	B	110	TYR	C-N-CA	5.07	131.22	121.54
1	M	6	ILE	N-CA-C	-5.06	107.21	111.56
1	O	13	VAL	CA-CB-CG2	5.05	118.99	110.40
1	G	107	VAL	N-CA-C	-5.02	107.96	113.43

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3710	0	3766	96	0
1	B	3710	0	3766	84	0
1	C	3710	0	3766	75	0
1	D	3710	0	3766	90	0
1	E	3710	0	3766	86	0
1	F	3710	0	3766	89	0
1	G	3710	0	3766	80	0
1	H	3710	0	3766	80	0
1	I	102	0	99	1	0
1	J	102	0	99	3	0
1	K	102	0	99	5	0
1	L	102	0	99	1	0
1	M	102	0	99	1	0
1	N	102	0	99	3	0
1	O	102	0	99	1	0
1	P	102	0	99	0	0
2	A	23	0	11	3	0
2	B	23	0	11	0	0
2	C	23	0	11	2	0
2	D	23	0	11	3	0
2	E	23	0	11	3	0
2	F	23	0	11	2	0
2	G	23	0	11	4	0
2	H	23	0	11	1	0
3	A	44	0	24	2	0
3	B	44	0	24	0	0
3	C	44	0	24	1	0
3	D	44	0	24	0	0
3	E	44	0	22	1	0
3	F	44	0	24	1	0
3	G	44	0	24	1	0
3	H	44	0	24	3	0
4	A	62	0	24	1	0
4	B	62	0	24	1	0
4	C	62	0	24	2	0
4	D	62	0	23	3	0
4	E	62	0	24	2	0
4	F	62	0	24	1	0
4	G	62	0	24	0	0
4	H	62	0	24	2	0
All	All	31528	0	31389	637	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (637) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:474:LYS:H	1:H:478:GLN:HE21	1.27	0.82
1:E:200:ILE:O	1:E:204:SER:HB3	1.82	0.80
1:E:36:LEU:HD13	1:E:493:ARG:HD2	1.65	0.78
1:A:36:LEU:HD13	1:A:493:ARG:HD2	1.71	0.72
1:F:283:GLN:HE22	1:F:302:GLY:H	1.37	0.71
1:F:58:LYS:HB2	1:F:298:GLN:HE22	1.55	0.71
1:A:306:THR:H	1:A:309:GLN:HE21	1.40	0.70
1:E:186:VAL:H	4:E:603:ATP:HN62	1.39	0.70
1:D:37:ILE:HD12	1:D:471:ILE:HD12	1.73	0.70
1:A:200:ILE:O	1:A:204:SER:HB3	1.91	0.70
1:A:80:ILE:O	1:A:84:LEU:HB2	1.91	0.69
1:E:306:THR:H	1:E:309:GLN:HE21	1.40	0.69
1:A:186:VAL:H	4:A:603:ATP:HN62	1.39	0.68
1:G:475:SER:H	1:G:478:GLN:HE21	1.41	0.68
1:B:283:GLN:HE22	1:B:302:GLY:H	1.42	0.68
1:F:55:LEU:HD23	1:F:56:THR:HG23	1.76	0.66
1:H:471:ILE:HD11	1:H:488:LEU:HD13	1.78	0.66
1:B:58:LYS:HB2	1:B:298:GLN:HE22	1.61	0.66
1:A:91:ILE:H	1:A:248:ALA:HA	1.60	0.65
1:C:67:SER:OG	1:C:82:MET:SD	2.55	0.65
1:A:304:VAL:HG13	1:A:309:GLN:HG3	1.77	0.65
1:H:37:ILE:HD12	1:H:471:ILE:HD12	1.78	0.65
1:A:97:PRO:HG3	1:A:259:ARG:HG2	1.79	0.65
1:B:97:PRO:HG3	1:B:259:ARG:HG2	1.78	0.65
1:D:166:LEU:HD13	1:D:168:GLU:H	1.60	0.64
1:D:19:THR:H	1:D:22:GLN:HE21	1.46	0.64
1:D:140:CYS:HB3	1:D:160:SER:HB3	1.80	0.64
1:A:56:THR:HG21	1:A:298:GLN:HG3	1.80	0.64
1:G:45:THR:H	1:G:48:GLN:HE21	1.46	0.64
1:G:168:GLU:HB2	1:G:171:HIS:HB2	1.80	0.64
1:C:55:LEU:HD23	1:C:56:THR:HG23	1.79	0.63
1:B:108:LYS:HG3	1:B:109:LYS:HD3	1.80	0.63
1:H:339:CYS:SG	1:H:340:GLY:N	2.72	0.63
1:F:187:VAL:HG11	1:F:212:VAL:HG22	1.81	0.63
1:H:201:LEU:HD11	1:H:224:ARG:HD2	1.79	0.63
1:B:132:GLU:HG3	1:B:136:ARG:HE	1.64	0.63
1:D:70:MET:HB2	1:D:73:VAL:HG12	1.79	0.62
1:H:61:LEU:HD21	1:H:87:GLY:HA2	1.81	0.62
1:A:161:ARG:HB3	1:H:224:ARG:HH22	1.64	0.62
1:D:168:GLU:O	1:D:171:HIS:ND1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:VAL:HG13	1:E:309:GLN:HG3	1.79	0.62
1:H:184:ASP:O	1:H:206:LYS:NZ	2.32	0.62
1:H:202:GLN:HA	1:H:205:LYS:HE3	1.79	0.62
1:D:126:ARG:NH2	1:D:173:CYS:SG	2.73	0.62
1:A:56:THR:HG23	1:A:58:LYS:H	1.65	0.62
1:A:115:ILE:HG23	1:A:221:ILE:HG23	1.82	0.62
1:A:327:SER:OG	1:A:343:GLN:NE2	2.33	0.62
1:C:339:CYS:SG	1:C:340:GLY:N	2.72	0.62
1:B:343:GLN:NE2	1:B:364:ASP:O	2.33	0.62
1:C:280:SER:HA	1:D:42:ILE:HB	1.81	0.62
1:F:166:LEU:HD13	1:F:168:GLU:H	1.65	0.61
1:F:333:THR:O	1:F:337:LEU:N	2.30	0.61
1:G:212:VAL:HA	1:G:218:LEU:HA	1.81	0.61
1:H:62:LYS:HE2	1:H:235:LEU:HA	1.82	0.61
1:D:339:CYS:SG	1:D:340:GLY:N	2.71	0.61
1:G:91:ILE:H	1:G:248:ALA:HA	1.66	0.61
1:H:321:LEU:HB2	1:H:361:VAL:HG12	1.82	0.61
1:G:476:LEU:HA	1:G:479:VAL:HG12	1.83	0.60
1:C:71:ASP:H	1:C:414:MET:HE1	1.67	0.60
1:E:115:ILE:HB	1:E:221:ILE:HG23	1.82	0.60
1:F:343:GLN:NE2	1:F:364:ASP:O	2.35	0.60
1:E:273:LEU:HD23	1:E:283:GLN:HG3	1.83	0.60
1:G:280:SER:HA	1:H:42:ILE:HB	1.83	0.60
1:G:306:THR:HG21	1:H:38:LEU:HD13	1.82	0.60
1:A:329:SER:OG	1:B:504:HIS:O	2.19	0.60
1:B:280:SER:HA	1:C:42:ILE:HB	1.83	0.60
1:C:277:GLN:NE2	1:C:309:GLN:OE1	2.35	0.60
1:H:305:VAL:HG21	1:H:325:MET:HG2	1.83	0.60
1:A:335:GLU:O	1:B:369:ASN:ND2	2.35	0.60
1:H:82:MET:O	1:H:87:GLY:N	2.35	0.60
1:A:246:CYS:SG	1:A:247:GLY:N	2.75	0.59
1:C:101:ALA:HB1	1:C:262:LEU:HD22	1.82	0.59
1:C:303:ASN:ND2	3:C:604:NAD:O7N	2.35	0.59
1:A:353:TYR:HD1	1:A:356:ARG:HH11	1.50	0.59
1:C:85:THR:HG21	1:C:457:VAL:HG21	1.84	0.59
1:A:281:ILE:HD12	1:A:284:ILE:HD11	1.84	0.59
1:D:471:ILE:HD11	1:D:488:LEU:HD13	1.84	0.59
1:E:97:PRO:HG3	1:E:259:ARG:HG2	1.84	0.59
1:C:212:VAL:HA	1:C:218:LEU:HA	1.83	0.59
1:H:132:GLU:O	1:H:136:ARG:N	2.35	0.59
1:E:102:ASN:HA	1:E:105:ARG:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:LYS:NZ	1:E:267:GLY:O	2.36	0.59
1:A:188:ALA:HB3	1:A:211:ILE:HG22	1.84	0.59
1:B:323:VAL:HG11	1:B:350:VAL:HG11	1.85	0.59
1:C:72:THR:HG21	1:C:411:TYR:HA	1.83	0.59
1:F:188:ALA:H	1:F:209:LEU:HD21	1.67	0.59
1:A:134:LYS:HB2	1:A:140:CYS:HB3	1.85	0.58
1:C:82:MET:HA	1:C:85:THR:HG22	1.84	0.58
1:F:105:ARG:HA	1:F:108:LYS:HE3	1.85	0.58
3:A:602:NAD:O2B	1:B:469:GLN:NE2	2.36	0.58
1:G:71:ASP:H	1:G:414:MET:HE1	1.68	0.58
1:A:280:SER:HA	1:B:42:ILE:HB	1.84	0.58
1:F:71:ASP:HB3	1:F:94:ASN:HD21	1.69	0.58
1:F:280:SER:HA	1:G:42:ILE:HB	1.86	0.58
1:B:373:ILE:HD11	1:B:464:ILE:HG21	1.86	0.58
1:H:100:GLN:OE1	1:H:259:ARG:NH2	2.36	0.58
1:A:100:GLN:OE1	1:A:259:ARG:NH2	2.36	0.58
1:E:246:CYS:SG	1:E:247:GLY:N	2.77	0.58
1:F:355:ARG:NH1	1:K:11:SER:O	2.35	0.58
1:A:38:LEU:HD12	1:D:306:THR:HG22	1.85	0.58
1:C:306:THR:H	1:C:309:GLN:HE21	1.50	0.58
1:E:188:ALA:HB3	1:E:211:ILE:HG22	1.85	0.58
1:E:392:ALA:HA	1:E:409:LYS:HD2	1.86	0.57
1:F:161:ARG:NH1	4:F:601:ATP:O3G	2.34	0.57
1:B:335:GLU:O	1:C:369:ASN:ND2	2.37	0.57
1:D:201:LEU:HA	1:D:204:SER:HB3	1.86	0.57
1:A:356:ARG:NH2	1:N:12:TYR:OH	2.35	0.57
1:B:145:THR:HA	1:B:154:LEU:HA	1.86	0.57
1:D:57:LYS:NZ	1:D:358:GLY:O	2.37	0.57
1:D:333:THR:HG22	1:D:441:GLN:HB2	1.86	0.57
1:F:92:HIS:ND1	1:F:94:ASN:OD1	2.38	0.57
1:F:326:GLY:O	1:F:334:GLN:NE2	2.36	0.57
1:E:200:ILE:HA	1:E:203:ARG:HD2	1.87	0.57
1:F:126:ARG:NH2	1:F:170:GLU:O	2.37	0.57
1:G:56:THR:HG21	1:G:270:VAL:HG21	1.87	0.57
1:H:166:LEU:HD13	1:H:168:GLU:H	1.68	0.57
1:D:46:ALA:HA	1:D:469:GLN:HG3	1.87	0.56
1:D:241:LYS:O	1:D:243:GLN:NE2	2.37	0.56
1:A:339:CYS:SG	1:A:340:GLY:N	2.78	0.56
1:C:168:GLU:HB2	1:C:171:HIS:HB2	1.85	0.56
1:D:100:GLN:OE1	1:D:259:ARG:NH2	2.38	0.56
1:E:100:GLN:OE1	1:E:259:ARG:NH2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:GLU:O	1:F:369:ASN:ND2	2.39	0.56
1:F:88:ILE:HD13	1:F:245:LEU:HB3	1.87	0.56
1:G:126:ARG:HG3	1:G:128:ARG:H	1.71	0.56
1:D:54:ALA:HB2	1:M:5:LEU:HD21	1.87	0.56
1:G:306:THR:HG22	1:G:341:ARG:HH11	1.70	0.56
1:B:506:LEU:HD11	1:B:509:TYR:HB3	1.87	0.56
1:C:78:MET:HG3	1:C:82:MET:HE3	1.88	0.56
1:C:79:ALA:HB3	1:C:107:VAL:HG21	1.88	0.56
1:D:304:VAL:HG23	1:D:309:GLN:HG2	1.88	0.56
1:E:31:THR:OG1	1:E:32:TYR:N	2.39	0.56
1:F:403:SER:HB3	1:F:408:LEU:HD21	1.87	0.56
1:G:322:ARG:HA	1:G:362:ILE:HG23	1.87	0.56
1:H:63:THR:HG23	1:H:65:LEU:H	1.71	0.56
1:H:414:MET:HB3	3:H:604:NAD:H4D	1.88	0.56
1:C:82:MET:O	1:C:87:GLY:N	2.32	0.56
1:A:102:ASN:HA	1:A:105:ARG:HG2	1.86	0.56
1:F:250:ILE:HD11	1:F:273:LEU:HG	1.86	0.56
1:C:330:ILE:HG23	1:C:443:VAL:HG12	1.88	0.55
1:E:275:SER:O	1:E:303:ASN:ND2	2.39	0.55
1:D:377:LEU:HD13	1:D:476:LEU:HD21	1.88	0.55
1:H:112:GLN:NE2	1:H:230:ASN:OD1	2.39	0.55
1:B:373:ILE:HB	1:B:384:VAL:HG11	1.89	0.55
1:D:108:LYS:NZ	1:D:267:GLY:O	2.34	0.55
1:B:92:HIS:ND1	1:B:94:ASN:OD1	2.39	0.55
1:B:305:VAL:H	1:B:309:GLN:HE21	1.55	0.55
1:E:281:ILE:HD12	1:E:284:ILE:HD11	1.88	0.55
1:F:199:GLU:HA	1:F:202:GLN:HG2	1.89	0.55
1:G:377:LEU:HD13	1:G:476:LEU:HD21	1.88	0.55
1:A:329:SER:N	2:A:601:IMP:O3P	2.38	0.54
1:D:80:ILE:O	1:D:84:LEU:HB2	2.08	0.54
1:B:33:ASN:O	1:B:498:GLN:NE2	2.38	0.54
1:A:361:VAL:HG13	1:A:381:ALA:HA	1.88	0.54
1:A:369:ASN:ND2	1:D:335:GLU:O	2.40	0.54
1:E:75:GLU:HA	1:E:91:ILE:HD13	1.88	0.54
3:E:602:NAD:O2B	1:F:469:GLN:NE2	2.40	0.54
1:A:109:LYS:HA	1:A:112:GLN:HE22	1.73	0.54
1:E:339:CYS:SG	1:E:340:GLY:N	2.80	0.54
1:E:28:ASP:N	1:E:28:ASP:OD1	2.39	0.54
1:E:280:SER:HA	1:F:42:ILE:HB	1.88	0.54
1:G:453:ILE:HA	1:G:456:PHE:HB3	1.89	0.54
1:E:369:ASN:ND2	1:H:335:GLU:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:VAL:HG11	1:F:350:VAL:HG11	1.87	0.54
1:D:161:ARG:HD3	4:D:601:ATP:H5'1	1.89	0.54
1:A:412:ARG:HD2	1:A:418:ASP:HB2	1.89	0.54
1:D:212:VAL:HG22	1:D:218:LEU:HD23	1.90	0.54
1:E:161:ARG:HA	1:E:164:ASP:HB2	1.89	0.54
1:G:200:ILE:O	1:G:204:SER:HB2	2.07	0.54
1:G:381:ALA:O	1:G:480:ARG:NH2	2.40	0.54
1:B:108:LYS:NZ	1:B:266:ALA:O	2.34	0.54
1:C:272:VAL:HG13	1:C:300:ILE:HD11	1.89	0.54
1:G:72:THR:HG21	1:G:411:TYR:HA	1.91	0.53
1:G:334:GLN:OE1	1:H:493:ARG:NH1	2.41	0.53
1:H:147:THR:OG1	1:H:152:SER:OG	2.23	0.53
1:A:108:LYS:O	1:A:112:GLN:NE2	2.41	0.53
1:C:329:SER:OG	1:C:388:SER:OG	2.25	0.53
1:F:38:LEU:HD11	1:F:489:LYS:HG3	1.90	0.53
1:B:175:LEU:HD13	1:B:178:ILE:HD13	1.90	0.53
1:D:364:ASP:OD2	2:D:603:IMP:O2'	2.24	0.53
1:F:145:THR:HA	1:F:154:LEU:HA	1.91	0.53
1:F:200:ILE:HG22	1:F:203:ARG:HH11	1.74	0.53
1:G:195:LYS:HA	1:G:198:ASN:HD22	1.73	0.53
1:G:283:GLN:HE22	1:G:302:GLY:H	1.55	0.53
1:A:303:ASN:ND2	3:A:602:NAD:O7N	2.39	0.53
1:B:329:SER:OG	1:C:504:HIS:O	2.26	0.53
1:C:158:ILE:HG22	1:C:179:MET:HG2	1.91	0.53
1:G:50:ASP:OD1	1:G:475:SER:OG	2.23	0.53
1:G:363:ALA:HB3	1:G:384:VAL:HG12	1.90	0.53
1:B:55:LEU:HD23	1:B:56:THR:HG23	1.91	0.53
1:D:181:LYS:HG3	1:D:182:ARG:HG2	1.91	0.53
1:A:71:ASP:OD2	1:A:412:ARG:NH1	2.43	0.52
1:H:304:VAL:HG23	1:H:309:GLN:HG2	1.91	0.52
1:A:80:ILE:O	1:A:84:LEU:CB	2.56	0.52
1:C:394:THR:OG1	1:C:395:GLU:OE1	2.26	0.52
1:G:132:GLU:O	1:G:136:ARG:N	2.41	0.52
1:A:70:MET:SD	2:A:601:IMP:H8	2.50	0.52
1:C:198:ASN:HB3	1:C:227:LEU:HD13	1.90	0.52
1:D:132:GLU:O	1:D:136:ARG:N	2.41	0.52
1:E:325:MET:HG3	1:E:340:GLY:HA2	1.91	0.52
1:F:97:PRO:HG3	1:F:259:ARG:HG2	1.89	0.52
1:H:377:LEU:HD13	1:H:476:LEU:HD21	1.91	0.52
1:E:85:THR:HG21	1:E:457:VAL:HG11	1.92	0.52
1:A:355:ARG:HH12	1:N:12:TYR:HA	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ARG:HD2	1:D:173:CYS:H	1.73	0.52
1:E:71:ASP:OD2	1:E:412:ARG:NH1	2.42	0.52
1:E:159:SER:OG	4:E:603:ATP:O1B	2.24	0.52
1:G:272:VAL:HA	1:G:300:ILE:HG13	1.90	0.52
1:H:181:LYS:O	1:H:182:ARG:NH1	2.38	0.52
1:D:388:SER:N	2:D:603:IMP:O1P	2.36	0.52
1:F:452:SER:OG	1:F:453:ILE:N	2.43	0.52
1:B:304:VAL:HG13	1:B:309:GLN:HG2	1.90	0.52
1:C:453:ILE:HA	1:C:456:PHE:HB3	1.91	0.52
1:D:115:ILE:HG23	1:D:221:ILE:HG23	1.92	0.52
1:A:415:GLY:N	2:A:601:IMP:O6	2.37	0.52
1:C:272:VAL:HA	1:C:300:ILE:HG13	1.92	0.52
1:G:332:ILE:HD11	1:G:443:VAL:HG13	1.92	0.52
1:A:108:LYS:HE2	1:A:268:VAL:HA	1.92	0.52
1:B:91:ILE:H	1:B:248:ALA:HA	1.75	0.52
1:E:336:VAL:HG12	1:E:337:LEU:HD22	1.90	0.52
1:E:387:GLY:HA3	2:E:601:IMP:H5'1	1.90	0.52
1:H:274:ASP:OD2	3:H:604:NAD:O2D	2.27	0.52
1:A:170:GLU:HA	1:A:173:CYS:HB2	1.91	0.51
1:A:474:LYS:H	1:A:478:GLN:HE21	1.57	0.51
1:B:452:SER:OG	1:B:453:ILE:N	2.44	0.51
1:E:91:ILE:HG23	1:E:100:GLN:HE21	1.74	0.51
1:F:355:ARG:HH12	1:K:12:TYR:HA	1.75	0.51
1:G:325:MET:HE1	1:H:39:PRO:HG3	1.93	0.51
1:A:105:ARG:O	1:A:109:LYS:N	2.42	0.51
1:B:71:ASP:OD2	1:B:412:ARG:NH1	2.43	0.51
1:C:128:ARG:HH11	1:C:170:GLU:HG2	1.76	0.51
1:D:49:VAL:HG11	1:D:465:GLN:HB2	1.91	0.51
1:C:201:LEU:HD11	1:C:224:ARG:HG3	1.92	0.51
1:E:412:ARG:NH2	1:E:418:ASP:O	2.44	0.51
1:H:193:THR:OG1	1:H:196:GLU:OE1	2.27	0.51
1:H:208:LYS:HB3	1:H:221:ILE:HD11	1.93	0.51
1:C:159:SER:HB3	4:C:601:ATP:H3'	1.93	0.51
1:E:276:SER:OG	1:E:277:GLN:N	2.44	0.51
1:G:19:THR:H	1:G:22:GLN:HE21	1.57	0.51
1:A:373:ILE:HG23	1:A:384:VAL:HG11	1.92	0.51
1:D:100:GLN:HE21	1:D:248:ALA:HB1	1.76	0.51
1:F:71:ASP:OD2	1:F:412:ARG:NH1	2.44	0.51
1:A:161:ARG:HE	1:H:224:ARG:NH2	2.09	0.51
1:C:100:GLN:HA	1:C:103:GLU:HB3	1.92	0.51
1:E:140:CYS:HG	1:E:160:SER:HG	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ARG:HD2	1:E:418:ASP:HB2	1.92	0.51
1:F:108:LYS:O	1:F:243:GLN:NE2	2.43	0.51
1:H:328:GLY:N	1:H:331:CYS:SG	2.84	0.51
1:A:56:THR:OG1	1:A:319:ASP:OD2	2.25	0.50
1:A:276:SER:OG	1:A:277:GLN:N	2.44	0.50
1:A:335:GLU:OE2	1:B:369:ASN:ND2	2.44	0.50
1:E:67:SER:HB2	1:E:82:MET:HE1	1.92	0.50
1:H:213:ASN:HB3	1:H:217:GLU:HB2	1.92	0.50
1:H:330:ILE:HD13	1:H:413:GLY:HA3	1.93	0.50
1:E:126:ARG:HG2	1:E:170:GLU:HB2	1.92	0.50
1:E:469:GLN:NE2	3:H:604:NAD:O3B	2.44	0.50
1:G:339:CYS:SG	1:G:340:GLY:N	2.83	0.50
1:E:134:LYS:HB2	1:E:140:CYS:HB3	1.92	0.50
1:D:126:ARG:NE	1:D:169:GLU:O	2.45	0.50
1:G:394:THR:OG1	1:G:395:GLU:OE1	2.25	0.50
1:C:104:VAL:HA	1:C:107:VAL:HG12	1.94	0.50
1:E:74:THR:HG23	1:E:78:MET:HB2	1.93	0.50
1:E:353:TYR:HD1	1:E:356:ARG:HH11	1.58	0.50
1:H:91:ILE:H	1:H:248:ALA:HA	1.76	0.50
1:H:119:VAL:HG13	1:H:142:ILE:HD11	1.93	0.50
1:A:280:SER:OG	1:A:283:GLN:N	2.39	0.50
1:A:51:LEU:HD11	1:A:464:ILE:HG23	1.93	0.50
1:E:355:ARG:HH12	1:J:12:TYR:HA	1.77	0.50
1:B:120:VAL:HG12	1:B:143:PRO:HG2	1.93	0.49
1:C:386:MET:HG2	1:C:390:LEU:HD13	1.94	0.49
1:B:114:PHE:HD1	1:B:222:ILE:HD11	1.77	0.49
1:B:322:ARG:HA	1:B:362:ILE:HB	1.93	0.49
1:E:335:GLU:OE2	1:F:369:ASN:ND2	2.45	0.49
1:B:38:LEU:HD11	1:B:489:LYS:HG3	1.94	0.49
1:C:68:SER:OG	1:C:70:MET:SD	2.63	0.49
1:D:328:GLY:N	1:D:331:CYS:SG	2.86	0.49
1:E:356:ARG:NH2	1:J:12:TYR:OH	2.45	0.49
1:B:61:LEU:HD21	1:B:88:ILE:HG22	1.94	0.49
1:E:51:LEU:HD11	1:E:464:ILE:HG23	1.94	0.49
1:C:305:VAL:H	1:C:309:GLN:NE2	2.10	0.49
1:E:105:ARG:O	1:E:109:LYS:N	2.40	0.49
1:G:70:MET:HB2	1:G:73:VAL:HG12	1.95	0.49
1:B:333:THR:HG23	1:B:337:LEU:HB2	1.94	0.49
1:D:393:THR:O	1:D:409:LYS:NZ	2.40	0.49
1:E:416:SER:OG	1:E:417:LEU:N	2.46	0.49
1:B:187:VAL:HG11	1:B:212:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ALA:HB1	1:B:478:GLN:HB3	1.95	0.49
1:D:329:SER:N	2:D:603:IMP:O3P	2.36	0.49
1:E:42:ILE:HG23	1:H:280:SER:HA	1.94	0.49
1:E:70:MET:SD	2:E:601:IMP:H8	2.53	0.49
1:F:61:LEU:HD21	1:F:88:ILE:HG22	1.94	0.49
1:D:62:LYS:HE2	1:D:235:LEU:HA	1.93	0.49
1:H:155:VAL:O	1:H:182:ARG:NH1	2.39	0.49
1:B:105:ARG:HA	1:B:108:LYS:HE3	1.94	0.49
1:F:211:ILE:HD11	1:F:220:ALA:HB3	1.95	0.49
1:H:329:SER:N	2:H:603:IMP:O2P	2.46	0.49
1:E:91:ILE:H	1:E:248:ALA:HA	1.78	0.48
1:G:303:ASN:ND2	3:G:604:NAD:O7N	2.46	0.48
1:G:333:THR:HG22	1:G:441:GLN:HB2	1.95	0.48
1:H:188:ALA:HB3	1:H:211:ILE:HD13	1.95	0.48
1:C:341:ARG:NH2	1:D:491:GLU:OE1	2.46	0.48
1:D:126:ARG:HG2	1:D:127:VAL:H	1.78	0.48
1:D:283:GLN:HE22	1:D:302:GLY:H	1.61	0.48
1:F:361:VAL:HG13	1:F:381:ALA:HA	1.95	0.48
1:H:336:VAL:HG12	1:H:337:LEU:HD12	1.95	0.48
1:E:82:MET:HA	1:E:85:THR:HG22	1.94	0.48
1:F:212:VAL:HG12	1:F:218:LEU:HA	1.96	0.48
1:A:236:ALA:HB3	1:A:238:LYS:HE3	1.96	0.48
1:A:248:ALA:HB3	1:A:263:LEU:HD21	1.94	0.48
1:B:361:VAL:HG13	1:B:381:ALA:HA	1.94	0.48
1:D:142:ILE:HD12	1:D:143:PRO:HD2	1.96	0.48
1:H:80:ILE:HG23	1:H:107:VAL:HG22	1.93	0.48
1:B:21:GLN:OE1	1:B:348:TYR:OH	2.26	0.48
1:G:341:ARG:NH2	1:H:491:GLU:OE1	2.47	0.48
1:G:362:ILE:HG12	1:G:385:MET:HE3	1.95	0.48
1:F:33:ASN:O	1:F:498:GLN:NE2	2.40	0.48
1:H:70:MET:HB2	1:H:73:VAL:HG12	1.95	0.48
1:H:190:ALA:HA	1:H:211:ILE:HD11	1.94	0.48
1:A:252:THR:HG23	1:A:286:MET:HE2	1.95	0.48
1:D:263:LEU:HD12	1:D:268:VAL:HB	1.95	0.48
1:C:384:VAL:HG13	1:C:386:MET:HE1	1.96	0.48
1:B:36:LEU:HD22	1:B:493:ARG:HD2	1.96	0.48
1:C:322:ARG:HG3	1:C:362:ILE:HD11	1.96	0.48
1:D:165:PHE:HE1	1:E:231:ARG:HG2	1.78	0.48
1:H:131:PHE:HA	1:H:134:LYS:HE2	1.96	0.48
1:A:42:ILE:HG13	1:D:280:SER:HA	1.96	0.47
1:B:212:VAL:HG12	1:B:218:LEU:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:LEU:HA	1:C:479:VAL:HG12	1.96	0.47
1:F:506:LEU:HD11	1:F:509:TYR:HB3	1.96	0.47
1:A:263:LEU:HD23	1:A:268:VAL:HG11	1.95	0.47
1:C:186:VAL:O	4:C:601:ATP:N6	2.47	0.47
1:D:97:PRO:HG3	1:D:259:ARG:HG2	1.95	0.47
1:D:181:LYS:O	1:D:182:ARG:NH2	2.40	0.47
3:F:604:NAD:O3B	1:G:469:GLN:NE2	2.47	0.47
1:F:373:ILE:HG23	1:F:384:VAL:HG11	1.95	0.47
1:F:476:LEU:HA	1:F:479:VAL:HG12	1.96	0.47
1:C:165:PHE:HD2	1:F:202:GLN:HB3	1.79	0.47
1:E:184:ASP:OD1	1:E:184:ASP:N	2.44	0.47
1:H:79:ALA:HB3	1:H:107:VAL:HG21	1.95	0.47
1:H:304:VAL:HG11	1:H:321:LEU:HD22	1.95	0.47
1:C:70:MET:HG2	1:C:73:VAL:HG12	1.96	0.47
1:G:207:GLY:HA2	1:G:224:ARG:HD2	1.96	0.47
1:C:80:ILE:HG13	1:C:107:VAL:HG23	1.96	0.47
1:E:12:TYR:HB3	1:H:311:LYS:HE2	1.96	0.47
1:F:335:GLU:O	1:G:369:ASN:ND2	2.46	0.47
1:G:329:SER:N	2:G:603:IMP:O2P	2.44	0.47
1:A:31:THR:OG1	1:A:32:TYR:N	2.43	0.47
1:C:109:LYS:HA	1:C:243:GLN:HE21	1.80	0.47
1:C:260:LEU:HD22	1:C:290:ILE:HD11	1.97	0.47
1:C:332:ILE:HD11	1:C:443:VAL:HB	1.96	0.47
1:C:393:THR:O	1:C:409:LYS:NZ	2.39	0.47
1:D:80:ILE:HG23	1:D:107:VAL:HG22	1.96	0.47
1:D:330:ILE:HD13	1:D:413:GLY:HA3	1.97	0.47
1:E:329:SER:N	2:E:601:IMP:O1P	2.42	0.47
1:F:51:LEU:HD11	1:F:464:ILE:HD11	1.96	0.47
1:G:64:PRO:HA	1:G:383:THR:HG22	1.97	0.47
1:E:154:LEU:N	1:E:216:ASP:OD2	2.47	0.47
1:F:80:ILE:O	1:F:84:LEU:HB2	2.14	0.47
1:F:306:THR:OG1	1:G:16:ASP:OD2	2.28	0.47
1:G:206:LYS:O	1:G:224:ARG:NH1	2.47	0.47
1:C:112:GLN:NE2	1:C:230:ASN:OD1	2.48	0.47
1:C:302:GLY:HA2	1:C:303:ASN:HA	1.72	0.47
1:F:36:LEU:HD22	1:F:493:ARG:HD2	1.97	0.47
1:A:70:MET:HB2	1:A:73:VAL:HG22	1.97	0.47
1:A:308:ALA:HA	1:B:14:PRO:HD2	1.96	0.47
1:C:300:ILE:HG22	1:C:320:ALA:HB3	1.96	0.47
1:D:476:LEU:HA	1:D:479:VAL:HG12	1.97	0.47
1:B:272:VAL:HG23	1:B:300:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ILE:HG21	1:C:413:GLY:H	1.79	0.46
1:C:370:VAL:HG12	1:C:460:LEU:HG	1.97	0.46
1:G:305:VAL:H	1:G:309:GLN:NE2	2.13	0.46
1:B:80:ILE:HD11	1:B:110:TYR:CG	2.51	0.46
1:D:414:MET:HE2	1:D:414:MET:HB2	1.75	0.46
1:E:334:GLN:HG3	1:F:36:LEU:HD13	1.96	0.46
1:F:234:PRO:HG2	1:F:235:LEU:HD22	1.96	0.46
1:G:364:ASP:OD2	2:G:603:IMP:O2'	2.24	0.46
1:B:62:LYS:HB3	1:B:235:LEU:HD12	1.96	0.46
1:D:144:ILE:HG23	1:D:155:VAL:HG23	1.98	0.46
1:F:210:PRO:HA	1:F:221:ILE:HA	1.97	0.46
1:F:211:ILE:HD12	1:F:219:VAL:HG23	1.97	0.46
1:A:85:THR:HG21	1:A:457:VAL:HG11	1.97	0.46
1:A:343:GLN:O	1:A:346:ALA:N	2.48	0.46
1:D:393:THR:OG1	1:D:396:ALA:N	2.49	0.46
1:G:200:ILE:O	1:G:204:SER:CB	2.64	0.46
1:E:337:LEU:HD13	1:E:337:LEU:HA	1.71	0.46
1:E:360:PRO:HG3	1:J:6:ILE:HD11	1.97	0.46
1:A:162:ASP:OD1	1:A:162:ASP:N	2.48	0.46
1:B:121:LEU:HD22	1:B:122:SER:H	1.80	0.46
1:C:329:SER:N	2:C:603:IMP:O2P	2.49	0.46
1:F:222:ILE:HD13	1:F:222:ILE:HA	1.84	0.46
1:F:286:MET:HE3	1:F:286:MET:HB3	1.77	0.46
1:H:100:GLN:HE21	1:H:248:ALA:HB1	1.80	0.46
1:B:71:ASP:HB3	1:B:94:ASN:HD21	1.81	0.46
1:B:121:LEU:HD11	1:B:125:ASP:HB3	1.97	0.46
1:B:224:ARG:NH2	1:G:164:ASP:OD2	2.49	0.46
1:B:417:LEU:HD21	1:C:512:ARG:HD2	1.97	0.46
1:D:246:CYS:N	1:D:269:ASP:OD2	2.48	0.46
1:H:97:PRO:HG3	1:H:259:ARG:HG2	1.97	0.46
1:A:14:PRO:HD2	1:D:308:ALA:HA	1.98	0.46
1:A:412:ARG:NH2	1:A:418:ASP:O	2.48	0.46
1:G:187:VAL:HG22	1:G:210:PRO:HB2	1.98	0.46
1:D:61:LEU:HD21	1:D:88:ILE:HG23	1.98	0.46
1:B:211:ILE:HD11	1:B:220:ALA:HB3	1.98	0.45
1:C:281:ILE:HG12	1:D:43:ASP:HA	1.98	0.45
1:G:70:MET:SD	2:G:603:IMP:H8	2.55	0.45
1:H:95:CYS:O	1:H:259:ARG:NH1	2.47	0.45
1:F:104:VAL:HA	1:F:107:VAL:HG12	1.97	0.45
1:E:75:GLU:OE1	1:E:397:PRO:HB3	2.17	0.45
1:G:306:THR:OG1	1:G:309:GLN:OE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:HA	1:B:381:ALA:HB3	1.98	0.45
1:F:304:VAL:HG13	1:F:309:GLN:HG2	1.99	0.45
1:G:126:ARG:HA	1:G:126:ARG:HD2	1.83	0.45
1:H:305:VAL:H	1:H:309:GLN:HE21	1.65	0.45
1:D:255:ASP:OD1	1:D:255:ASP:N	2.48	0.45
1:A:50:ASP:OD1	1:A:50:ASP:N	2.50	0.45
1:F:250:ILE:HG21	1:F:260:LEU:HD23	1.97	0.45
1:G:79:ALA:O	1:G:83:ALA:HB2	2.16	0.45
1:G:61:LEU:HD23	1:G:87:GLY:HA2	1.99	0.45
1:G:496:SER:HA	1:G:499:VAL:HG12	1.98	0.45
1:A:71:ASP:HA	1:A:92:HIS:CD2	2.52	0.45
1:A:112:GLN:HG3	1:A:243:GLN:HE21	1.81	0.45
1:A:208:LYS:HB3	1:A:221:ILE:HD11	1.98	0.45
1:A:231:ARG:HH22	1:H:164:ASP:HB3	1.82	0.45
1:C:306:THR:HG22	1:D:38:LEU:HD23	1.98	0.45
1:F:417:LEU:HD21	1:G:512:ARG:HD2	1.98	0.45
1:G:305:VAL:H	1:G:309:GLN:HE21	1.65	0.45
1:A:184:ASP:OD1	1:A:184:ASP:N	2.49	0.45
1:A:300:ILE:HD12	1:A:320:ALA:HB3	1.99	0.45
1:B:333:THR:O	1:B:337:LEU:N	2.39	0.45
1:E:504:HIS:CE1	1:H:368:GLN:HE21	2.35	0.45
1:F:324:GLY:HA3	1:F:343:GLN:HE22	1.81	0.45
1:C:373:ILE:HG23	1:C:384:VAL:HG11	1.98	0.44
1:B:88:ILE:HD13	1:B:245:LEU:HB3	1.99	0.44
1:B:118:PRO:HB3	4:B:602:ATP:HN62	1.82	0.44
1:C:37:ILE:HD13	1:C:37:ILE:HG21	1.81	0.44
1:D:91:ILE:H	1:D:248:ALA:HA	1.82	0.44
1:E:71:ASP:HA	1:E:92:HIS:CD2	2.53	0.44
1:F:389:LEU:H	1:F:389:LEU:HD23	1.82	0.44
1:B:305:VAL:HG21	1:B:325:MET:HG2	1.99	0.44
1:C:387:GLY:HA3	2:C:603:IMP:H5'1	1.98	0.44
1:F:71:ASP:HA	1:F:92:HIS:CD2	2.52	0.44
1:G:373:ILE:H	1:G:373:ILE:HG13	1.62	0.44
1:B:269:ASP:OD1	1:B:270:VAL:N	2.49	0.44
1:B:367:ILE:HG21	1:B:386:MET:HE2	2.00	0.44
1:F:239:ASP:OD1	1:F:243:GLN:N	2.38	0.44
1:G:16:ASP:N	1:G:16:ASP:OD1	2.42	0.44
1:D:126:ARG:HG2	1:D:127:VAL:HG23	1.99	0.44
1:H:263:LEU:O	1:H:267:GLY:N	2.51	0.44
1:H:461:ILE:HA	1:H:464:ILE:HG22	1.99	0.44
1:C:354:ALA:HB1	1:C:359:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:VAL:HG11	1:D:321:LEU:HD22	2.00	0.44
1:E:133:ALA:O	1:E:137:HIS:N	2.46	0.44
1:F:229:LYS:HA	1:F:231:ARG:HH21	1.82	0.44
1:H:286:MET:HE2	1:H:286:MET:HB3	1.72	0.44
1:A:12:TYR:HB3	1:D:311:LYS:HE2	2.00	0.44
1:B:354:ALA:HB1	1:B:359:VAL:HG13	2.00	0.44
1:G:223:ALA:HB3	1:G:226:ASP:HB2	2.00	0.44
1:A:212:VAL:HG22	1:A:218:LEU:HA	2.00	0.43
1:B:386:MET:HE2	1:B:386:MET:HB3	1.64	0.43
1:E:305:VAL:H	1:E:309:GLN:NE2	2.15	0.43
1:F:327:SER:OG	1:F:343:GLN:NE2	2.46	0.43
1:G:145:THR:HA	1:G:155:VAL:HB	1.99	0.43
1:G:370:VAL:HG11	1:G:463:GLY:HA3	2.00	0.43
1:C:492:LYS:HE3	1:C:492:LYS:HB2	1.82	0.43
1:D:58:LYS:HB3	1:D:298:GLN:HE22	1.81	0.43
1:D:285:ASN:HA	1:D:288:LYS:HZ2	1.83	0.43
1:E:212:VAL:HG22	1:E:218:LEU:HA	2.00	0.43
1:A:143:PRO:HA	1:A:157:ILE:HA	2.00	0.43
1:B:187:VAL:HG13	1:B:211:ILE:HA	2.01	0.43
1:D:155:VAL:O	1:D:182:ARG:NH2	2.49	0.43
1:D:492:LYS:HE3	1:D:492:LYS:HB2	1.87	0.43
1:A:309:GLN:HE22	1:B:39:PRO:HG2	1.83	0.43
1:B:104:VAL:HA	1:B:107:VAL:HG12	1.99	0.43
1:H:304:VAL:HG11	1:H:321:LEU:HD13	2.00	0.43
1:B:70:MET:HE2	1:B:70:MET:HB2	1.91	0.43
1:E:128:ARG:HG2	1:E:170:GLU:HB3	2.01	0.43
1:H:370:VAL:HG21	1:H:463:GLY:HA3	2.01	0.43
1:A:82:MET:HE2	1:A:82:MET:HB3	1.90	0.43
1:A:164:ASP:OD1	1:A:164:ASP:N	2.51	0.43
1:F:43:ASP:OD1	1:F:43:ASP:N	2.50	0.43
1:G:61:LEU:HD21	1:G:88:ILE:HG22	2.00	0.43
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.81	0.43
1:B:386:MET:HG3	1:B:390:LEU:HD22	2.01	0.43
1:G:329:SER:OG	1:G:388:SER:OG	2.24	0.43
1:B:31:THR:OG1	1:B:32:TYR:N	2.51	0.43
1:C:386:MET:SD	1:C:386:MET:N	2.92	0.43
1:E:314:ILE:HA	1:E:318:VAL:HG12	2.01	0.43
1:C:377:LEU:HA	1:C:381:ALA:HB3	1.99	0.43
1:E:56:THR:OG1	1:E:57:LYS:N	2.46	0.43
1:G:88:ILE:HD13	1:G:245:LEU:HB3	2.01	0.43
1:A:332:ILE:O	1:A:336:VAL:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:VAL:HG12	1:B:298:GLN:HB2	2.01	0.43
1:C:496:SER:HA	1:C:499:VAL:HG12	2.01	0.43
1:E:330:ILE:H	1:E:330:ILE:HG13	1.63	0.43
1:F:356:ARG:HG2	1:K:12:TYR:CE1	2.53	0.43
1:F:386:MET:HE1	1:F:460:LEU:HD21	1.99	0.43
1:H:108:LYS:NZ	1:H:267:GLY:O	2.32	0.43
1:H:255:ASP:OD1	1:H:255:ASP:N	2.49	0.43
1:I:7:SER:OG	1:I:10:THR:N	2.52	0.43
1:B:222:ILE:HD13	1:B:222:ILE:HA	1.83	0.42
1:B:305:VAL:H	1:B:309:GLN:NE2	2.17	0.42
1:G:281:ILE:HG12	1:H:43:ASP:HA	2.00	0.42
1:A:305:VAL:H	1:A:309:GLN:NE2	2.16	0.42
1:B:492:LYS:HE3	1:B:492:LYS:HB2	1.86	0.42
1:A:67:SER:HB3	1:A:82:MET:SD	2.60	0.42
1:A:504:HIS:CE1	1:D:368:GLN:HE21	2.38	0.42
1:D:72:THR:HG21	1:D:412:ARG:H	1.85	0.42
1:D:369:ASN:OD1	1:D:369:ASN:N	2.49	0.42
1:E:459:TYR:HE1	1:H:439:VAL:HG23	1.84	0.42
1:F:109:LYS:HG2	1:F:110:TYR:H	1.85	0.42
1:H:158:ILE:HD11	1:H:178:ILE:HG22	2.00	0.42
1:H:377:LEU:HD23	1:H:377:LEU:HA	1.87	0.42
1:D:184:ASP:OD1	1:D:184:ASP:N	2.48	0.42
1:A:73:VAL:O	1:A:78:MET:HG3	2.19	0.42
1:B:80:ILE:HD11	1:B:110:TYR:CD1	2.54	0.42
1:B:116:THR:HG22	1:B:117:ASP:H	1.85	0.42
1:E:194:LEU:O	1:E:198:ASN:ND2	2.52	0.42
1:F:109:LYS:C	1:F:111:GLU:H	2.27	0.42
1:F:302:GLY:HA3	1:F:303:ASN:HA	1.83	0.42
1:A:126:ARG:HG3	1:A:170:GLU:HG2	2.02	0.42
1:A:154:LEU:N	1:A:216:ASP:OD2	2.51	0.42
1:D:140:CYS:N	4:D:602:ATP:O2A	2.51	0.42
1:E:83:ALA:O	1:E:237:SER:OG	2.32	0.42
1:H:389:LEU:H	1:H:389:LEU:HD23	1.83	0.42
1:A:161:ARG:HE	1:H:224:ARG:HH22	1.68	0.42
1:B:80:ILE:HD13	1:B:80:ILE:HG21	1.79	0.42
1:B:403:SER:HB3	1:B:408:LEU:HD21	2.01	0.42
1:F:153:ARG:HH11	1:F:216:ASP:HB3	1.85	0.42
1:A:360:PRO:HG3	1:N:6:ILE:HD11	2.01	0.42
1:B:130:VAL:O	1:B:134:LYS:NZ	2.41	0.42
1:C:473:ALA:HB1	1:C:478:GLN:HG2	2.02	0.42
1:E:67:SER:HB3	1:E:89:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:LEU:HA	1:E:381:ALA:HB3	2.00	0.42
1:H:283:GLN:HE22	1:H:302:GLY:H	1.66	0.42
1:E:80:ILE:HG13	1:E:107:VAL:HG23	2.02	0.42
1:A:95:CYS:O	1:A:259:ARG:NH1	2.44	0.42
1:B:140:CYS:HB2	1:B:160:SER:HB2	2.02	0.42
1:C:309:GLN:HE22	1:D:39:PRO:HG2	1.84	0.42
1:E:395:GLU:CD	1:E:453:ILE:H	2.28	0.42
1:G:97:PRO:HG3	1:G:259:ARG:HE	1.85	0.42
1:G:503:VAL:HG21	1:G:509:TYR:CZ	2.55	0.42
1:H:71:ASP:H	1:H:414:MET:HE1	1.84	0.42
1:H:269:ASP:OD1	1:H:269:ASP:N	2.45	0.42
1:A:100:GLN:NE2	1:A:248:ALA:HB1	2.35	0.41
1:D:47:ASP:OD1	1:D:47:ASP:N	2.53	0.41
1:D:114:PHE:HD1	1:D:222:ILE:HD13	1.84	0.41
1:D:330:ILE:H	1:D:330:ILE:HG13	1.55	0.41
1:E:211:ILE:HD11	1:E:220:ALA:HB3	2.00	0.41
1:H:494:THR:HG23	1:H:496:SER:H	1.85	0.41
1:C:97:PRO:O	1:C:101:ALA:HB2	2.20	0.41
1:C:471:ILE:H	1:C:471:ILE:HG13	1.78	0.41
1:D:45:THR:OG1	1:D:46:ALA:N	2.51	0.41
1:E:280:SER:OG	1:E:283:GLN:N	2.45	0.41
1:F:18:LEU:HD12	1:F:22:GLN:HG3	2.02	0.41
1:F:73:VAL:HG13	1:F:74:THR:HG22	2.02	0.41
1:F:387:GLY:HA3	2:F:603:IMP:H5'1	2.01	0.41
1:G:272:VAL:HG13	1:G:300:ILE:HD11	2.01	0.41
1:A:47:ASP:OD1	1:A:47:ASP:N	2.47	0.41
1:A:362:ILE:HG21	1:A:385:MET:HE3	2.02	0.41
1:D:124:LYS:NZ	1:D:172:ASP:O	2.54	0.41
1:D:461:ILE:HA	1:D:464:ILE:HG22	2.02	0.41
1:F:120:VAL:HG12	1:F:143:PRO:HG2	2.02	0.41
1:F:126:ARG:NH2	1:F:128:ARG:HE	2.19	0.41
1:F:246:CYS:SG	1:F:247:GLY:N	2.93	0.41
2:F:603:IMP:H8	2:F:603:IMP:H2'	1.79	0.41
1:G:325:MET:HE3	1:G:340:GLY:HA2	2.02	0.41
1:G:387:GLY:HA3	2:G:603:IMP:H5'1	2.00	0.41
1:G:478:GLN:HA	1:G:481:ALA:HB3	2.01	0.41
1:A:386:MET:HB2	1:A:390:LEU:HD22	2.02	0.41
1:D:269:ASP:OD1	1:D:269:ASP:N	2.43	0.41
4:D:601:ATP:O2G	1:E:161:ARG:NH1	2.54	0.41
1:G:492:LYS:HE3	1:G:492:LYS:HB2	1.81	0.41
1:L:10:THR:OG1	1:L:11:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HD13	1:A:337:LEU:HA	1.79	0.41
1:G:127:VAL:HG12	1:G:175:LEU:HD11	2.03	0.41
1:H:273:LEU:HD13	1:H:283:GLN:HG3	2.02	0.41
1:H:369:ASN:OD1	1:H:369:ASN:N	2.51	0.41
1:A:491:GLU:OE1	1:D:341:ARG:NH2	2.53	0.41
1:B:30:LEU:H	1:B:30:LEU:HG	1.57	0.41
1:C:129:ASP:OD1	1:C:130:VAL:N	2.54	0.41
1:F:388:SER:OG	1:F:389:LEU:N	2.53	0.41
1:H:206:LYS:HE3	4:H:601:ATP:C6	2.56	0.41
1:H:306:THR:OG1	1:H:307:ALA:N	2.54	0.41
1:B:91:ILE:HD12	1:B:91:ILE:HA	1.89	0.41
1:E:142:ILE:HD12	1:E:142:ILE:HA	1.89	0.41
1:A:82:MET:HA	1:A:85:THR:HG22	2.02	0.41
1:A:492:LYS:HE3	1:A:492:LYS:HB2	1.92	0.41
1:D:38:LEU:HD11	1:D:491:GLU:HG2	2.03	0.41
1:D:58:LYS:HD2	1:D:298:GLN:HE22	1.86	0.41
1:D:366:GLY:O	1:D:368:GLN:NE2	2.54	0.41
1:F:126:ARG:HH22	1:F:128:ARG:HE	1.68	0.41
1:H:160:SER:OG	4:H:601:ATP:O1B	2.29	0.41
1:A:449:ASP:OD1	1:A:450:LYS:N	2.54	0.41
1:B:43:ASP:OD1	1:B:43:ASP:N	2.52	0.41
1:D:263:LEU:O	1:D:267:GLY:N	2.54	0.41
1:F:121:LEU:HD21	1:F:125:ASP:HB3	2.03	0.41
1:F:305:VAL:H	1:F:309:GLN:NE2	2.19	0.41
1:G:149:ARG:HG3	1:G:151:GLY:H	1.86	0.41
1:B:77:GLY:HA2	1:B:80:ILE:HG22	2.03	0.41
1:C:145:THR:HG21	1:C:149:ARG:O	2.21	0.41
1:C:323:VAL:HG21	1:C:347:VAL:HG12	2.03	0.41
1:D:79:ALA:HB3	1:D:107:VAL:HG21	2.02	0.41
1:E:49:VAL:HG23	1:E:475:SER:HA	2.03	0.41
1:F:205:LYS:HE3	1:F:205:LYS:HB3	1.90	0.41
1:F:495:SER:HA	1:F:498:GLN:HG2	2.01	0.41
1:H:126:ARG:HH21	1:H:126:ARG:HD2	1.78	0.41
1:H:281:ILE:HA	1:H:284:ILE:HG22	2.02	0.41
1:K:10:THR:OG1	1:K:11:SER:N	2.54	0.41
1:D:209:LEU:HB3	1:D:222:ILE:HG22	2.04	0.40
1:G:158:ILE:HG22	1:G:179:MET:HG2	2.02	0.40
1:B:327:SER:O	1:B:327:SER:OG	2.39	0.40
1:E:47:ASP:OD1	1:E:47:ASP:N	2.48	0.40
1:E:67:SER:OG	1:E:68:SER:N	2.54	0.40
1:E:82:MET:O	1:E:87:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ILE:HD12	1:E:250:ILE:HG23	1.85	0.40
1:O:10:THR:OG1	1:O:11:SER:N	2.54	0.40
1:A:56:THR:HG22	1:A:59:ILE:HG13	2.03	0.40
1:A:88:ILE:HD12	1:A:88:ILE:HA	1.85	0.40
1:D:213:ASN:HB3	1:D:217:GLU:HB2	2.03	0.40
1:F:283:GLN:HA	1:F:286:MET:SD	2.61	0.40
1:F:339:CYS:SG	1:F:340:GLY:N	2.93	0.40
1:G:354:ALA:HB1	1:G:359:VAL:HG13	2.03	0.40
1:C:65:LEU:HA	1:C:65:LEU:HD13	1.90	0.40
1:C:128:ARG:HE	1:C:170:GLU:HG2	1.87	0.40
1:C:332:ILE:HG22	1:C:336:VAL:HG13	2.02	0.40
1:D:304:VAL:HG11	1:D:321:LEU:HD13	2.04	0.40
1:D:477:THR:H	1:D:477:THR:HG23	1.60	0.40
1:F:304:VAL:HA	1:F:309:GLN:HE21	1.85	0.40
1:G:58:LYS:HB2	1:G:298:GLN:HE22	1.87	0.40
1:K:3:ASP:OD1	1:K:3:ASP:N	2.53	0.40
1:B:306:THR:OG1	1:B:307:ALA:N	2.54	0.40
1:F:65:LEU:HD11	1:F:373:ILE:HD13	2.03	0.40
1:F:176:GLU:HA	1:F:179:MET:HE3	2.03	0.40
1:F:280:SER:HB2	1:F:282:PHE:HD2	1.86	0.40
1:F:417:LEU:HD21	1:G:512:ARG:HB3	2.03	0.40
1:G:65:LEU:HD13	1:G:65:LEU:HA	1.82	0.40
1:G:466:HIS:O	1:G:470:ASP:HB2	2.21	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
1	B	484/519 (93%)	446 (92%)	37 (8%)	1 (0%)	43	75

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

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	111	GLU
1	B	110	TYR
1	D	111	GLU
1	D	110	TYR
1	F	110	TYR
1	F	111	GLU
1	G	110	TYR
1	G	111	GLU
1	H	110	TYR
1	H	111	GLU
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%)	387 (97%)	11 (3%)	38	59
1	B	398/425 (94%)	387 (97%)	11 (3%)	38	59
1	C	398/425 (94%)	386 (97%)	12 (3%)	36	57
1	D	398/425 (94%)	381 (96%)	17 (4%)	26	49
1	E	398/425 (94%)	389 (98%)	9 (2%)	44	63
1	F	398/425 (94%)	383 (96%)	15 (4%)	29	51
1	G	398/425 (94%)	381 (96%)	17 (4%)	26	49
1	H	398/425 (94%)	385 (97%)	13 (3%)	33	55
1	I	11/425 (3%)	11 (100%)	0	100	100
1	J	11/425 (3%)	11 (100%)	0	100	100
1	K	11/425 (3%)	11 (100%)	0	100	100
1	L	11/425 (3%)	11 (100%)	0	100	100
1	M	11/425 (3%)	11 (100%)	0	100	100
1	N	11/425 (3%)	11 (100%)	0	100	100
1	O	11/425 (3%)	11 (100%)	0	100	100
1	P	11/425 (3%)	11 (100%)	0	100	100
All	All	3272/6800 (48%)	3167 (97%)	105 (3%)	35	56

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	49	VAL
1	A	66	VAL
1	A	103	GLU
1	A	163	ILE
1	A	201	LEU
1	A	287	ILE
1	A	314	ILE
1	A	361	VAL
1	A	377	LEU
1	A	461	ILE
1	B	30	LEU
1	B	72	THR
1	B	163	ILE

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Mol	Chain	Res	Type
1	B	250	ILE
1	B	284	ILE
1	B	332	ILE
1	B	359	VAL
1	B	361	VAL
1	B	373	ILE
1	B	384	VAL
1	B	455	LYS
1	C	36	LEU
1	C	51	LEU
1	C	72	THR
1	C	78	MET
1	C	88	ILE
1	C	91	ILE
1	C	163	ILE
1	C	200	ILE
1	C	250	ILE
1	C	262	LEU
1	C	377	LEU
1	C	465	GLN
1	D	49	VAL
1	D	51	LEU
1	D	142	ILE
1	D	166	LEU
1	D	201	LEU
1	D	235	LEU
1	D	250	ILE
1	D	252	THR
1	D	287	ILE
1	D	297	LEU
1	D	300	ILE
1	D	304	VAL
1	D	314	ILE
1	D	330	ILE
1	D	389	LEU
1	D	465	GLN
1	D	488	LEU
1	E	36	LEU
1	E	49	VAL
1	E	66	VAL
1	E	103	GLU
1	E	314	ILE

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Mol	Chain	Res	Type
1	E	330	ILE
1	E	367	ILE
1	E	377	LEU
1	E	465	GLN
1	F	51	LEU
1	F	66	VAL
1	F	91	ILE
1	F	103	GLU
1	F	132	GLU
1	F	163	ILE
1	F	166	LEU
1	F	201	LEU
1	F	284	ILE
1	F	287	ILE
1	F	300	ILE
1	F	332	ILE
1	F	384	VAL
1	F	455	LYS
1	F	465	GLN
1	G	31	THR
1	G	36	LEU
1	G	51	LEU
1	G	66	VAL
1	G	72	THR
1	G	78	MET
1	G	84	LEU
1	G	91	ILE
1	G	200	ILE
1	G	201	LEU
1	G	202	GLN
1	G	250	ILE
1	G	287	ILE
1	G	362	ILE
1	G	373	ILE
1	G	465	GLN
1	G	483	MET
1	H	49	VAL
1	H	51	LEU
1	H	88	ILE
1	H	130	VAL
1	H	166	LEU
1	H	281	ILE

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Mol	Chain	Res	Type
1	H	287	ILE
1	H	300	ILE
1	H	304	VAL
1	H	314	ILE
1	H	330	ILE
1	H	465	GLN
1	H	488	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	171	HIS
1	A	230	ASN
1	A	283	GLN
1	A	309	GLN
1	A	343	GLN
1	A	478	GLN
1	A	498	GLN
1	B	112	GLN
1	B	137	HIS
1	B	243	GLN
1	B	283	GLN
1	B	312	ASN
1	B	343	GLN
1	C	112	GLN
1	C	243	GLN
1	C	277	GLN
1	C	309	GLN
1	C	368	GLN
1	D	22	GLN
1	D	25	ASN
1	D	112	GLN
1	D	137	HIS
1	D	298	GLN
1	D	343	GLN
1	D	368	GLN
1	D	372	HIS
1	E	202	GLN
1	E	230	ASN
1	E	283	GLN
1	E	298	GLN

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Mol	Chain	Res	Type
1	E	309	GLN
1	E	504	HIS
1	F	137	HIS
1	F	243	GLN
1	F	283	GLN
1	F	309	GLN
1	F	312	ASN
1	F	343	GLN
1	F	507	HIS
1	G	22	GLN
1	G	25	ASN
1	G	48	GLN
1	G	112	GLN
1	G	198	ASN
1	G	368	GLN
1	G	469	GLN
1	G	478	GLN
1	H	25	ASN
1	H	112	GLN
1	H	230	ASN
1	H	243	GLN
1	H	253	HIS
1	H	277	GLN
1	H	309	GLN
1	H	372	HIS
1	H	478	GLN
1	H	507	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	G	602	-	32,33,33	3.17	17 (53%)	48,52,52	2.87	12 (25%)
2	IMP	B	603	-	25,25,25	2.63	7 (28%)	37,38,38	2.17	12 (32%)
4	ATP	D	602	-	32,33,33	3.18	16 (50%)	48,52,52	2.89	12 (25%)
4	ATP	A	603	-	32,33,33	3.17	18 (56%)	48,52,52	2.97	14 (29%)
4	ATP	C	602	-	32,33,33	3.20	17 (53%)	48,52,52	2.86	12 (25%)
2	IMP	F	603	-	25,25,25	2.60	7 (28%)	37,38,38	2.08	10 (27%)
4	ATP	F	601	-	32,33,33	3.21	16 (50%)	48,52,52	2.89	13 (27%)
4	ATP	C	601	-	32,33,33	3.16	16 (50%)	48,52,52	2.91	15 (31%)
3	NAD	B	604	-	46,48,48	3.45	21 (45%)	64,73,73	2.40	17 (26%)
4	ATP	E	603	-	32,33,33	3.19	18 (56%)	48,52,52	2.96	13 (27%)
2	IMP	A	601	-	25,25,25	2.54	6 (24%)	37,38,38	2.37	9 (24%)
4	ATP	D	601	-	32,33,33	3.21	18 (56%)	48,52,52	2.94	12 (25%)
4	ATP	H	602	-	32,33,33	3.15	16 (50%)	48,52,52	2.85	14 (29%)
2	IMP	D	603	-	25,25,25	2.62	7 (28%)	37,38,38	2.33	10 (27%)
3	NAD	H	604	-	46,48,48	3.47	21 (45%)	64,73,73	2.39	13 (20%)
4	ATP	H	601	-	32,33,33	3.21	18 (56%)	48,52,52	2.82	12 (25%)
3	NAD	G	604	-	46,48,48	3.46	21 (45%)	64,73,73	2.40	15 (23%)
4	ATP	B	602	-	32,33,33	3.21	17 (53%)	48,52,52	2.84	11 (22%)
4	ATP	F	602	-	32,33,33	3.33	16 (50%)	48,52,52	2.87	11 (22%)
3	NAD	A	602	-	46,48,48	3.47	21 (45%)	64,73,73	2.28	13 (20%)
4	ATP	G	601	-	32,33,33	3.18	17 (53%)	48,52,52	3.06	13 (27%)
3	NAD	C	604	-	46,48,48	3.52	21 (45%)	64,73,73	2.38	14 (21%)
4	ATP	A	604	-	32,33,33	3.21	18 (56%)	48,52,52	2.82	11 (22%)
4	ATP	E	604	-	32,33,33	3.21	16 (50%)	48,52,52	2.91	12 (25%)
4	ATP	B	601	-	32,33,33	3.10	16 (50%)	48,52,52	2.92	12 (25%)
2	IMP	G	603	-	25,25,25	2.64	7 (28%)	37,38,38	2.10	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	E	602	-	46,48,48	3.51	22 (47%)	64,73,73	2.44	15 (23%)
2	IMP	C	603	-	25,25,25	2.63	7 (28%)	37,38,38	2.26	8 (21%)
2	IMP	E	601	-	25,25,25	2.64	6 (24%)	37,38,38	2.25	9 (24%)
3	NAD	D	604	-	46,48,48	3.48	21 (45%)	64,73,73	2.38	15 (23%)
3	NAD	F	604	-	46,48,48	3.50	21 (45%)	64,73,73	2.36	16 (25%)
2	IMP	H	603	-	25,25,25	2.62	7 (28%)	37,38,38	2.29	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (493) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ATP	C2'-C3'	-10.51	1.24	1.53
4	H	602	ATP	C2'-C3'	-10.50	1.24	1.53
4	E	603	ATP	C2'-C3'	-10.49	1.25	1.53
4	A	604	ATP	C2'-C3'	-10.48	1.25	1.53
4	E	604	ATP	C2'-C3'	-10.45	1.25	1.53
4	G	601	ATP	C2'-C3'	-10.38	1.25	1.53
4	D	602	ATP	C2'-C3'	-10.37	1.25	1.53
4	G	602	ATP	C2'-C3'	-10.35	1.25	1.53
4	H	601	ATP	C2'-C3'	-10.35	1.25	1.53
4	D	601	ATP	C2'-C3'	-10.32	1.25	1.53
4	C	602	ATP	C2'-C3'	-10.29	1.25	1.53
4	B	602	ATP	C2'-C3'	-10.29	1.25	1.53
4	C	601	ATP	C2'-C3'	-10.26	1.25	1.53
4	B	601	ATP	C2'-C3'	-10.23	1.25	1.53
4	F	602	ATP	C2'-C3'	-10.23	1.25	1.53
4	F	601	ATP	C2'-C3'	-10.13	1.25	1.53
3	A	602	NAD	C3D-C4D	-9.44	1.29	1.53
3	A	602	NAD	C3B-C4B	-9.24	1.29	1.53
3	E	602	NAD	C3B-C4B	-9.21	1.29	1.53
3	C	604	NAD	C3D-C4D	-9.14	1.29	1.53
3	G	604	NAD	C3B-C4B	-9.08	1.30	1.53
3	E	602	NAD	C3D-C4D	-9.05	1.30	1.53
3	B	604	NAD	C3D-C4D	-8.95	1.30	1.53
3	F	604	NAD	C3B-C4B	-8.95	1.30	1.53
3	B	604	NAD	C3B-C4B	-8.90	1.30	1.53
3	C	604	NAD	C3B-C4B	-8.84	1.30	1.53
3	H	604	NAD	C3B-C4B	-8.81	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	604	NAD	C3D-C4D	-8.80	1.30	1.53
3	F	604	NAD	C3D-C4D	-8.78	1.30	1.53
3	D	604	NAD	C3B-C4B	-8.76	1.30	1.53
3	G	604	NAD	C3D-C4D	-8.74	1.30	1.53
3	D	604	NAD	C3D-C4D	-8.72	1.30	1.53
2	E	601	IMP	C2-N3	8.65	1.45	1.30
2	B	603	IMP	C2-N3	8.46	1.45	1.30
2	H	603	IMP	C2-N3	8.37	1.45	1.30
2	G	603	IMP	C2-N3	8.34	1.45	1.30
3	H	604	NAD	O4D-C1D	-8.27	1.30	1.40
3	D	604	NAD	O4D-C1D	-8.22	1.30	1.40
2	F	603	IMP	C2-N3	8.21	1.44	1.30
2	D	603	IMP	C2-N3	8.21	1.44	1.30
2	C	603	IMP	C2-N3	8.10	1.44	1.30
2	A	601	IMP	C2-N3	8.03	1.44	1.30
3	F	604	NAD	O4D-C1D	-8.01	1.30	1.40
3	G	604	NAD	O4D-C1D	-7.91	1.30	1.40
3	E	602	NAD	O4D-C1D	-7.82	1.30	1.40
3	C	604	NAD	O4D-C1D	-7.73	1.30	1.40
3	B	604	NAD	O4D-C4D	7.66	1.62	1.45
3	F	604	NAD	O4B-C4B	7.66	1.62	1.45
3	C	604	NAD	O4B-C4B	7.59	1.61	1.45
3	B	604	NAD	O4D-C1D	-7.57	1.31	1.40
3	D	604	NAD	O4B-C4B	7.57	1.61	1.45
3	E	602	NAD	O4D-C4D	7.57	1.61	1.45
3	B	604	NAD	O4B-C4B	7.57	1.61	1.45
3	A	602	NAD	O4D-C1D	-7.56	1.31	1.40
3	A	602	NAD	O4B-C4B	7.50	1.61	1.45
3	F	604	NAD	O4D-C4D	7.49	1.61	1.45
3	E	602	NAD	O4B-C4B	7.46	1.61	1.45
3	H	604	NAD	O4B-C4B	7.41	1.61	1.45
3	D	604	NAD	O4D-C4D	7.37	1.61	1.45
3	G	604	NAD	O4D-C4D	7.36	1.61	1.45
3	E	602	NAD	C7N-N7N	7.35	1.46	1.33
3	H	604	NAD	O4D-C4D	7.32	1.61	1.45
3	C	604	NAD	O4D-C4D	7.23	1.61	1.45
3	G	604	NAD	O4B-C4B	7.22	1.61	1.45
3	A	602	NAD	O4D-C4D	7.21	1.61	1.45
4	F	602	ATP	PA-O3A	7.07	1.67	1.59
4	F	602	ATP	PB-O3A	6.94	1.67	1.59
3	G	604	NAD	C7N-N7N	6.78	1.45	1.33
3	F	604	NAD	C7N-N7N	6.72	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	604	NAD	C7N-N7N	6.61	1.45	1.33
3	H	604	NAD	C7N-N7N	6.60	1.45	1.33
3	D	604	NAD	C7N-N7N	6.50	1.44	1.33
3	B	604	NAD	C7N-N7N	6.44	1.44	1.33
3	A	602	NAD	C7N-N7N	6.38	1.44	1.33
4	E	604	ATP	PA-O3A	6.13	1.66	1.59
2	E	601	IMP	C4-N3	6.11	1.48	1.35
4	A	604	ATP	PA-O3A	6.05	1.66	1.59
4	F	601	ATP	PA-O3A	6.00	1.66	1.59
4	C	601	ATP	PA-O3A	5.96	1.65	1.59
2	G	603	IMP	C4-N3	5.91	1.47	1.35
4	F	601	ATP	PB-O3A	5.82	1.65	1.59
4	G	601	ATP	PA-O3A	5.81	1.65	1.59
4	B	602	ATP	PA-O3A	5.77	1.65	1.59
4	H	601	ATP	PA-O3A	5.76	1.65	1.59
2	C	603	IMP	C4-N3	5.75	1.47	1.35
2	H	603	IMP	C4-N3	5.73	1.47	1.35
4	E	604	ATP	PB-O3A	5.71	1.65	1.59
2	B	603	IMP	C4-N3	5.70	1.47	1.35
4	C	602	ATP	PB-O3A	5.67	1.65	1.59
2	F	603	IMP	C4-N3	5.66	1.47	1.35
4	B	602	ATP	PB-O3A	5.64	1.65	1.59
4	H	601	ATP	PB-O3A	5.63	1.65	1.59
2	D	603	IMP	C4-N3	5.61	1.47	1.35
4	D	601	ATP	PB-O3A	5.60	1.65	1.59
4	D	601	ATP	PA-O3A	5.54	1.65	1.59
4	C	601	ATP	PB-O3A	5.50	1.65	1.59
2	A	601	IMP	C4-N3	5.49	1.46	1.35
4	G	602	ATP	PA-O3A	5.49	1.65	1.59
4	E	603	ATP	PA-O3A	5.48	1.65	1.59
4	D	602	ATP	PB-O3A	5.46	1.65	1.59
4	C	602	ATP	PA-O3A	5.42	1.65	1.59
4	G	601	ATP	PB-O3A	5.41	1.65	1.59
4	D	602	ATP	PA-O3A	5.38	1.65	1.59
4	H	602	ATP	PA-O3A	5.36	1.65	1.59
4	E	603	ATP	PB-O3A	5.33	1.65	1.59
4	A	603	ATP	PA-O3A	5.30	1.65	1.59
3	G	604	NAD	O4B-C1B	-5.20	1.30	1.42
4	G	602	ATP	PB-O3A	5.19	1.65	1.59
3	B	604	NAD	O4B-C1B	-5.17	1.30	1.42
3	D	604	NAD	O4B-C1B	-5.16	1.30	1.42
3	F	604	NAD	O4B-C1B	-5.16	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	604	NAD	O4B-C1B	-5.10	1.30	1.42
4	A	604	ATP	PB-O3A	5.09	1.65	1.59
4	B	601	ATP	PA-O3A	5.09	1.65	1.59
4	H	602	ATP	PB-O3A	5.08	1.65	1.59
3	C	604	NAD	PN-O3	5.04	1.64	1.59
3	C	604	NAD	O4B-C1B	-5.01	1.30	1.42
3	E	602	NAD	O4B-C1B	-4.87	1.30	1.42
3	A	602	NAD	O4B-C1B	-4.81	1.30	1.42
4	B	601	ATP	PB-O3A	4.72	1.64	1.59
4	A	603	ATP	PB-O3A	4.63	1.64	1.59
4	H	602	ATP	O4'-C1'	-4.53	1.31	1.42
4	C	602	ATP	O4'-C1'	-4.53	1.31	1.42
2	G	603	IMP	C2-N1	4.47	1.43	1.35
4	G	602	ATP	O4'-C1'	-4.47	1.31	1.42
4	D	601	ATP	O4'-C1'	-4.44	1.31	1.42
4	B	602	ATP	O4'-C1'	-4.44	1.31	1.42
4	G	601	ATP	O4'-C1'	-4.39	1.31	1.42
2	C	603	IMP	C2-N1	4.34	1.43	1.35
4	B	601	ATP	O4'-C1'	-4.31	1.32	1.42
4	A	603	ATP	O4'-C1'	-4.29	1.32	1.42
3	C	604	NAD	PA-O3	4.29	1.64	1.59
4	F	601	ATP	O4'-C1'	-4.27	1.32	1.42
4	H	601	ATP	O4'-C1'	-4.27	1.32	1.42
4	E	603	ATP	O4'-C1'	-4.25	1.32	1.42
4	D	602	ATP	O4'-C1'	-4.23	1.32	1.42
4	A	604	ATP	O4'-C1'	-4.22	1.32	1.42
2	B	603	IMP	C2-N1	4.22	1.42	1.35
4	F	602	ATP	O4'-C1'	-4.19	1.32	1.42
3	H	604	NAD	C6A-N6A	4.19	1.44	1.34
4	E	604	ATP	O4'-C1'	-4.18	1.32	1.42
3	C	604	NAD	C6A-N6A	4.18	1.44	1.34
3	D	604	NAD	C6A-N6A	4.17	1.44	1.34
3	B	604	NAD	C6A-N6A	4.16	1.44	1.34
3	G	604	NAD	C6A-N6A	4.15	1.44	1.34
2	F	603	IMP	C2-N1	4.13	1.42	1.35
4	G	601	ATP	C5'-C4'	-4.12	1.39	1.51
4	C	601	ATP	O4'-C1'	-4.10	1.32	1.42
3	F	604	NAD	C6A-N6A	4.09	1.44	1.34
3	F	604	NAD	PA-O3	4.09	1.63	1.59
2	H	603	IMP	C2-N1	4.08	1.42	1.35
4	B	601	ATP	C2'-C1'	4.06	1.66	1.53
4	H	602	ATP	C2'-C1'	4.06	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAD	C6A-N6A	4.04	1.44	1.34
3	E	602	NAD	C6A-N6A	4.01	1.44	1.34
4	C	601	ATP	C5'-C4'	-3.99	1.39	1.51
4	F	601	ATP	C2'-C1'	3.97	1.66	1.53
2	D	603	IMP	C2-N1	3.97	1.42	1.35
2	B	603	IMP	C5-N7	-3.96	1.31	1.39
2	F	603	IMP	C5-N7	-3.93	1.31	1.39
4	F	602	ATP	C2'-C1'	3.92	1.65	1.53
4	E	604	ATP	C2'-C1'	3.91	1.65	1.53
4	H	601	ATP	C2'-C1'	3.90	1.65	1.53
3	F	604	NAD	PN-O3	3.90	1.63	1.59
4	D	601	ATP	C2'-C1'	3.88	1.65	1.53
4	C	601	ATP	C6-N6	3.87	1.44	1.34
4	B	602	ATP	C2'-C1'	3.85	1.65	1.53
2	E	601	IMP	C5-N7	-3.84	1.31	1.39
4	A	604	ATP	C2'-C1'	3.80	1.65	1.53
3	G	604	NAD	C5A-C4A	-3.79	1.32	1.39
4	E	603	ATP	C2'-C1'	3.75	1.65	1.53
3	C	604	NAD	C5A-C4A	-3.75	1.32	1.39
2	A	601	IMP	C2-N1	3.75	1.42	1.35
2	H	603	IMP	C5-N7	-3.74	1.31	1.39
4	A	603	ATP	C2'-C1'	3.73	1.65	1.53
4	D	602	ATP	C2'-C1'	3.72	1.65	1.53
4	D	601	ATP	C5-C4	-3.72	1.32	1.39
2	E	601	IMP	C2-N1	3.72	1.42	1.35
4	D	602	ATP	C6-N6	3.72	1.43	1.34
2	A	601	IMP	C5-N7	-3.72	1.31	1.39
4	C	602	ATP	C6-N6	3.71	1.43	1.34
4	A	603	ATP	C6-N6	3.71	1.43	1.34
4	G	602	ATP	C6-N6	3.70	1.43	1.34
4	G	601	ATP	C2'-C1'	3.70	1.65	1.53
4	E	603	ATP	C6-N6	3.70	1.43	1.34
3	B	604	NAD	PA-O3	3.67	1.63	1.59
4	F	601	ATP	C6-N6	3.67	1.43	1.34
4	H	602	ATP	C5'-C4'	-3.66	1.40	1.51
4	B	602	ATP	C6-N6	3.66	1.43	1.34
4	D	601	ATP	C5'-C4'	-3.66	1.40	1.51
4	D	602	ATP	C5'-C4'	-3.65	1.40	1.51
3	A	602	NAD	PN-O3	3.64	1.63	1.59
4	E	604	ATP	C5'-C4'	-3.63	1.40	1.51
4	D	602	ATP	PB-O3B	3.63	1.63	1.59
2	D	603	IMP	C5-N7	-3.63	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	NAD	PN-O3	3.62	1.63	1.59
4	G	601	ATP	C6-N6	3.62	1.43	1.34
4	D	601	ATP	C6-N6	3.61	1.43	1.34
4	B	601	ATP	C5'-C4'	-3.61	1.40	1.51
4	A	603	ATP	C5'-C4'	-3.60	1.40	1.51
4	C	602	ATP	C2'-C1'	3.60	1.64	1.53
4	A	604	ATP	C5-C4	-3.59	1.32	1.39
2	G	603	IMP	C5-N7	-3.58	1.31	1.39
4	E	604	ATP	C6-N6	3.58	1.43	1.34
2	C	603	IMP	C4-N9	-3.58	1.28	1.38
3	D	604	NAD	C5A-C4A	-3.57	1.32	1.39
4	H	602	ATP	C6-N6	3.56	1.43	1.34
4	H	601	ATP	C6-N6	3.55	1.43	1.34
4	H	601	ATP	C5'-C4'	-3.54	1.40	1.51
4	F	602	ATP	C6-N6	3.54	1.43	1.34
3	B	604	NAD	PN-O3	3.53	1.63	1.59
3	H	604	NAD	C5A-C4A	-3.52	1.32	1.39
4	G	602	ATP	C2'-C1'	3.52	1.64	1.53
4	B	601	ATP	C6-N6	3.52	1.43	1.34
4	A	604	ATP	C5'-C4'	-3.50	1.41	1.51
4	E	603	ATP	C5'-C4'	-3.50	1.41	1.51
3	D	604	NAD	C4N-C3N	-3.49	1.34	1.39
4	F	601	ATP	C5-C4	-3.49	1.32	1.39
3	H	604	NAD	C4N-C3N	-3.48	1.34	1.39
4	C	601	ATP	C2'-C1'	3.48	1.64	1.53
4	G	601	ATP	C5-C4	-3.47	1.32	1.39
4	A	603	ATP	PB-O3B	3.47	1.63	1.59
4	C	602	ATP	C5'-C4'	-3.47	1.41	1.51
4	B	602	ATP	C5'-C4'	-3.45	1.41	1.51
3	D	604	NAD	PA-O3	3.42	1.63	1.59
3	H	604	NAD	PA-O3	3.42	1.63	1.59
4	E	603	ATP	C5-C4	-3.42	1.33	1.39
4	A	604	ATP	PB-O3B	3.41	1.63	1.59
4	C	602	ATP	C5-C4	-3.41	1.33	1.39
4	E	604	ATP	C5-C4	-3.40	1.33	1.39
3	C	604	NAD	O7N-C7N	-3.40	1.17	1.24
4	B	601	ATP	C5-C4	-3.40	1.33	1.39
3	E	602	NAD	PA-O3	3.39	1.63	1.59
3	E	602	NAD	C5A-C4A	-3.39	1.33	1.39
4	G	602	ATP	C5-C4	-3.39	1.33	1.39
4	A	603	ATP	C5-C4	-3.37	1.33	1.39
4	G	602	ATP	C5'-C4'	-3.37	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	ATP	C5-C4	-3.35	1.33	1.39
4	H	601	ATP	C5-C4	-3.35	1.33	1.39
4	B	602	ATP	C5-C4	-3.35	1.33	1.39
3	F	604	NAD	O7N-C7N	-3.33	1.17	1.24
4	B	602	ATP	PB-O3B	3.32	1.63	1.59
4	A	604	ATP	C6-N6	3.32	1.42	1.34
3	A	602	NAD	O7N-C7N	-3.32	1.17	1.24
4	H	602	ATP	C5-C4	-3.32	1.33	1.39
4	F	602	ATP	C5'-C4'	-3.32	1.41	1.51
3	A	602	NAD	C5A-C4A	-3.32	1.33	1.39
2	D	603	IMP	O6-C6	-3.31	1.17	1.23
3	G	604	NAD	O7N-C7N	-3.31	1.18	1.24
4	F	602	ATP	C5-C4	-3.30	1.33	1.39
3	A	602	NAD	C4N-C3N	-3.30	1.34	1.39
3	D	604	NAD	PN-O3	3.29	1.63	1.59
4	C	601	ATP	C5-C4	-3.29	1.33	1.39
3	B	604	NAD	C5A-C4A	-3.28	1.33	1.39
2	E	601	IMP	O6-C6	-3.28	1.17	1.23
3	A	602	NAD	PA-O3	3.27	1.63	1.59
3	F	604	NAD	O2D-C2D	-3.26	1.34	1.43
2	C	603	IMP	C5-N7	-3.24	1.32	1.39
2	C	603	IMP	O6-C6	-3.24	1.17	1.23
4	B	602	ATP	PA-O5'	3.23	1.72	1.59
2	D	603	IMP	C4-N9	-3.22	1.29	1.38
2	A	601	IMP	O6-C6	-3.21	1.17	1.23
4	H	601	ATP	C5-N7	-3.21	1.33	1.39
3	A	602	NAD	O2B-C2B	-3.21	1.35	1.43
4	F	602	ATP	PA-O5'	3.21	1.71	1.59
3	G	604	NAD	C4N-C3N	-3.20	1.34	1.39
2	G	603	IMP	C4-N9	-3.19	1.29	1.38
2	F	603	IMP	C4-N9	-3.18	1.30	1.38
3	F	604	NAD	C5A-C4A	-3.18	1.33	1.39
4	C	602	ATP	PB-O3B	3.17	1.62	1.59
4	E	604	ATP	PB-O3B	3.17	1.62	1.59
4	C	602	ATP	C8-N9	-3.17	1.32	1.37
3	B	604	NAD	O7N-C7N	-3.16	1.18	1.24
3	A	602	NAD	O2D-C2D	-3.16	1.35	1.43
3	G	604	NAD	PA-O3	3.16	1.62	1.59
4	B	602	ATP	C3'-C4'	3.16	1.61	1.53
3	D	604	NAD	O7N-C7N	-3.15	1.18	1.24
4	F	601	ATP	O3'-C3'	3.15	1.50	1.43
4	C	602	ATP	C3'-C4'	3.15	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	601	ATP	C5'-C4'	-3.15	1.42	1.51
4	G	602	ATP	C3'-C4'	3.14	1.61	1.53
4	C	602	ATP	O3'-C3'	3.14	1.50	1.43
3	E	602	NAD	O2B-C2B	-3.13	1.35	1.43
4	F	602	ATP	C3'-C4'	3.13	1.60	1.53
4	G	601	ATP	C3'-C4'	3.13	1.60	1.53
4	G	602	ATP	PB-O3B	3.13	1.62	1.59
4	G	602	ATP	O3'-C3'	3.13	1.50	1.43
4	B	602	ATP	O3'-C3'	3.13	1.50	1.43
3	F	604	NAD	C4N-C3N	-3.12	1.34	1.39
3	B	604	NAD	O2B-C2B	-3.12	1.35	1.43
3	B	604	NAD	C4N-C3N	-3.12	1.34	1.39
4	F	602	ATP	O3'-C3'	3.11	1.50	1.43
4	G	602	ATP	C8-N9	-3.11	1.32	1.37
4	F	601	ATP	C3'-C4'	3.11	1.60	1.53
3	E	602	NAD	O7N-C7N	-3.11	1.18	1.24
4	H	601	ATP	C8-N9	-3.11	1.32	1.37
4	D	601	ATP	C3'-C4'	3.11	1.60	1.53
4	B	601	ATP	O3'-C3'	3.10	1.50	1.43
4	C	601	ATP	O3'-C3'	3.10	1.50	1.43
3	G	604	NAD	PN-O3	3.09	1.62	1.59
4	A	603	ATP	C8-N9	-3.09	1.32	1.37
3	C	604	NAD	C5A-N7A	-3.09	1.33	1.39
3	F	604	NAD	O2B-C2B	-3.09	1.35	1.43
3	E	602	NAD	C5A-N7A	-3.09	1.33	1.39
4	H	601	ATP	C3'-C4'	3.09	1.60	1.53
3	H	604	NAD	O7N-C7N	-3.08	1.18	1.24
4	D	601	ATP	O3'-C3'	3.08	1.50	1.43
4	B	601	ATP	C3'-C4'	3.08	1.60	1.53
3	H	604	NAD	O2B-C2B	-3.08	1.35	1.43
4	F	601	ATP	PA-O5'	3.08	1.71	1.59
4	F	601	ATP	O4'-C4'	3.06	1.51	1.45
3	D	604	NAD	O2B-C2B	-3.06	1.35	1.43
3	A	602	NAD	C5A-N7A	-3.06	1.33	1.39
4	A	604	ATP	C3'-C4'	3.06	1.60	1.53
4	D	601	ATP	C8-N9	-3.06	1.32	1.37
3	H	604	NAD	C8A-N9A	-3.05	1.32	1.37
3	H	604	NAD	O2D-C2D	-3.05	1.35	1.43
3	B	604	NAD	O2D-C2D	-3.05	1.35	1.43
4	F	601	ATP	C8-N9	-3.04	1.32	1.37
4	A	604	ATP	PA-O5'	3.04	1.71	1.59
4	E	603	ATP	C8-N9	-3.04	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	ATP	PA-O5'	3.03	1.71	1.59
4	E	604	ATP	PA-O5'	3.03	1.71	1.59
4	D	602	ATP	O3'-C3'	3.02	1.50	1.43
3	E	602	NAD	O2D-C2D	-3.01	1.35	1.43
3	F	604	NAD	C5A-N7A	-3.01	1.33	1.39
3	G	604	NAD	O2D-C2D	-3.01	1.35	1.43
3	C	604	NAD	C4N-C3N	-3.00	1.34	1.39
4	H	602	ATP	C5-N7	-2.99	1.33	1.39
4	F	602	ATP	PB-O3B	2.99	1.62	1.59
4	G	601	ATP	O3'-C3'	2.99	1.50	1.43
4	F	601	ATP	C5-N7	-2.99	1.33	1.39
3	C	604	NAD	O2D-C2D	-2.98	1.35	1.43
3	G	604	NAD	C5A-N7A	-2.98	1.33	1.39
3	D	604	NAD	O2D-C2D	-2.97	1.35	1.43
4	H	601	ATP	PB-O3B	2.97	1.62	1.59
4	A	604	ATP	O3'-C3'	2.96	1.50	1.43
2	H	603	IMP	C4-N9	-2.96	1.30	1.38
4	E	603	ATP	O3'-C3'	2.96	1.50	1.43
4	B	602	ATP	C8-N9	-2.96	1.32	1.37
3	H	604	NAD	PN-O3	2.96	1.62	1.59
4	H	602	ATP	O3'-C3'	2.95	1.50	1.43
4	A	603	ATP	O3'-C3'	2.95	1.50	1.43
4	E	604	ATP	O3'-C3'	2.94	1.50	1.43
4	C	602	ATP	PA-O5'	2.94	1.70	1.59
4	E	603	ATP	PA-O5'	2.93	1.70	1.59
4	B	601	ATP	C5-N7	-2.93	1.33	1.39
3	G	604	NAD	C8A-N9A	-2.93	1.32	1.37
4	D	602	ATP	C3'-C4'	2.93	1.60	1.53
4	C	601	ATP	PB-O3B	2.92	1.62	1.59
4	D	602	ATP	C5-N7	-2.92	1.33	1.39
4	C	601	ATP	C8-N9	-2.92	1.32	1.37
4	H	601	ATP	O3'-C3'	2.92	1.50	1.43
4	E	604	ATP	C3'-C4'	2.92	1.60	1.53
4	D	602	ATP	C8-N9	-2.92	1.32	1.37
3	G	604	NAD	O2B-C2B	-2.90	1.35	1.43
3	H	604	NAD	C5A-N7A	-2.90	1.33	1.39
4	G	602	ATP	PA-O5'	2.90	1.70	1.59
4	H	602	ATP	PA-O5'	2.89	1.70	1.59
4	E	603	ATP	C3'-C4'	2.89	1.60	1.53
4	A	603	ATP	C3'-C4'	2.89	1.60	1.53
3	D	604	NAD	C5A-N7A	-2.89	1.33	1.39
4	C	601	ATP	C3'-C4'	2.89	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	603	ATP	PB-O3B	2.88	1.62	1.59
4	D	601	ATP	PB-O3B	2.88	1.62	1.59
4	B	601	ATP	O4'-C4'	2.88	1.51	1.45
4	H	601	ATP	PA-O5'	2.87	1.70	1.59
2	B	603	IMP	C4-N9	-2.87	1.30	1.38
4	F	602	ATP	C8-N9	-2.85	1.32	1.37
2	A	601	IMP	C4-N9	-2.84	1.30	1.38
3	D	604	NAD	C8A-N9A	-2.83	1.32	1.37
3	C	604	NAD	O2B-C2B	-2.83	1.35	1.43
4	B	601	ATP	PA-O5'	2.83	1.70	1.59
4	B	601	ATP	C8-N9	-2.83	1.32	1.37
4	C	601	ATP	PA-O5'	2.82	1.70	1.59
4	D	601	ATP	PA-O5'	2.81	1.70	1.59
4	A	603	ATP	C5-N7	-2.80	1.34	1.39
3	C	604	NAD	C8A-N9A	-2.80	1.32	1.37
4	D	601	ATP	C5-N7	-2.80	1.34	1.39
4	H	601	ATP	O4'-C4'	2.80	1.51	1.45
2	H	603	IMP	O6-C6	-2.80	1.18	1.23
2	F	603	IMP	O6-C6	-2.80	1.18	1.23
4	H	602	ATP	O4'-C4'	2.79	1.51	1.45
3	B	604	NAD	C5A-N7A	-2.79	1.34	1.39
4	A	604	ATP	C8-N9	-2.79	1.32	1.37
3	E	602	NAD	C8A-N9A	-2.78	1.32	1.37
4	D	602	ATP	PA-O5'	2.78	1.70	1.59
3	D	604	NAD	C5N-C4N	-2.77	1.34	1.38
4	E	604	ATP	C8-N9	-2.77	1.32	1.37
3	E	602	NAD	C4N-C3N	-2.77	1.35	1.39
4	C	602	ATP	C5-N7	-2.77	1.34	1.39
4	E	603	ATP	C5-N7	-2.75	1.34	1.39
3	F	604	NAD	C8A-N9A	-2.74	1.32	1.37
4	E	603	ATP	O4'-C4'	2.73	1.51	1.45
4	H	602	ATP	C8-N9	-2.73	1.32	1.37
4	H	602	ATP	C3'-C4'	2.72	1.59	1.53
2	G	603	IMP	O6-C6	-2.72	1.18	1.23
4	G	602	ATP	C5-N7	-2.71	1.34	1.39
4	G	601	ATP	C8-N9	-2.70	1.33	1.37
3	D	604	NAD	O3B-C3B	2.70	1.49	1.43
4	A	604	ATP	C5-N7	-2.70	1.34	1.39
3	A	602	NAD	C8A-N9A	-2.69	1.33	1.37
3	D	604	NAD	O3D-C3D	2.69	1.49	1.43
4	H	602	ATP	PB-O3B	2.67	1.62	1.59
3	H	604	NAD	O3D-C3D	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	602	ATP	C5-N7	-2.66	1.34	1.39
3	H	604	NAD	C5N-C4N	-2.65	1.34	1.38
2	B	603	IMP	O6-C6	-2.64	1.18	1.23
3	H	604	NAD	O3B-C3B	2.64	1.49	1.43
4	A	603	ATP	O4'-C4'	2.63	1.50	1.45
3	D	604	NAD	C4A-N9A	-2.63	1.32	1.37
3	F	604	NAD	O3B-C3B	2.62	1.49	1.43
4	G	601	ATP	C5-N7	-2.62	1.34	1.39
4	D	602	ATP	O4'-C4'	2.61	1.50	1.45
3	F	604	NAD	O3D-C3D	2.61	1.49	1.43
4	G	601	ATP	C1'-N9	-2.61	1.39	1.46
4	E	604	ATP	O4'-C4'	2.60	1.50	1.45
4	C	601	ATP	C5-N7	-2.60	1.34	1.39
3	B	604	NAD	O3D-C3D	2.59	1.49	1.43
3	G	604	NAD	O3B-C3B	2.58	1.49	1.43
4	G	602	ATP	O4'-C4'	2.58	1.50	1.45
4	G	601	ATP	PA-O5'	2.57	1.69	1.59
3	B	604	NAD	O3B-C3B	2.57	1.49	1.43
4	E	604	ATP	C5-N7	-2.55	1.34	1.39
3	C	604	NAD	O3B-C3B	2.54	1.49	1.43
3	G	604	NAD	O3D-C3D	2.54	1.49	1.43
3	B	604	NAD	C8A-N9A	-2.54	1.33	1.37
4	B	602	ATP	C5-N7	-2.53	1.34	1.39
4	D	601	ATP	O4'-C4'	2.52	1.50	1.45
4	F	602	ATP	O4'-C4'	2.52	1.50	1.45
3	G	604	NAD	C4A-N9A	-2.50	1.32	1.37
3	C	604	NAD	O3D-C3D	2.50	1.49	1.43
4	C	602	ATP	O4'-C4'	2.49	1.50	1.45
4	A	604	ATP	O4'-C4'	2.48	1.50	1.45
2	E	601	IMP	C4-N9	-2.46	1.31	1.38
3	H	604	NAD	C4A-N9A	-2.45	1.32	1.37
3	G	604	NAD	C5N-C4N	-2.45	1.34	1.38
3	A	602	NAD	O3B-C3B	2.44	1.49	1.43
4	B	602	ATP	O4'-C4'	2.44	1.50	1.45
3	E	602	NAD	O3B-C3B	2.44	1.49	1.43
3	F	604	NAD	C5N-C4N	-2.44	1.34	1.38
4	A	603	ATP	C1'-N9	-2.43	1.39	1.46
3	A	602	NAD	C4A-N9A	-2.42	1.32	1.37
3	A	602	NAD	O3D-C3D	2.42	1.48	1.43
3	C	604	NAD	C4A-N9A	-2.40	1.32	1.37
4	F	601	ATP	PB-O3B	2.40	1.62	1.59
3	E	602	NAD	O3D-C3D	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	ATP	PB-O3B	2.39	1.62	1.59
4	E	603	ATP	C1'-N9	-2.39	1.39	1.46
4	B	602	ATP	O2'-C2'	2.38	1.48	1.43
4	F	602	ATP	O2'-C2'	2.37	1.48	1.43
4	D	601	ATP	O2'-C2'	2.36	1.48	1.43
4	D	601	ATP	C1'-N9	-2.36	1.39	1.46
3	E	602	NAD	C4A-N9A	-2.36	1.32	1.37
4	C	602	ATP	C1'-N9	-2.36	1.39	1.46
4	H	601	ATP	O2'-C2'	2.35	1.48	1.43
3	B	604	NAD	C5N-C4N	-2.35	1.34	1.38
4	B	601	ATP	O2'-C2'	2.34	1.48	1.43
3	C	604	NAD	C5N-C4N	-2.34	1.34	1.38
4	G	602	ATP	C1'-N9	-2.34	1.39	1.46
4	G	601	ATP	O2'-C2'	2.34	1.48	1.43
4	A	604	ATP	O2'-C2'	2.32	1.48	1.43
4	F	601	ATP	O2'-C2'	2.32	1.48	1.43
4	C	602	ATP	O2'-C2'	2.31	1.48	1.43
2	H	603	IMP	C8-N9	-2.30	1.32	1.37
4	G	601	ATP	PB-O3B	2.29	1.62	1.59
4	E	603	ATP	O2'-C2'	2.29	1.48	1.43
3	A	602	NAD	C5N-C4N	-2.29	1.35	1.38
2	B	603	IMP	C8-N9	-2.29	1.32	1.37
4	D	602	ATP	O2'-C2'	2.28	1.48	1.43
4	G	602	ATP	O2'-C2'	2.27	1.48	1.43
4	A	603	ATP	O2'-C2'	2.27	1.48	1.43
4	H	602	ATP	O2'-C2'	2.26	1.48	1.43
4	E	604	ATP	O2'-C2'	2.26	1.48	1.43
4	B	602	ATP	C1'-N9	-2.23	1.40	1.46
3	E	602	NAD	C3N-C7N	2.22	1.53	1.50
4	C	601	ATP	O4'-C4'	2.22	1.49	1.45
2	D	603	IMP	C8-N9	-2.21	1.32	1.37
3	B	604	NAD	C4A-N9A	-2.20	1.33	1.37
4	D	601	ATP	C4-N9	-2.16	1.33	1.37
4	A	604	ATP	C1'-N9	-2.16	1.40	1.46
4	E	603	ATP	C4-N9	-2.15	1.33	1.37
4	G	601	ATP	O4'-C4'	2.14	1.49	1.45
4	H	601	ATP	C4-N9	-2.14	1.33	1.37
3	F	604	NAD	C4A-N9A	-2.14	1.33	1.37
4	A	603	ATP	C4-N9	-2.12	1.33	1.37
4	C	601	ATP	O2'-C2'	2.08	1.48	1.43
4	A	604	ATP	C4-N9	-2.08	1.33	1.37
3	E	602	NAD	C5N-C4N	-2.07	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	601	ATP	C1'-N9	-2.05	1.40	1.46
2	F	603	IMP	C8-N9	-2.04	1.32	1.37
2	C	603	IMP	C8-N9	-2.03	1.33	1.37
2	G	603	IMP	C8-N9	-2.00	1.33	1.37

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	604	ATP	N6-C6-N1	-9.40	97.44	118.38
4	C	601	ATP	N6-C6-N1	-9.35	97.55	118.38
4	A	603	ATP	N6-C6-N1	-9.34	97.57	118.38
4	B	601	ATP	N6-C6-N1	-9.29	97.70	118.38
4	D	601	ATP	N6-C6-N1	-9.22	97.84	118.38
4	E	603	ATP	N6-C6-N1	-9.20	97.88	118.38
4	H	602	ATP	N6-C6-N1	-9.20	97.90	118.38
4	G	602	ATP	N6-C6-N1	-9.16	97.97	118.38
4	G	601	ATP	N6-C6-N1	-9.16	97.97	118.38
4	F	601	ATP	N6-C6-N1	-9.14	98.03	118.38
4	C	602	ATP	N6-C6-N1	-9.12	98.07	118.38
4	F	602	ATP	N6-C6-N1	-9.09	98.12	118.38
4	H	601	ATP	N6-C6-N1	-9.07	98.17	118.38
4	D	602	ATP	N6-C6-N1	-9.05	98.22	118.38
4	B	602	ATP	N6-C6-N1	-8.92	98.52	118.38
4	A	604	ATP	N6-C6-N1	-8.74	98.90	118.38
4	G	601	ATP	C4-N9-C1'	-8.14	107.60	126.63
4	C	601	ATP	C5-C6-N6	8.01	143.11	123.29
4	A	603	ATP	C5-C6-N6	7.87	142.77	123.29
4	B	601	ATP	C4-N9-C1'	-7.87	108.23	126.63
4	A	604	ATP	C4-N9-C1'	-7.81	108.36	126.63
4	E	603	ATP	C5-C6-N6	7.77	142.51	123.29
4	E	603	ATP	C4-N9-C1'	-7.71	108.59	126.63
4	D	602	ATP	C5-C6-N6	7.65	142.23	123.29
4	F	601	ATP	C4-N9-C1'	-7.63	108.78	126.63
4	H	602	ATP	C5-C6-N6	7.61	142.13	123.29
4	D	601	ATP	C4-N9-C1'	-7.60	108.86	126.63
4	G	602	ATP	C5-C6-N6	7.58	142.06	123.29
4	H	601	ATP	C4-N9-C1'	-7.58	108.92	126.63
4	B	601	ATP	C5-C6-N6	7.53	141.92	123.29
4	F	601	ATP	C5-C6-N6	7.50	141.86	123.29
4	D	601	ATP	C5-C6-N6	7.49	141.83	123.29
4	D	602	ATP	C4-N9-C1'	-7.46	109.18	126.63
4	C	602	ATP	C5-C6-N6	7.46	141.75	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	604	ATP	C5-C6-N6	7.45	141.73	123.29
4	H	601	ATP	C5-C6-N6	7.41	141.63	123.29
4	A	603	ATP	C4-N9-C1'	-7.40	109.31	126.63
2	A	601	IMP	C5-C6-N1	7.38	121.39	110.78
3	B	604	NAD	N6A-C6A-N1A	-7.26	102.20	118.38
4	E	604	ATP	C4-N9-C1'	-7.26	109.66	126.63
4	G	601	ATP	C5-C6-N6	7.25	141.25	123.29
4	C	601	ATP	C4-N9-C1'	-7.24	109.69	126.63
4	F	602	ATP	C4-N9-C1'	-7.24	109.71	126.63
4	F	602	ATP	C5-C6-N6	7.23	141.19	123.29
3	G	604	NAD	C4A-N9A-C1B	-7.23	109.72	126.63
4	B	602	ATP	C5-C6-N6	7.21	141.13	123.29
4	H	602	ATP	C4-N9-C1'	-7.14	109.93	126.63
4	B	602	ATP	C4-N9-C1'	-7.13	109.95	126.63
4	A	604	ATP	C5-C6-N6	7.13	140.93	123.29
3	F	604	NAD	N6A-C6A-N1A	-7.12	102.51	118.38
4	G	602	ATP	C4-N9-C1'	-7.12	109.98	126.63
2	E	601	IMP	C5-C6-N1	7.12	121.02	110.78
2	C	603	IMP	C5-C6-N1	7.12	121.02	110.78
2	D	603	IMP	C5-C6-N1	7.10	121.00	110.78
3	D	604	NAD	C4A-N9A-C1B	-7.07	110.11	126.63
3	C	604	NAD	C4A-N9A-C1B	-7.06	110.11	126.63
4	C	602	ATP	C4-N9-C1'	-7.04	110.17	126.63
3	G	604	NAD	N6A-C6A-N1A	-7.01	102.77	118.38
3	D	604	NAD	N6A-C6A-N1A	-6.99	102.82	118.38
3	A	602	NAD	N6A-C6A-N1A	-6.97	102.84	118.38
3	H	604	NAD	N6A-C6A-N1A	-6.94	102.91	118.38
3	A	602	NAD	C4A-N9A-C1B	-6.89	110.52	126.63
3	B	604	NAD	C4A-N9A-C1B	-6.87	110.56	126.63
3	E	602	NAD	N6A-C6A-N1A	-6.85	103.12	118.38
3	E	602	NAD	C4A-N9A-C1B	-6.85	110.62	126.63
3	H	604	NAD	C4D-O4D-C1D	-6.78	103.72	109.92
3	C	604	NAD	N6A-C6A-N1A	-6.71	103.42	118.38
3	H	604	NAD	C4A-N9A-C1B	-6.54	111.33	126.63
2	H	603	IMP	C5-C6-N1	6.53	120.17	110.78
2	G	603	IMP	C5-C6-N1	6.46	120.06	110.78
4	B	601	ATP	C1'-N9-C8	6.45	141.40	127.09
3	E	602	NAD	C3N-C7N-N7N	6.40	125.63	117.74
4	F	601	ATP	C1'-N9-C8	6.36	141.20	127.09
2	F	603	IMP	C5-C6-N1	6.34	119.89	110.78
4	G	601	ATP	N9-C8-N7	-6.31	104.98	113.94
3	F	604	NAD	C4A-N9A-C1B	-6.28	111.95	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	ATP	C1'-N9-C8	6.22	140.89	127.09
2	B	603	IMP	C5-C6-N1	6.17	119.65	110.78
4	H	601	ATP	C1'-N9-C8	6.15	140.74	127.09
4	D	601	ATP	N3-C2-N1	-6.09	119.36	128.58
4	E	603	ATP	N3-C2-N1	-6.09	119.36	128.58
4	G	601	ATP	C1'-N9-C8	6.07	140.56	127.09
4	F	602	ATP	N3-C2-N1	-6.06	119.41	128.58
4	D	602	ATP	C1'-N9-C8	6.05	140.53	127.09
4	H	602	ATP	C1'-N9-C8	6.01	140.44	127.09
3	G	604	NAD	N3A-C2A-N1A	-6.01	119.48	128.58
3	C	604	NAD	N3A-C2A-N1A	-6.00	119.50	128.58
4	E	604	ATP	N3-C2-N1	-6.00	119.51	128.58
4	A	603	ATP	N3-C2-N1	-5.98	119.52	128.58
4	B	601	ATP	N3-C2-N1	-5.93	119.60	128.58
3	B	604	NAD	N3A-C2A-N1A	-5.92	119.61	128.58
4	E	603	ATP	N9-C8-N7	-5.90	105.56	113.94
4	C	601	ATP	C1'-N9-C8	5.90	140.18	127.09
4	E	603	ATP	C1'-N9-C8	5.89	140.17	127.09
4	F	601	ATP	N3-C2-N1	-5.89	119.67	128.58
4	A	603	ATP	N9-C8-N7	-5.88	105.59	113.94
3	H	604	NAD	N3A-C2A-N1A	-5.87	119.69	128.58
4	B	602	ATP	N3-C2-N1	-5.87	119.70	128.58
3	F	604	NAD	N3A-C2A-N1A	-5.84	119.73	128.58
4	B	602	ATP	N9-C8-N7	-5.83	105.66	113.94
3	E	602	NAD	N3A-C2A-N1A	-5.81	119.78	128.58
4	D	601	ATP	C1'-N9-C8	5.81	139.99	127.09
4	G	601	ATP	C4-N9-C8	5.81	111.84	105.74
4	D	601	ATP	N9-C8-N7	-5.81	105.69	113.94
3	D	604	NAD	N3A-C2A-N1A	-5.81	119.79	128.58
3	A	602	NAD	N3A-C2A-N1A	-5.79	119.81	128.58
4	H	602	ATP	N3-C2-N1	-5.79	119.82	128.58
4	D	602	ATP	N3-C2-N1	-5.77	119.84	128.58
2	C	603	IMP	N1-C2-N3	-5.77	118.85	125.50
4	A	604	ATP	N3-C2-N1	-5.75	119.87	128.58
3	B	604	NAD	C5A-C6A-N6A	5.75	137.51	123.29
4	E	604	ATP	N9-C8-N7	-5.74	105.80	113.94
4	G	602	ATP	N3-C2-N1	-5.74	119.90	128.58
4	H	601	ATP	N3-C2-N1	-5.73	119.91	128.58
4	C	602	ATP	N3-C2-N1	-5.72	119.93	128.58
3	B	604	NAD	C1B-N9A-C8A	5.70	139.74	127.09
4	G	602	ATP	N9-C8-N7	-5.66	105.90	113.94
3	G	604	NAD	C1B-N9A-C8A	5.66	139.66	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAD	C1B-N9A-C8A	5.66	139.66	127.09
4	F	602	ATP	C1'-N9-C8	5.65	139.62	127.09
4	G	601	ATP	N3-C2-N1	-5.63	120.05	128.58
3	G	604	NAD	N9A-C8A-N7A	-5.63	105.95	113.94
3	D	604	NAD	C1B-N9A-C8A	5.62	139.58	127.09
3	C	604	NAD	C1B-N9A-C8A	5.61	139.55	127.09
3	F	604	NAD	C5A-C6A-N6A	5.61	137.18	123.29
4	E	604	ATP	C1'-N9-C8	5.61	139.54	127.09
4	C	601	ATP	N9-C8-N7	-5.60	105.99	113.94
3	E	602	NAD	C1B-N9A-C8A	5.58	139.49	127.09
4	C	602	ATP	N9-C8-N7	-5.56	106.05	113.94
4	A	603	ATP	C1'-N9-C8	5.54	139.40	127.09
3	D	604	NAD	C5A-C6A-N6A	5.54	137.00	123.29
4	F	602	ATP	N9-C8-N7	-5.51	106.11	113.94
2	A	601	IMP	C2-N3-C4	5.50	121.19	111.53
3	A	602	NAD	C5A-C6A-N6A	5.49	136.88	123.29
3	H	604	NAD	C5A-C6A-N6A	5.48	136.87	123.29
4	A	604	ATP	N9-C8-N7	-5.44	106.21	113.94
3	G	604	NAD	C5A-C6A-N6A	5.43	136.73	123.29
3	E	602	NAD	C5A-C6A-N6A	5.42	136.70	123.29
3	C	604	NAD	N9A-C8A-N7A	-5.41	106.27	113.94
4	D	602	ATP	N9-C8-N7	-5.40	106.28	113.94
4	G	602	ATP	C1'-N9-C8	5.40	139.07	127.09
4	B	601	ATP	N9-C8-N7	-5.39	106.28	113.94
2	A	601	IMP	N1-C2-N3	-5.36	119.32	125.50
4	C	602	ATP	C1'-N9-C8	5.35	138.97	127.09
4	B	602	ATP	C1'-N9-C8	5.33	138.91	127.09
2	E	601	IMP	C5-C4-N3	-5.31	119.45	127.27
4	A	603	ATP	C4-N9-C8	5.27	111.28	105.74
4	E	603	ATP	C4-N9-C8	5.23	111.23	105.74
3	C	604	NAD	C5A-C6A-N6A	5.21	136.19	123.29
3	D	604	NAD	N9A-C8A-N7A	-5.21	106.55	113.94
2	E	601	IMP	C2-N1-C6	-5.18	118.00	125.09
4	D	601	ATP	C4-N9-C8	5.16	111.15	105.74
4	B	602	ATP	C4-N9-C8	5.13	111.12	105.74
3	H	604	NAD	C1B-N9A-C8A	5.10	138.41	127.09
4	H	601	ATP	N9-C8-N7	-5.07	106.74	113.94
3	A	602	NAD	N9A-C8A-N7A	-5.05	106.77	113.94
3	F	604	NAD	C1B-N9A-C8A	5.04	138.29	127.09
3	E	602	NAD	N9A-C8A-N7A	-5.04	106.79	113.94
4	F	601	ATP	N9-C8-N7	-5.01	106.83	113.94
3	B	604	NAD	N9A-C8A-N7A	-4.99	106.86	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	604	NAD	N9A-C8A-N7A	-4.98	106.88	113.94
4	H	602	ATP	N9-C8-N7	-4.97	106.89	113.94
4	G	602	ATP	C4-N9-C8	4.96	110.95	105.74
3	H	604	NAD	N9A-C8A-N7A	-4.96	106.90	113.94
3	C	604	NAD	C4D-O4D-C1D	-4.93	105.41	109.92
2	A	601	IMP	C5-C4-N3	-4.88	120.08	127.27
4	C	602	ATP	C4-N9-C8	4.87	110.85	105.74
2	H	603	IMP	C5-C4-N3	-4.86	120.11	127.27
4	E	604	ATP	C4-N9-C8	4.82	110.80	105.74
3	D	604	NAD	C4D-O4D-C1D	-4.81	105.52	109.92
4	A	604	ATP	C4-N9-C8	4.76	110.74	105.74
2	D	603	IMP	N1-C2-N3	-4.75	120.03	125.50
2	C	603	IMP	C2-N3-C4	4.74	119.87	111.53
2	B	603	IMP	C2-N1-C6	-4.72	118.61	125.09
2	A	601	IMP	C2-N1-C6	-4.72	118.63	125.09
4	C	601	ATP	N3-C2-N1	-4.71	121.45	128.58
4	H	602	ATP	C5-C4-N3	-4.68	120.28	126.72
4	F	602	ATP	C4-N9-C8	4.68	110.65	105.74
2	D	603	IMP	C2-N1-C6	-4.67	118.68	125.09
2	D	603	IMP	C2-N3-C4	4.67	119.75	111.53
4	F	602	ATP	C5-C4-N3	-4.67	120.29	126.72
3	G	604	NAD	C4A-N9A-C8A	4.63	110.60	105.74
2	H	603	IMP	C2-N1-C6	-4.62	118.75	125.09
2	B	603	IMP	C5-C4-N3	-4.62	120.47	127.27
2	F	603	IMP	C2-N1-C6	-4.61	118.77	125.09
4	E	604	ATP	C5-C4-N3	-4.61	120.37	126.72
2	H	603	IMP	C2-N3-C4	4.55	119.53	111.53
4	B	602	ATP	C5-C4-N3	-4.53	120.48	126.72
3	F	604	NAD	C5A-C4A-N3A	-4.49	120.53	126.72
4	C	601	ATP	C5-C4-N3	-4.47	120.56	126.72
4	C	602	ATP	C5-C4-N3	-4.44	120.60	126.72
4	B	601	ATP	C4-N9-C8	4.40	110.36	105.74
3	B	604	NAD	C5A-C4A-N3A	-4.40	120.66	126.72
2	E	601	IMP	C2-N3-C4	4.40	119.26	111.53
3	C	604	NAD	C5A-C4A-N3A	-4.39	120.67	126.72
4	H	601	ATP	C4-N9-C8	4.39	110.34	105.74
3	C	604	NAD	C4A-N9A-C8A	4.38	110.34	105.74
2	D	603	IMP	C5-C4-N3	-4.36	120.85	127.27
3	D	604	NAD	C4A-N9A-C8A	4.36	110.32	105.74
2	G	603	IMP	C2-N1-C6	-4.36	119.12	125.09
4	G	602	ATP	C5-C4-N3	-4.34	120.75	126.72
4	D	602	ATP	C4-N9-C8	4.31	110.26	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	604	NAD	C4A-N9A-C8A	4.30	110.25	105.74
3	E	602	NAD	C5A-C4A-N3A	-4.29	120.80	126.72
3	H	604	NAD	C5A-C4A-N3A	-4.28	120.83	126.72
4	B	601	ATP	C5-C4-N3	-4.26	120.85	126.72
2	H	603	IMP	N1-C2-N3	-4.23	120.63	125.50
4	F	601	ATP	C5-C4-N3	-4.23	120.90	126.72
3	A	602	NAD	C5A-C4A-N3A	-4.21	120.92	126.72
2	C	603	IMP	N9-C8-N7	-4.21	105.60	113.40
4	G	601	ATP	C5-C4-N3	-4.18	120.97	126.72
3	G	604	NAD	C5A-C4A-N3A	-4.17	120.98	126.72
2	G	603	IMP	N1-C2-N3	-4.16	120.71	125.50
2	F	603	IMP	C5-C4-N3	-4.16	121.15	127.27
4	D	602	ATP	C5-C4-N3	-4.13	121.03	126.72
4	D	601	ATP	C5-C4-N3	-4.11	121.06	126.72
2	G	603	IMP	C2-N3-C4	4.11	118.76	111.53
4	C	601	ATP	C4-N9-C8	4.10	110.05	105.74
2	D	603	IMP	N9-C8-N7	-4.10	105.80	113.40
4	F	601	ATP	C4-N9-C8	4.05	109.99	105.74
3	D	604	NAD	C5A-C4A-N3A	-4.04	121.16	126.72
4	H	601	ATP	C5-C4-N3	-3.99	121.22	126.72
2	G	603	IMP	C5-C4-N3	-3.98	121.42	127.27
3	E	602	NAD	C4A-N9A-C8A	3.95	109.88	105.74
4	A	603	ATP	C5-C4-N3	-3.94	121.29	126.72
3	A	602	NAD	C4A-N9A-C8A	3.89	109.82	105.74
4	F	602	ATP	N3-C4-N9	3.86	133.74	127.17
2	C	603	IMP	C2-N1-C6	-3.86	119.80	125.09
2	B	603	IMP	C2-N3-C4	3.86	118.31	111.53
3	F	604	NAD	C4A-N9A-C8A	3.83	109.75	105.74
4	A	604	ATP	C5-C4-N3	-3.82	121.45	126.72
4	E	603	ATP	C5-C4-N3	-3.81	121.46	126.72
2	B	603	IMP	N9-C8-N7	-3.80	106.35	113.40
4	B	602	ATP	N3-C4-N9	3.80	133.62	127.17
3	B	604	NAD	C4A-N9A-C8A	3.77	109.70	105.74
4	G	601	ATP	N3-C4-N9	3.77	133.58	127.17
2	F	603	IMP	C2-N3-C4	3.73	118.10	111.53
4	E	604	ATP	N3-C4-N9	3.72	133.50	127.17
2	H	603	IMP	N9-C8-N7	-3.71	106.52	113.40
4	G	601	ATP	C4'-O4'-C1'	-3.71	101.27	109.47
4	H	602	ATP	C4-N9-C8	3.71	109.63	105.74
3	E	602	NAD	O7N-C7N-N7N	-3.66	117.33	122.62
3	B	604	NAD	C4B-O4B-C1B	-3.65	101.41	109.47
4	C	602	ATP	N3-C4-N9	3.63	133.34	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	603	IMP	N9-C8-N7	-3.61	106.70	113.40
2	E	601	IMP	N1-C2-N3	-3.60	121.36	125.50
4	C	601	ATP	C5-N7-C8	3.54	109.01	103.45
2	H	603	IMP	O3P-P-O2P	3.52	120.98	107.80
4	H	602	ATP	N3-C4-N9	3.50	133.12	127.17
3	F	604	NAD	O4B-C1B-C2B	-3.49	99.14	106.62
4	G	602	ATP	N3-C4-N9	3.49	133.10	127.17
3	D	604	NAD	C2N-C3N-C4N	3.46	122.28	118.26
4	F	602	ATP	C2-N3-C4	3.46	120.27	111.83
4	E	604	ATP	C2-N3-C4	3.45	120.26	111.83
3	B	604	NAD	O4B-C1B-C2B	-3.45	99.24	106.62
2	G	603	IMP	N9-C8-N7	-3.44	107.01	113.40
2	F	603	IMP	N1-C2-N3	-3.44	121.53	125.50
3	C	604	NAD	N3A-C4A-N9A	3.44	133.01	127.17
4	D	601	ATP	N3-C4-N9	3.40	132.95	127.17
4	F	601	ATP	C3'-C2'-C1'	3.40	107.89	101.46
4	H	601	ATP	N3-C4-N9	3.40	132.94	127.17
4	G	601	ATP	C5-N7-C8	3.39	108.78	103.45
3	H	604	NAD	N3A-C4A-N9A	3.39	132.93	127.17
4	B	602	ATP	C5-N7-C8	3.34	108.70	103.45
3	A	602	NAD	C4D-O4D-C1D	-3.34	106.86	109.92
3	B	604	NAD	C2A-N3A-C4A	3.33	119.96	111.83
4	B	601	ATP	N3-C4-N9	3.33	132.82	127.17
2	H	603	IMP	O6-C6-C5	-3.32	117.75	126.53
3	F	604	NAD	N3A-C4A-N9A	3.32	132.82	127.17
4	E	604	ATP	C5-N7-C8	3.32	108.67	103.45
3	C	604	NAD	C2A-N3A-C4A	3.32	119.93	111.83
2	E	601	IMP	O6-C6-C5	-3.32	117.78	126.53
4	F	601	ATP	N3-C4-N9	3.30	132.79	127.17
4	B	602	ATP	C2-N3-C4	3.30	119.90	111.83
2	A	601	IMP	N9-C8-N7	-3.30	107.28	113.40
2	D	603	IMP	O6-C6-C5	-3.30	117.83	126.53
3	G	604	NAD	C2A-N3A-C4A	3.29	119.86	111.83
2	G	603	IMP	O6-C6-C5	-3.29	117.86	126.53
4	D	601	ATP	C2-N3-C4	3.28	119.84	111.83
4	H	602	ATP	C2-N3-C4	3.28	119.84	111.83
3	F	604	NAD	C2A-N3A-C4A	3.27	119.83	111.83
2	B	603	IMP	N1-C2-N3	-3.26	121.74	125.50
4	A	603	ATP	N3-C4-N9	3.26	132.71	127.17
2	E	601	IMP	N9-C4-N3	3.26	134.32	126.90
3	H	604	NAD	C2A-N3A-C4A	3.25	119.77	111.83
2	C	603	IMP	C5-C4-N3	-3.24	122.50	127.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	ATP	C3'-C2'-C1'	3.24	107.59	101.46
4	B	601	ATP	C2-N3-C4	3.24	119.74	111.83
4	C	602	ATP	C2-N3-C4	3.23	119.72	111.83
3	B	604	NAD	C2N-C3N-C4N	3.23	122.01	118.26
3	H	604	NAD	C2N-C3N-C4N	3.22	122.01	118.26
4	A	603	ATP	C5-N7-C8	3.21	108.50	103.45
4	E	603	ATP	C5-N7-C8	3.20	108.48	103.45
4	G	602	ATP	C5-N7-C8	3.20	108.48	103.45
4	G	602	ATP	C2-N3-C4	3.18	119.60	111.83
4	F	602	ATP	C5-N7-C8	3.17	108.44	103.45
3	E	602	NAD	N3A-C4A-N9A	3.16	132.54	127.17
4	A	604	ATP	N3-C4-N9	3.16	132.54	127.17
4	G	601	ATP	C2-N3-C4	3.16	119.55	111.83
3	G	604	NAD	N3A-C4A-N9A	3.15	132.53	127.17
4	C	602	ATP	C5-N7-C8	3.15	108.40	103.45
3	G	604	NAD	C5A-N7A-C8A	3.15	108.39	103.45
3	E	602	NAD	C2A-N3A-C4A	3.14	119.50	111.83
2	H	603	IMP	N9-C4-N3	3.14	134.05	126.90
3	A	602	NAD	C2A-N3A-C4A	3.14	119.50	111.83
3	D	604	NAD	C2A-N3A-C4A	3.14	119.50	111.83
4	D	602	ATP	N3-C4-N9	3.12	132.48	127.17
4	E	603	ATP	C2-N3-C4	3.11	119.43	111.83
3	B	604	NAD	N3A-C4A-N9A	3.11	132.45	127.17
4	F	601	ATP	C2-N3-C4	3.10	119.41	111.83
4	D	602	ATP	C5-N7-C8	3.10	108.33	103.45
4	E	603	ATP	N3-C4-N9	3.08	132.41	127.17
4	A	603	ATP	C2-N3-C4	3.08	119.34	111.83
2	A	601	IMP	O6-C6-C5	-3.07	118.43	126.53
2	B	603	IMP	N9-C4-N3	3.06	133.88	126.90
2	F	603	IMP	O6-C6-C5	-3.06	118.46	126.53
4	H	601	ATP	C2-N3-C4	3.06	119.30	111.83
4	D	602	ATP	C2-N3-C4	3.05	119.29	111.83
2	B	603	IMP	O6-C6-C5	-3.05	118.48	126.53
3	A	602	NAD	C2N-C3N-C4N	3.04	121.79	118.26
3	D	604	NAD	N3A-C4A-N9A	3.04	132.33	127.17
3	C	604	NAD	C5A-N7A-C8A	3.03	108.22	103.45
4	D	601	ATP	C5-N7-C8	3.03	108.20	103.45
4	B	601	ATP	C5-N7-C8	3.02	108.19	103.45
3	A	602	NAD	N3A-C4A-N9A	3.01	132.28	127.17
4	A	604	ATP	C2-N3-C4	3.00	119.15	111.83
3	G	604	NAD	C2N-C3N-C4N	2.99	121.74	118.26
3	F	604	NAD	C4B-O4B-C1B	-2.99	102.86	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	604	NAD	C5A-N7A-C8A	2.99	108.15	103.45
2	D	603	IMP	O3P-P-O2P	2.99	119.00	107.80
2	E	601	IMP	N9-C8-N7	-2.97	107.90	113.40
4	B	601	ATP	C3'-C2'-C1'	2.96	107.07	101.46
2	C	603	IMP	O6-C6-C5	-2.95	118.75	126.53
3	F	604	NAD	C2N-C3N-C4N	2.92	121.65	118.26
2	A	601	IMP	O3P-P-O2P	2.90	118.68	107.80
3	B	604	NAD	C5A-N7A-C8A	2.90	108.00	103.45
3	A	602	NAD	C5A-N7A-C8A	2.89	108.00	103.45
4	H	602	ATP	C5-N7-C8	2.87	107.97	103.45
4	C	602	ATP	C3'-C2'-C1'	2.85	106.86	101.46
4	C	601	ATP	C3'-C2'-C1'	2.85	106.85	101.46
4	H	601	ATP	C5-N7-C8	2.84	107.92	103.45
4	C	601	ATP	C2-N3-C4	2.84	118.77	111.83
4	F	601	ATP	C5-N7-C8	2.84	107.91	103.45
3	E	602	NAD	C5A-N7A-C8A	2.83	107.90	103.45
4	C	601	ATP	N3-C4-N9	2.83	131.97	127.17
3	D	604	NAD	C5A-N7A-C8A	2.78	107.83	103.45
2	C	603	IMP	C8-N9-C4	2.76	111.20	106.03
2	D	603	IMP	C8-N9-C4	2.76	111.19	106.03
2	D	603	IMP	N9-C4-N3	2.75	133.17	126.90
4	A	604	ATP	C5-N7-C8	2.74	107.75	103.45
4	C	601	ATP	C4-C5-N7	-2.72	107.47	110.58
4	E	603	ATP	C3'-C2'-C1'	2.68	106.54	101.46
2	G	603	IMP	O3P-P-O2P	2.68	117.84	107.80
4	G	601	ATP	C3'-C2'-C1'	2.64	106.45	101.46
4	A	603	ATP	C2'-C1'-N9	-2.64	106.75	113.30
3	H	604	NAD	C5A-N7A-C8A	2.63	107.58	103.45
3	B	604	NAD	O4B-C1B-N9A	2.60	113.09	108.09
4	H	602	ATP	C3'-C2'-C1'	2.60	106.39	101.46
3	F	604	NAD	C2D-C3D-C4D	2.60	107.64	102.61
2	F	603	IMP	N9-C4-N3	2.58	132.77	126.90
4	A	603	ATP	O3G-PG-O3B	2.57	113.25	104.64
3	F	604	NAD	O4B-C1B-N9A	2.56	113.00	108.09
3	G	604	NAD	C2D-C3D-C4D	2.55	107.54	102.61
2	G	603	IMP	N9-C4-N3	2.54	132.70	126.90
2	B	603	IMP	C8-N9-C4	2.54	110.79	106.03
4	A	603	ATP	C3'-C2'-C1'	2.52	106.22	101.46
3	C	604	NAD	C3N-C7N-N7N	2.51	120.83	117.74
2	A	601	IMP	N9-C4-N3	2.50	132.59	126.90
3	C	604	NAD	C2N-C3N-C4N	2.50	121.16	118.26
2	H	603	IMP	C8-N9-C4	2.49	110.70	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	602	ATP	C3'-C2'-C1'	2.49	106.17	101.46
3	G	604	NAD	C3B-C2B-C1B	2.42	106.03	101.46
2	B	603	IMP	C1'-N9-C8	-2.38	119.96	126.73
4	C	601	ATP	C2'-C3'-C4'	2.38	107.20	102.61
2	F	603	IMP	O3P-P-O2P	2.38	116.71	107.80
2	G	603	IMP	C8-N9-C4	2.37	110.46	106.03
4	E	603	ATP	C2'-C1'-N9	-2.36	107.43	113.30
4	D	601	ATP	C3'-C2'-C1'	2.32	105.84	101.46
3	B	604	NAD	C4D-O4D-C1D	-2.31	107.81	109.92
2	F	603	IMP	C8-N9-C4	2.30	110.34	106.03
3	E	602	NAD	C2D-C3D-C4D	2.25	106.96	102.61
4	F	601	ATP	C2'-C3'-C4'	2.25	106.95	102.61
2	E	601	IMP	O2P-P-O1P	2.24	119.55	110.83
3	B	604	NAD	C6N-N1N-C2N	-2.22	119.99	121.88
3	G	604	NAD	C2B-C3B-C4B	2.21	106.88	102.61
3	E	602	NAD	O7N-C7N-C3N	-2.18	116.93	119.60
4	C	601	ATP	C6-C5-C4	2.11	120.06	117.18
2	B	603	IMP	C8-N7-C5	2.08	107.96	104.26
4	H	601	ATP	C3'-C2'-C1'	2.06	105.36	101.46
3	D	604	NAD	C4B-O4B-C1B	-2.06	104.93	109.47
2	B	603	IMP	O2P-P-O1P	2.05	118.83	110.83
4	H	602	ATP	C6-C5-C4	2.04	119.97	117.18
4	H	602	ATP	O4'-C1'-N9	2.04	112.01	108.09
3	D	604	NAD	C2D-C3D-C4D	2.04	106.55	102.61
4	E	604	ATP	C3'-C2'-C1'	2.03	105.30	101.46

There are no chirality outliers.

All (214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	603	IMP	C5'-O5'-P-O2P
2	B	603	IMP	C5'-O5'-P-O3P
2	B	603	IMP	O4'-C4'-C5'-O5'
2	C	603	IMP	C5'-O5'-P-O1P
2	C	603	IMP	C5'-O5'-P-O2P
2	C	603	IMP	C5'-O5'-P-O3P
2	E	601	IMP	C5'-O5'-P-O1P
2	E	601	IMP	C5'-O5'-P-O2P
2	E	601	IMP	C5'-O5'-P-O3P
2	F	603	IMP	C5'-O5'-P-O2P
2	G	603	IMP	C5'-O5'-P-O2P
2	G	603	IMP	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
3	A	602	NAD	PA-O3-PN-O5D
3	A	602	NAD	C5D-O5D-PN-O3
3	A	602	NAD	C5D-O5D-PN-O1N
3	A	602	NAD	C5D-O5D-PN-O2N
3	A	602	NAD	C2N-C3N-C7N-O7N
3	A	602	NAD	C2N-C3N-C7N-N7N
3	B	604	NAD	C2B-C1B-N9A-C8A
3	B	604	NAD	C2B-C1B-N9A-C4A
3	C	604	NAD	O4D-C4D-C5D-O5D
3	D	604	NAD	PA-O3-PN-O5D
3	E	602	NAD	C5D-O5D-PN-O1N
3	F	604	NAD	C5B-O5B-PA-O1A
3	F	604	NAD	C5B-O5B-PA-O3
3	F	604	NAD	O4B-C4B-C5B-O5B
3	F	604	NAD	C3B-C4B-C5B-O5B
3	F	604	NAD	C2B-C1B-N9A-C8A
3	F	604	NAD	C2N-C3N-C7N-O7N
3	F	604	NAD	C2N-C3N-C7N-N7N
3	G	604	NAD	C5B-O5B-PA-O1A
3	G	604	NAD	O4B-C4B-C5B-O5B
3	H	604	NAD	C5B-O5B-PA-O1A
3	H	604	NAD	C5B-O5B-PA-O2A
3	H	604	NAD	C5B-O5B-PA-O3
3	H	604	NAD	C2B-C1B-N9A-C8A
3	H	604	NAD	PA-O3-PN-O5D
4	A	603	ATP	C5'-O5'-PA-O1A
4	A	603	ATP	C5'-O5'-PA-O2A
4	A	603	ATP	C5'-O5'-PA-O3A
4	A	604	ATP	C5'-O5'-PA-O1A
4	A	604	ATP	C5'-O5'-PA-O2A
4	A	604	ATP	C5'-O5'-PA-O3A
4	B	601	ATP	C5'-O5'-PA-O2A
4	B	602	ATP	C5'-O5'-PA-O1A
4	B	602	ATP	C5'-O5'-PA-O2A
4	B	602	ATP	C5'-O5'-PA-O3A
4	C	601	ATP	C5'-O5'-PA-O2A
4	C	601	ATP	C5'-O5'-PA-O3A
4	D	602	ATP	C5'-O5'-PA-O2A
4	D	602	ATP	O4'-C4'-C5'-O5'
4	D	602	ATP	C3'-C4'-C5'-O5'
4	E	603	ATP	C5'-O5'-PA-O1A
4	E	603	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	E	604	ATP	C5'-O5'-PA-O1A
4	E	604	ATP	C5'-O5'-PA-O2A
4	E	604	ATP	C5'-O5'-PA-O3A
4	F	601	ATP	C5'-O5'-PA-O1A
4	F	601	ATP	C5'-O5'-PA-O2A
4	F	601	ATP	C5'-O5'-PA-O3A
4	F	602	ATP	C5'-O5'-PA-O2A
4	F	602	ATP	C5'-O5'-PA-O3A
4	G	601	ATP	O4'-C4'-C5'-O5'
4	H	601	ATP	C5'-O5'-PA-O1A
4	H	601	ATP	C5'-O5'-PA-O2A
4	H	601	ATP	C5'-O5'-PA-O3A
3	F	604	NAD	C4N-C3N-C7N-O7N
3	F	604	NAD	C4N-C3N-C7N-N7N
3	A	602	NAD	C4N-C3N-C7N-O7N
3	A	602	NAD	C4N-C3N-C7N-N7N
2	B	603	IMP	C3'-C4'-C5'-O5'
2	D	603	IMP	C3'-C4'-C5'-O5'
2	E	601	IMP	C3'-C4'-C5'-O5'
3	B	604	NAD	O4B-C4B-C5B-O5B
3	B	604	NAD	O4D-C4D-C5D-O5D
3	C	604	NAD	C3D-C4D-C5D-O5D
3	D	604	NAD	O4B-C4B-C5B-O5B
4	C	602	ATP	O4'-C4'-C5'-O5'
2	D	603	IMP	O4'-C4'-C5'-O5'
2	E	601	IMP	O4'-C4'-C5'-O5'
3	A	602	NAD	O4B-C4B-C5B-O5B
3	B	604	NAD	C3D-C4D-C5D-O5D
3	E	602	NAD	O4B-C4B-C5B-O5B
3	H	604	NAD	O4B-C4B-C5B-O5B
4	F	601	ATP	O4'-C4'-C5'-O5'
4	F	601	ATP	C3'-C4'-C5'-O5'
4	F	602	ATP	C3'-C4'-C5'-O5'
4	G	602	ATP	O4'-C4'-C5'-O5'
4	H	601	ATP	O4'-C4'-C5'-O5'
4	H	601	ATP	C3'-C4'-C5'-O5'
3	F	604	NAD	C2B-C1B-N9A-C4A
3	H	604	NAD	C2B-C1B-N9A-C4A
3	G	604	NAD	C3B-C4B-C5B-O5B
4	F	602	ATP	O4'-C4'-C5'-O5'
4	G	601	ATP	C3'-C4'-C5'-O5'
3	B	604	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	D	604	NAD	C3B-C4B-C5B-O5B
4	A	604	ATP	C3'-C4'-C5'-O5'
4	C	601	ATP	C3'-C4'-C5'-O5'
3	D	604	NAD	C2B-C1B-N9A-C8A
2	C	603	IMP	C3'-C4'-C5'-O5'
3	F	604	NAD	O4D-C4D-C5D-O5D
4	C	602	ATP	C3'-C4'-C5'-O5'
3	A	602	NAD	C3B-C4B-C5B-O5B
3	E	602	NAD	C3B-C4B-C5B-O5B
4	E	603	ATP	O4'-C4'-C5'-O5'
3	D	604	NAD	C2B-C1B-N9A-C4A
4	C	601	ATP	C4'-C5'-O5'-PA
2	B	603	IMP	C5'-O5'-P-O1P
2	G	603	IMP	C5'-O5'-P-O1P
3	A	602	NAD	C2B-C1B-N9A-C8A
3	E	602	NAD	C2B-C1B-N9A-C8A
4	A	603	ATP	C2'-C1'-N9-C8
3	F	604	NAD	C3D-C4D-C5D-O5D
3	E	602	NAD	PA-O3-PN-O1N
4	A	603	ATP	PA-O3A-PB-O1B
3	E	602	NAD	O4D-C4D-C5D-O5D
3	H	604	NAD	O4D-C4D-C5D-O5D
4	D	601	ATP	O4'-C4'-C5'-O5'
4	G	602	ATP	C3'-C4'-C5'-O5'
4	C	601	ATP	PG-O3B-PB-O3A
3	H	604	NAD	C3B-C4B-C5B-O5B
3	E	602	NAD	PA-O3-PN-O5D
4	A	604	ATP	PB-O3A-PA-O5'
4	B	602	ATP	PB-O3A-PA-O5'
4	E	604	ATP	PB-O3A-PA-O5'
2	G	603	IMP	C3'-C4'-C5'-O5'
3	E	602	NAD	C3D-C4D-C5D-O5D
3	H	604	NAD	C3D-C4D-C5D-O5D
3	G	604	NAD	C2B-C1B-N9A-C8A
4	E	603	ATP	C2'-C1'-N9-C8
4	C	601	ATP	PA-O3A-PB-O2B
3	A	602	NAD	C4B-C5B-O5B-PA
3	E	602	NAD	C4B-C5B-O5B-PA
3	C	604	NAD	C2B-C1B-N9A-C8A
3	E	602	NAD	C2B-C1B-N9A-C4A
2	C	603	IMP	O4'-C4'-C5'-O5'
3	B	604	NAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	C	604	NAD	C5B-O5B-PA-O1A
3	C	604	NAD	C5B-O5B-PA-O2A
3	C	604	NAD	C5B-O5B-PA-O3
3	D	604	NAD	C5B-O5B-PA-O1A
3	D	604	NAD	C5B-O5B-PA-O2A
3	D	604	NAD	C5B-O5B-PA-O3
3	E	602	NAD	C5D-O5D-PN-O3
3	E	602	NAD	C5D-O5D-PN-O2N
3	F	604	NAD	C5D-O5D-PN-O3
3	F	604	NAD	C5D-O5D-PN-O1N
3	F	604	NAD	C5D-O5D-PN-O2N
3	G	604	NAD	C5D-O5D-PN-O3
3	G	604	NAD	C5D-O5D-PN-O1N
3	G	604	NAD	C5D-O5D-PN-O2N
4	B	601	ATP	C5'-O5'-PA-O1A
4	B	601	ATP	C5'-O5'-PA-O3A
4	D	602	ATP	C5'-O5'-PA-O1A
4	D	602	ATP	C5'-O5'-PA-O3A
4	F	602	ATP	C5'-O5'-PA-O1A
4	G	602	ATP	C5'-O5'-PA-O1A
4	G	602	ATP	C5'-O5'-PA-O2A
4	G	602	ATP	C5'-O5'-PA-O3A
3	B	604	NAD	C4D-C5D-O5D-PN
4	D	602	ATP	C4'-C5'-O5'-PA
3	D	604	NAD	O4D-C4D-C5D-O5D
3	A	602	NAD	C2B-C1B-N9A-C4A
3	G	604	NAD	C2B-C1B-N9A-C4A
4	A	603	ATP	C2'-C1'-N9-C4
4	E	604	ATP	C3'-C4'-C5'-O5'
4	F	601	ATP	C2'-C1'-N9-C8
3	C	604	NAD	C4D-C5D-O5D-PN
3	A	602	NAD	C2D-C1D-N1N-C6N
4	A	603	ATP	O4'-C4'-C5'-O5'
3	H	604	NAD	C4B-C5B-O5B-PA
4	E	603	ATP	C2'-C1'-N9-C4
3	B	604	NAD	C4B-C5B-O5B-PA
3	D	604	NAD	C4B-C5B-O5B-PA
3	D	604	NAD	C4D-C5D-O5D-PN
3	D	604	NAD	C3D-C4D-C5D-O5D
4	C	601	ATP	O4'-C4'-C5'-O5'
4	A	603	ATP	PG-O3B-PB-O1B
4	E	604	ATP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	F	602	ATP	PG-O3B-PB-O1B
3	F	604	NAD	C4B-C5B-O5B-PA
3	G	604	NAD	C4B-C5B-O5B-PA
3	H	604	NAD	C4D-C5D-O5D-PN
3	G	604	NAD	O4B-C1B-N9A-C8A
4	E	603	ATP	O4'-C1'-N9-C8
4	G	601	ATP	C4'-C5'-O5'-PA
4	A	604	ATP	O4'-C4'-C5'-O5'
4	A	603	ATP	O4'-C1'-N9-C8
4	F	601	ATP	PB-O3B-PG-O3G
4	G	601	ATP	PB-O3B-PG-O2G
4	C	602	ATP	C4'-C5'-O5'-PA
3	A	602	NAD	O4B-C1B-N9A-C8A
3	E	602	NAD	O4B-C1B-N9A-C8A
4	B	601	ATP	C2'-C1'-N9-C8
3	C	604	NAD	PA-O3-PN-O2N
4	C	602	ATP	PG-O3B-PB-O2B
4	F	601	ATP	PB-O3A-PA-O2A
3	D	604	NAD	O4B-C1B-N9A-C8A
3	H	604	NAD	O4B-C1B-N9A-C8A
2	G	603	IMP	O4'-C4'-C5'-O5'
4	H	602	ATP	C3'-C4'-C5'-O5'
2	F	603	IMP	C4'-C5'-O5'-P
3	C	604	NAD	O4B-C1B-N9A-C8A
4	A	604	ATP	PB-O3A-PA-O2A
4	B	602	ATP	PB-O3A-PA-O2A
4	C	601	ATP	PG-O3B-PB-O2B
4	D	602	ATP	PG-O3B-PB-O1B
4	D	602	ATP	PG-O3B-PB-O2B
4	D	602	ATP	PA-O3A-PB-O2B
4	E	603	ATP	PB-O3A-PA-O2A
4	F	602	ATP	PB-O3A-PA-O2A
4	H	602	ATP	PG-O3B-PB-O2B
4	D	601	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

21 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	ATP	1	0
4	A	603	ATP	1	0
2	F	603	IMP	2	0

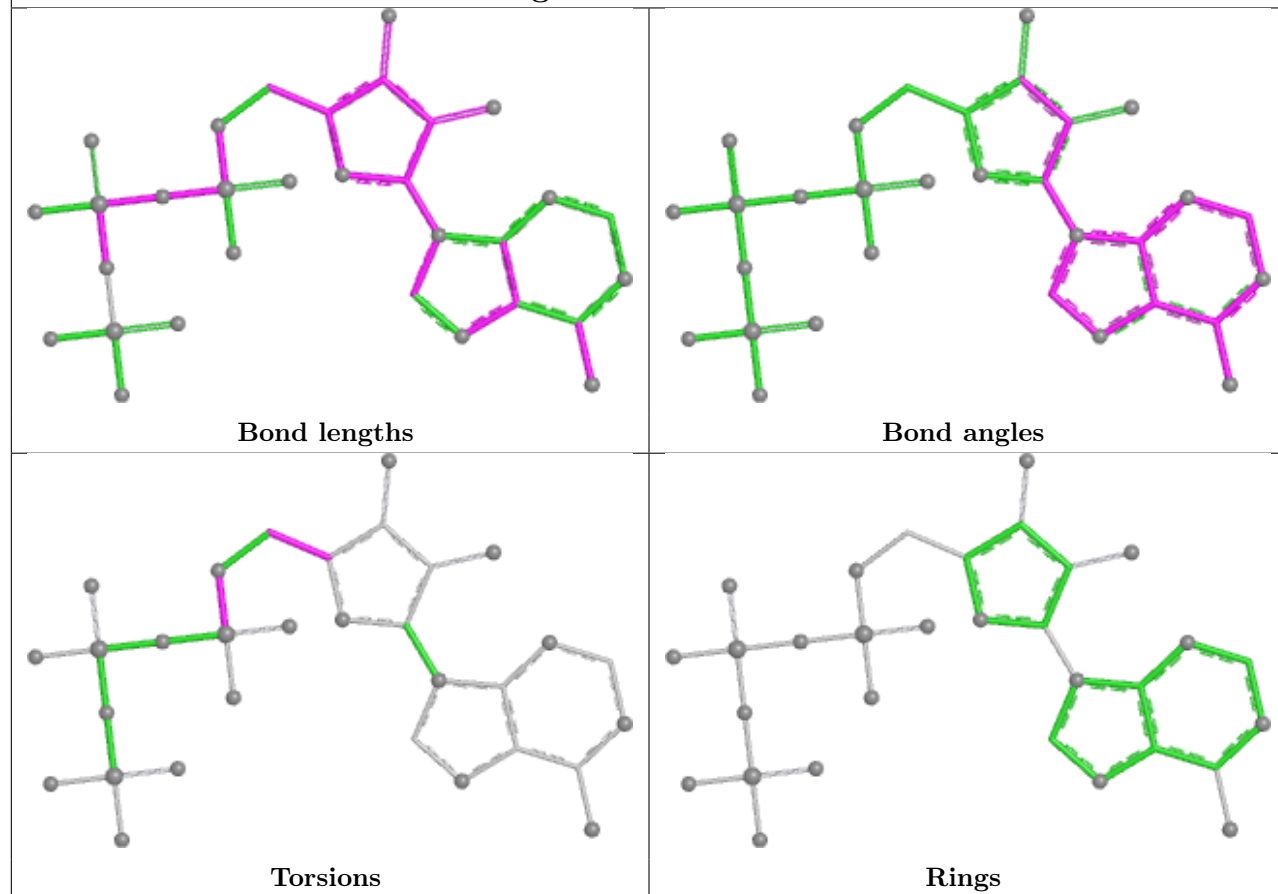
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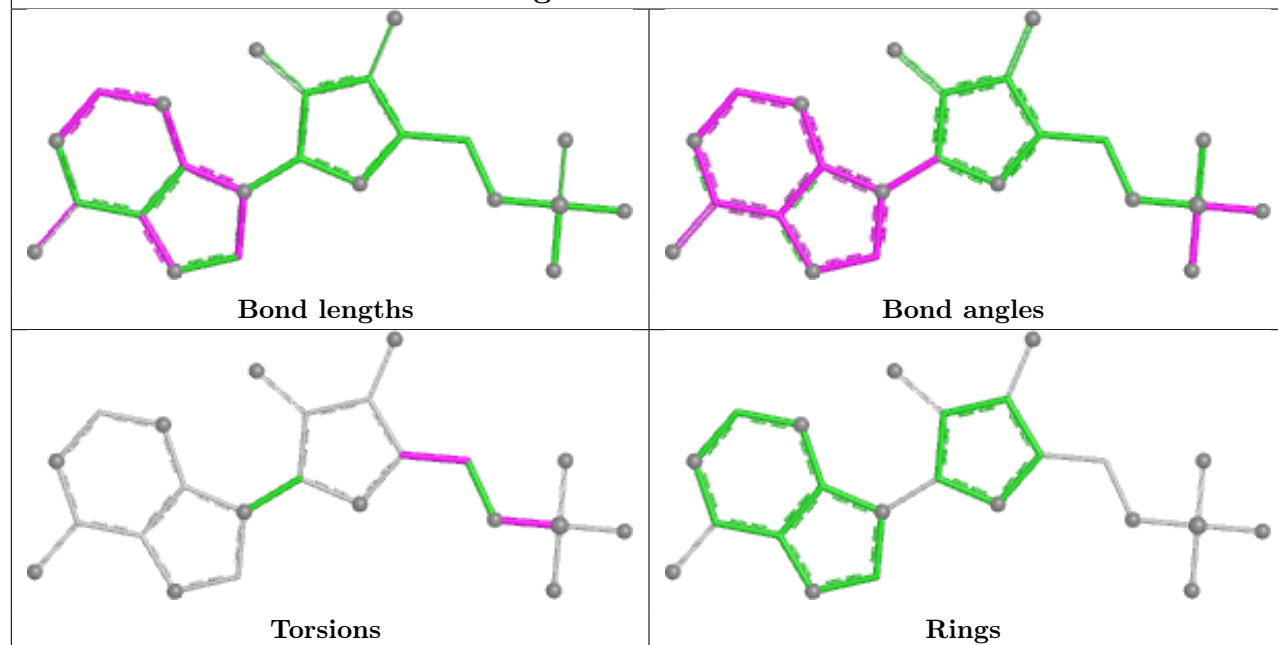
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	601	ATP	1	0
4	C	601	ATP	2	0
4	E	603	ATP	2	0
2	A	601	IMP	3	0
4	D	601	ATP	2	0
2	D	603	IMP	3	0
3	H	604	NAD	3	0
4	H	601	ATP	2	0
3	G	604	NAD	1	0
4	B	602	ATP	1	0
3	A	602	NAD	2	0
3	C	604	NAD	1	0
2	G	603	IMP	4	0
3	E	602	NAD	1	0
2	C	603	IMP	2	0
2	E	601	IMP	3	0
3	F	604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

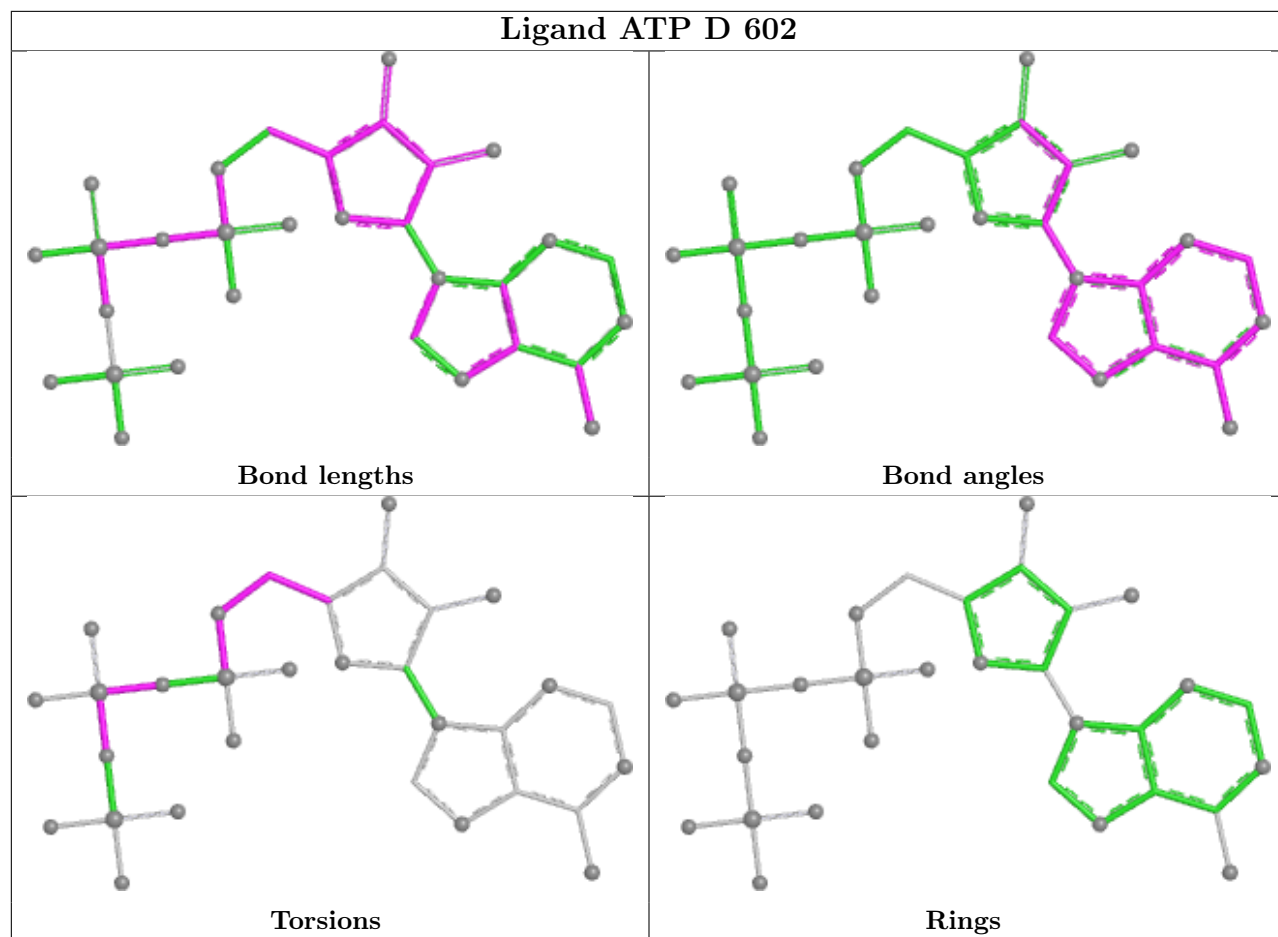
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

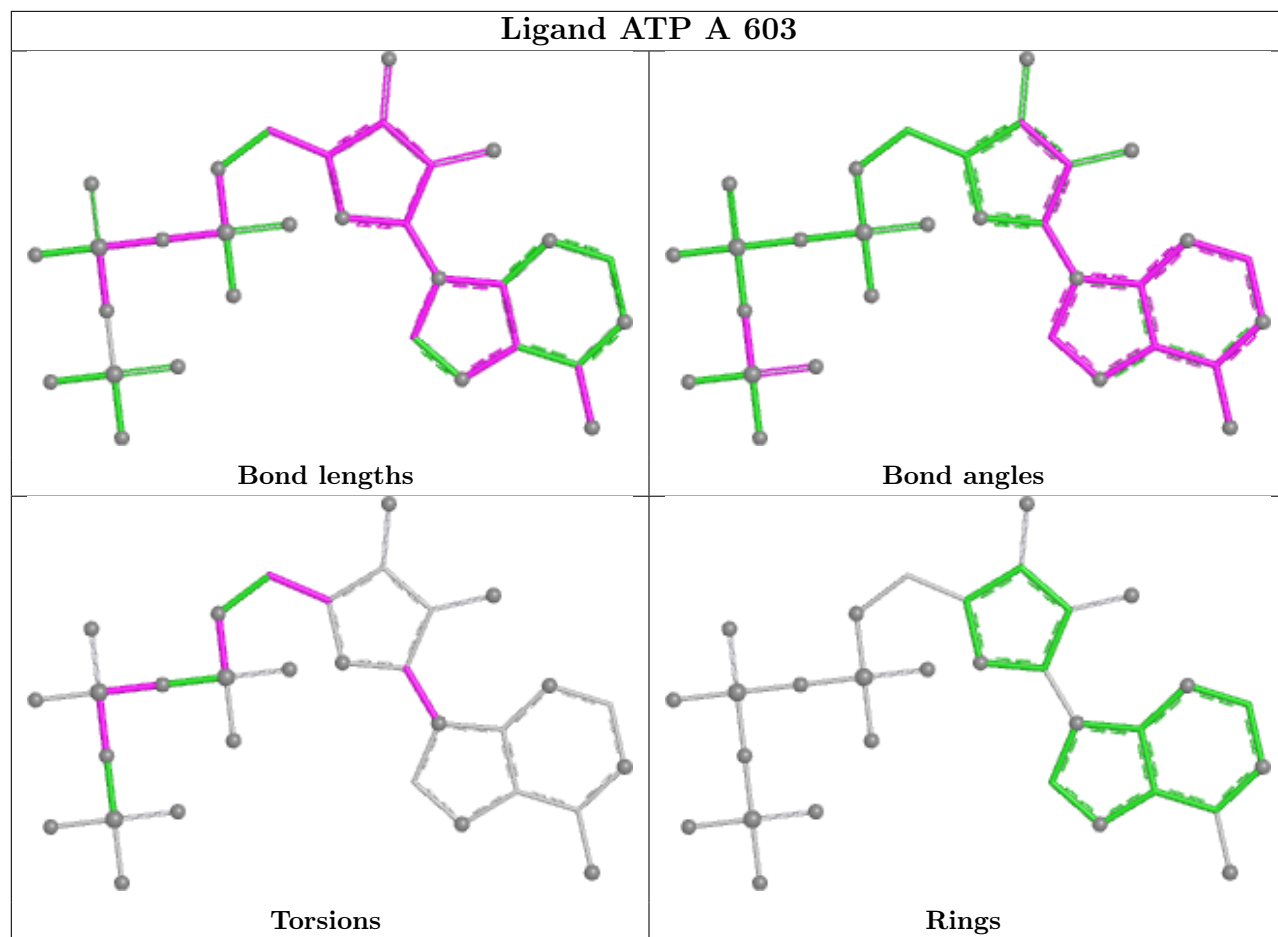
Ligand ATP G 602



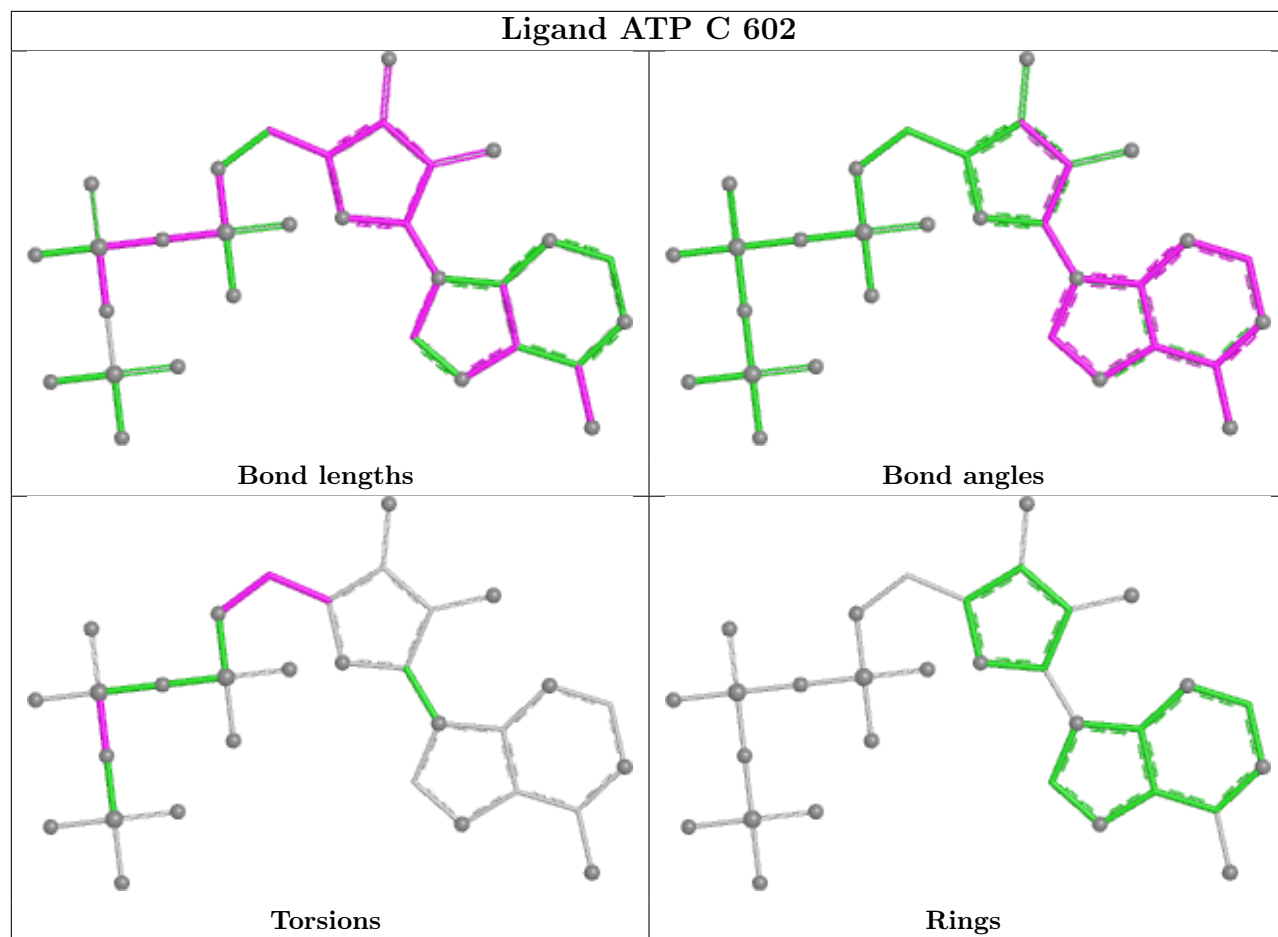
Ligand IMP B 603



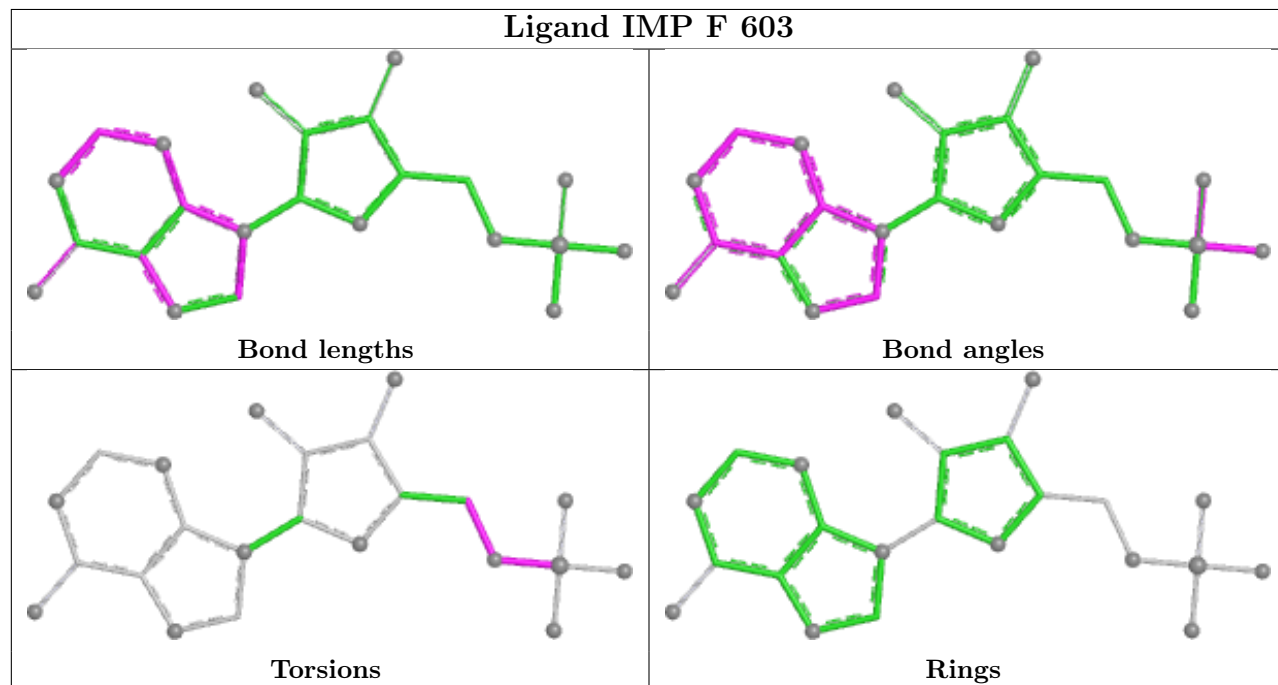




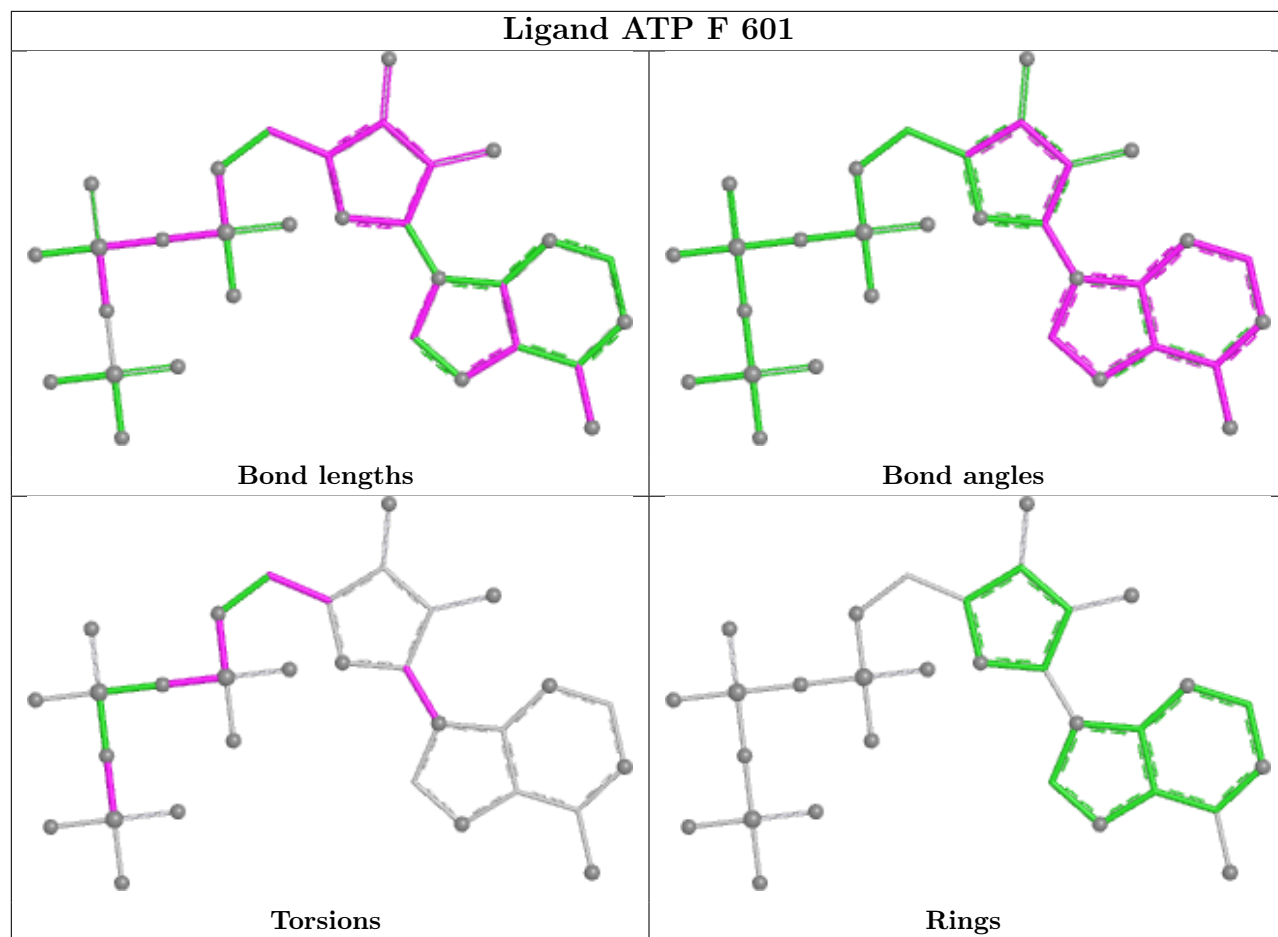
Ligand ATP C 602

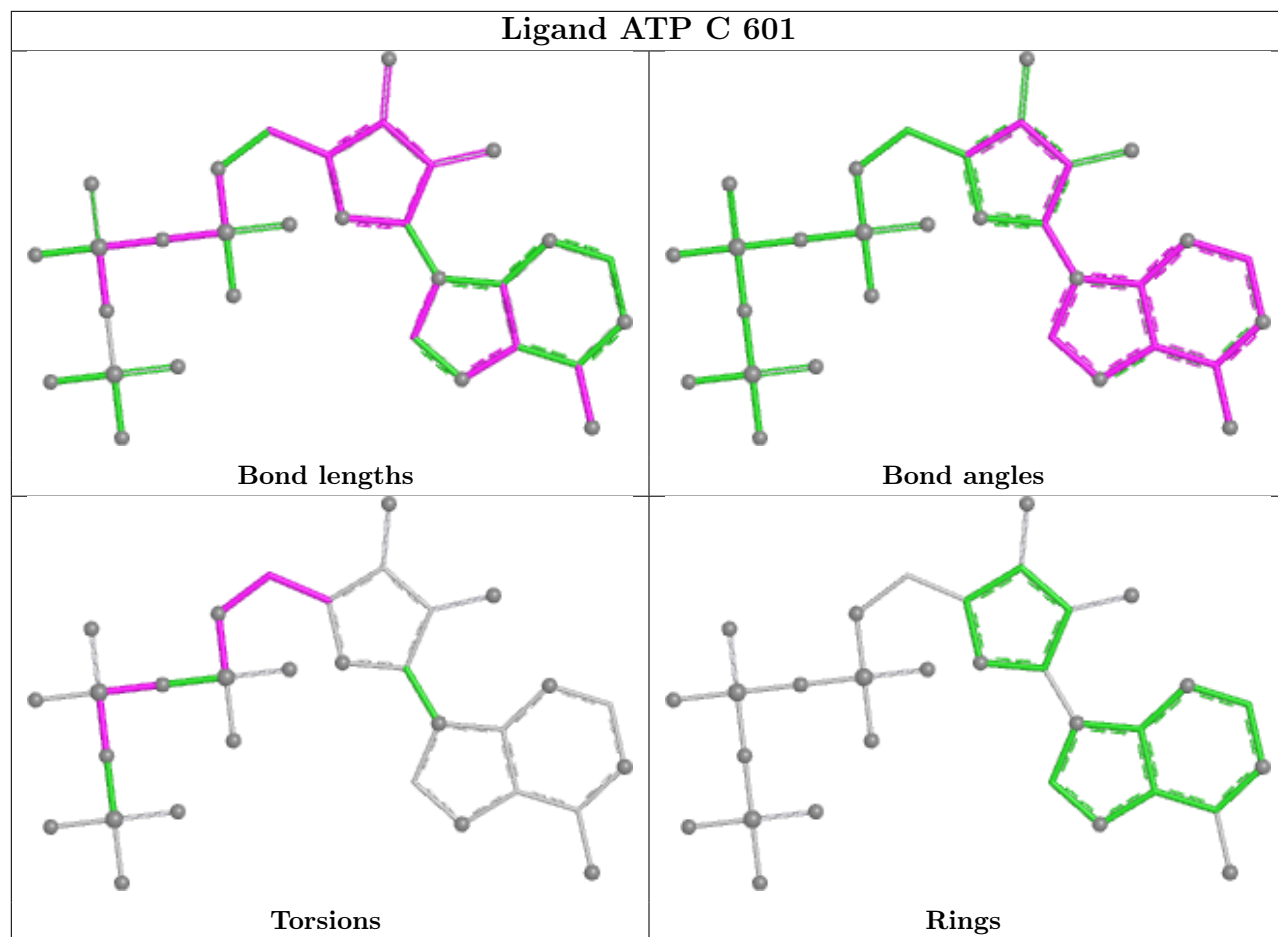


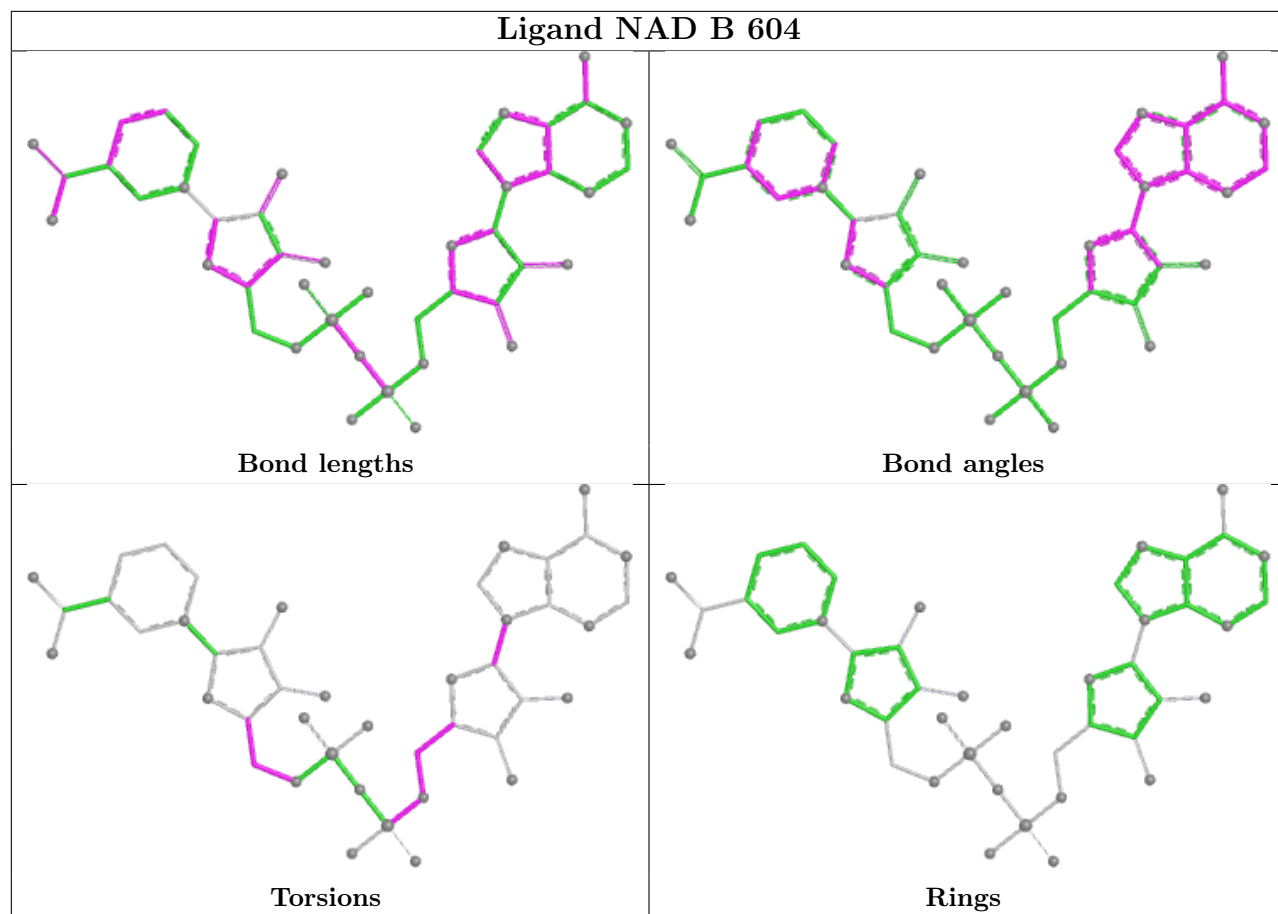
Ligand IMP F 603



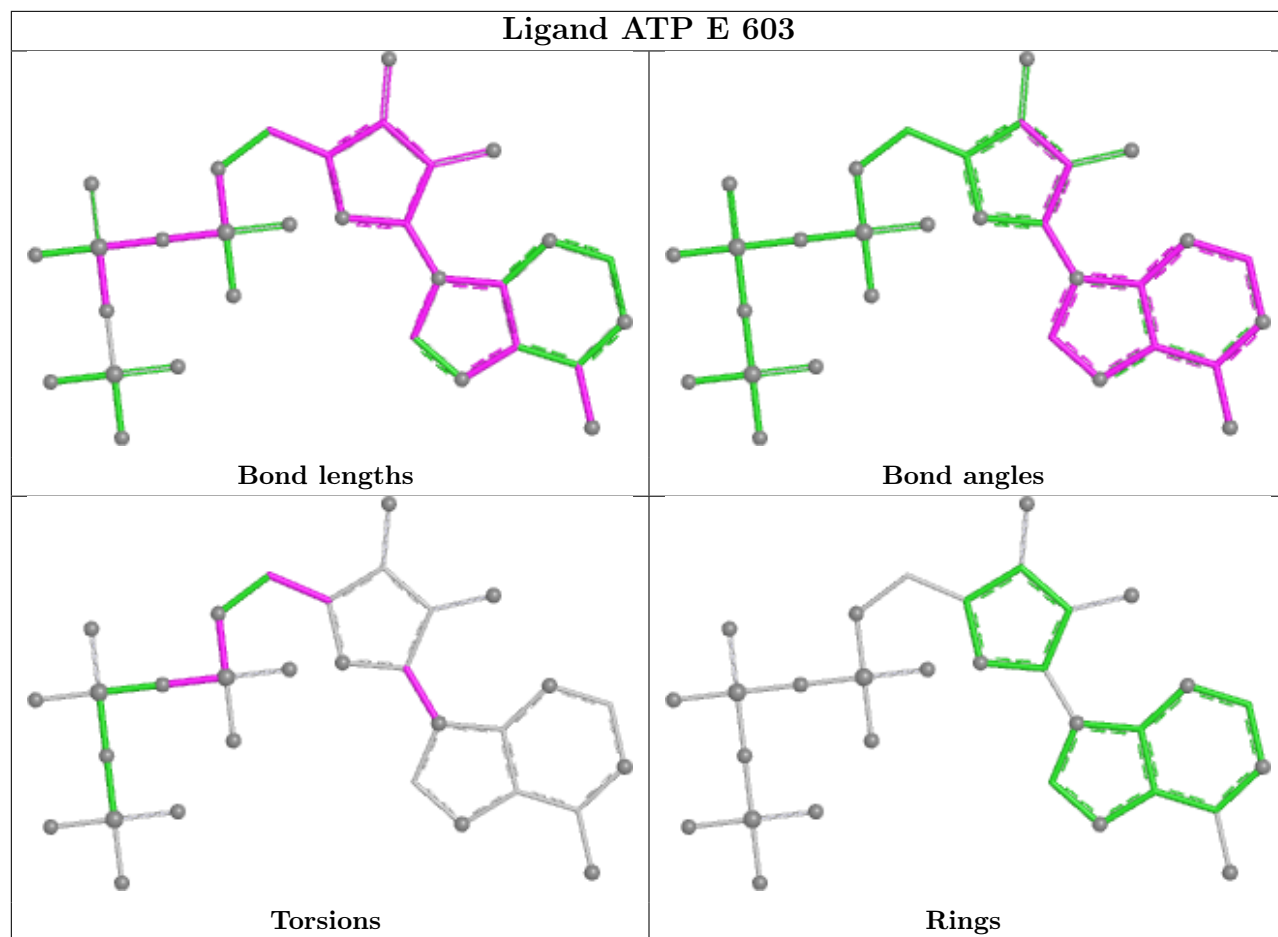
Ligand ATP F 601



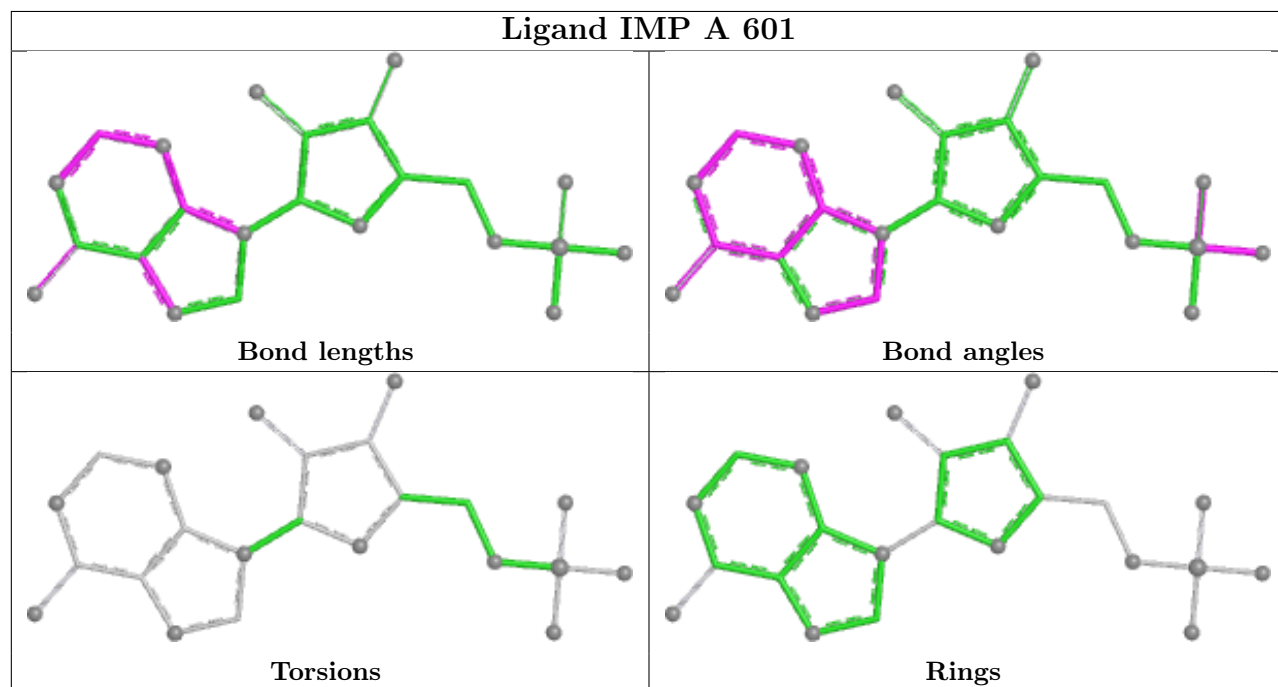


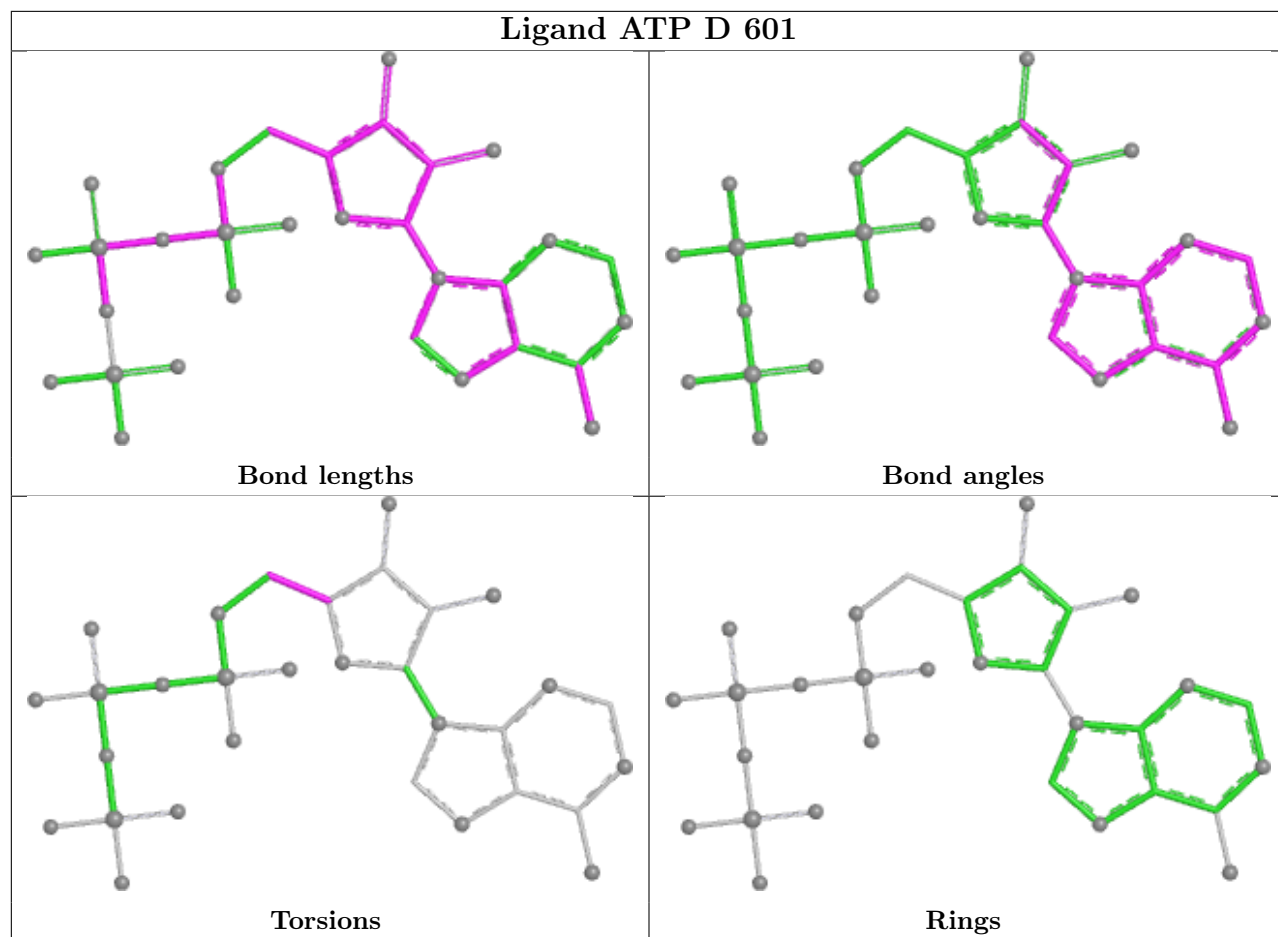


Ligand ATP E 603

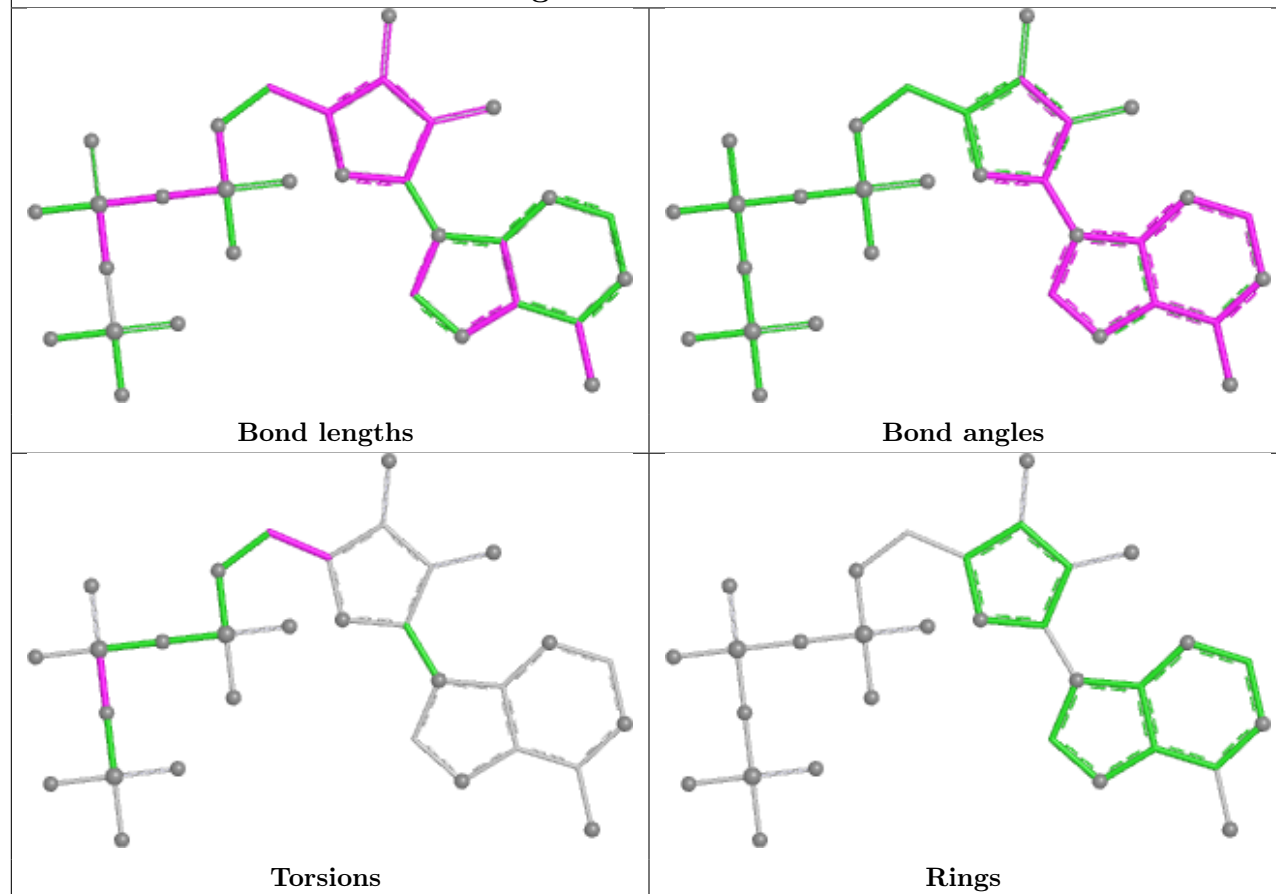


Ligand IMP A 601

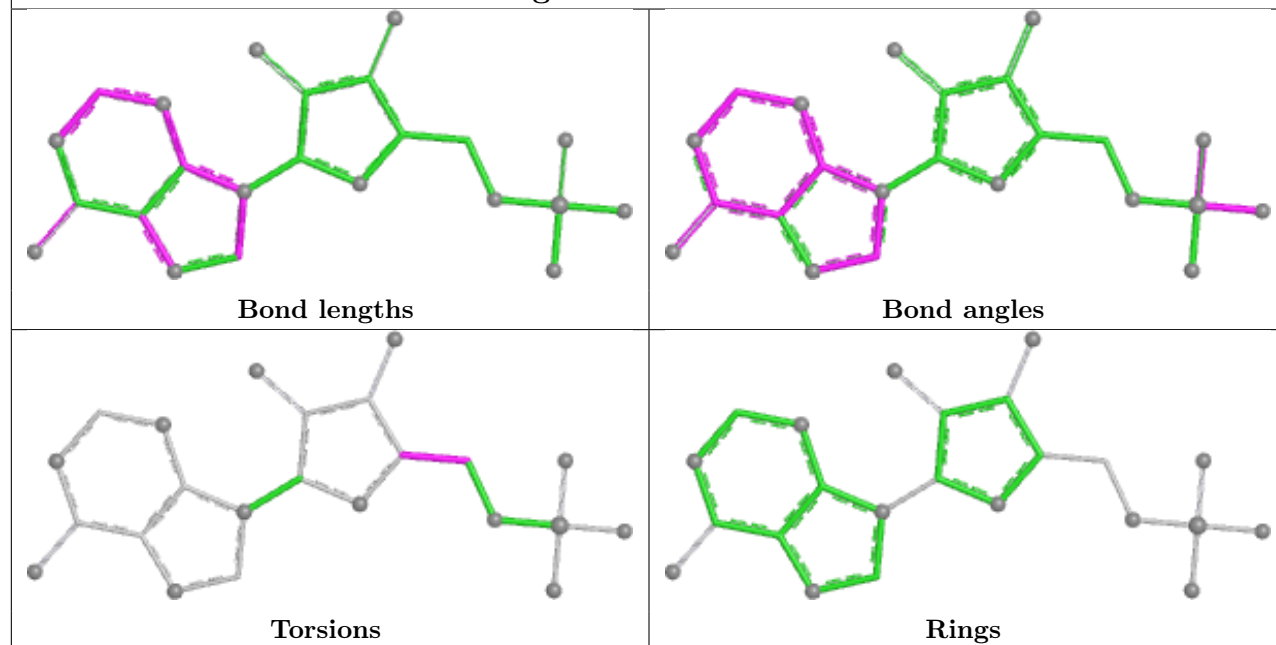


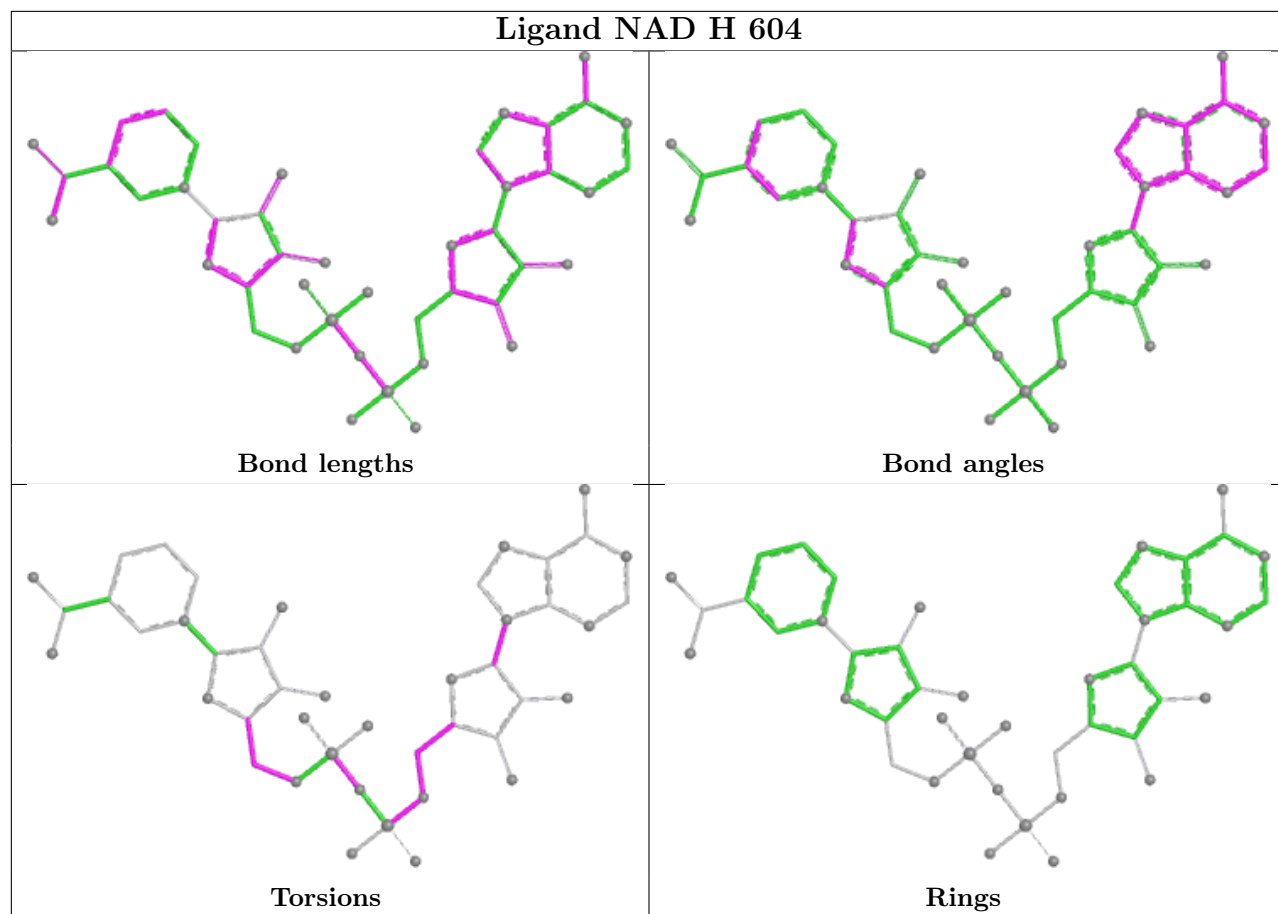


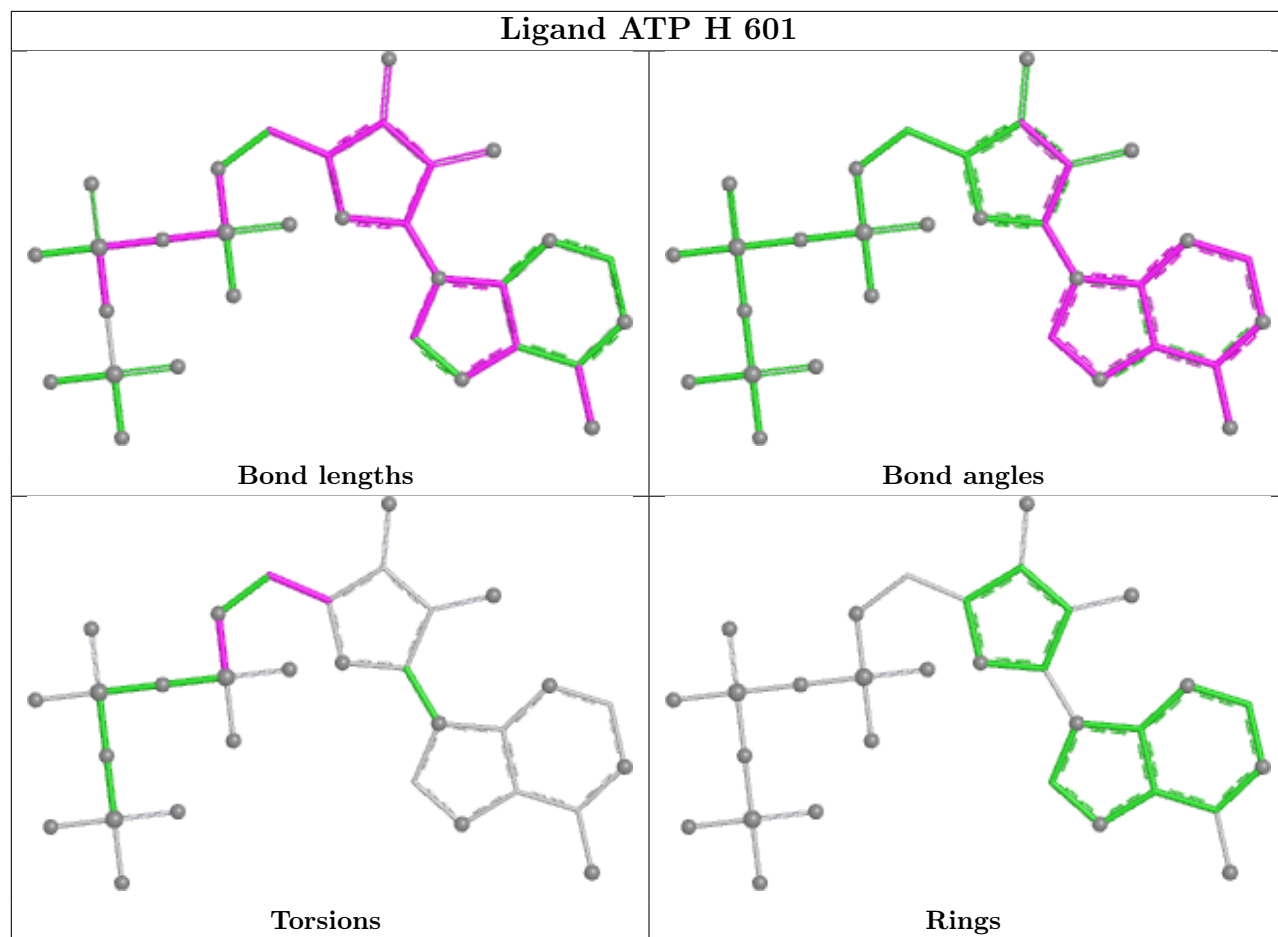
Ligand ATP H 602

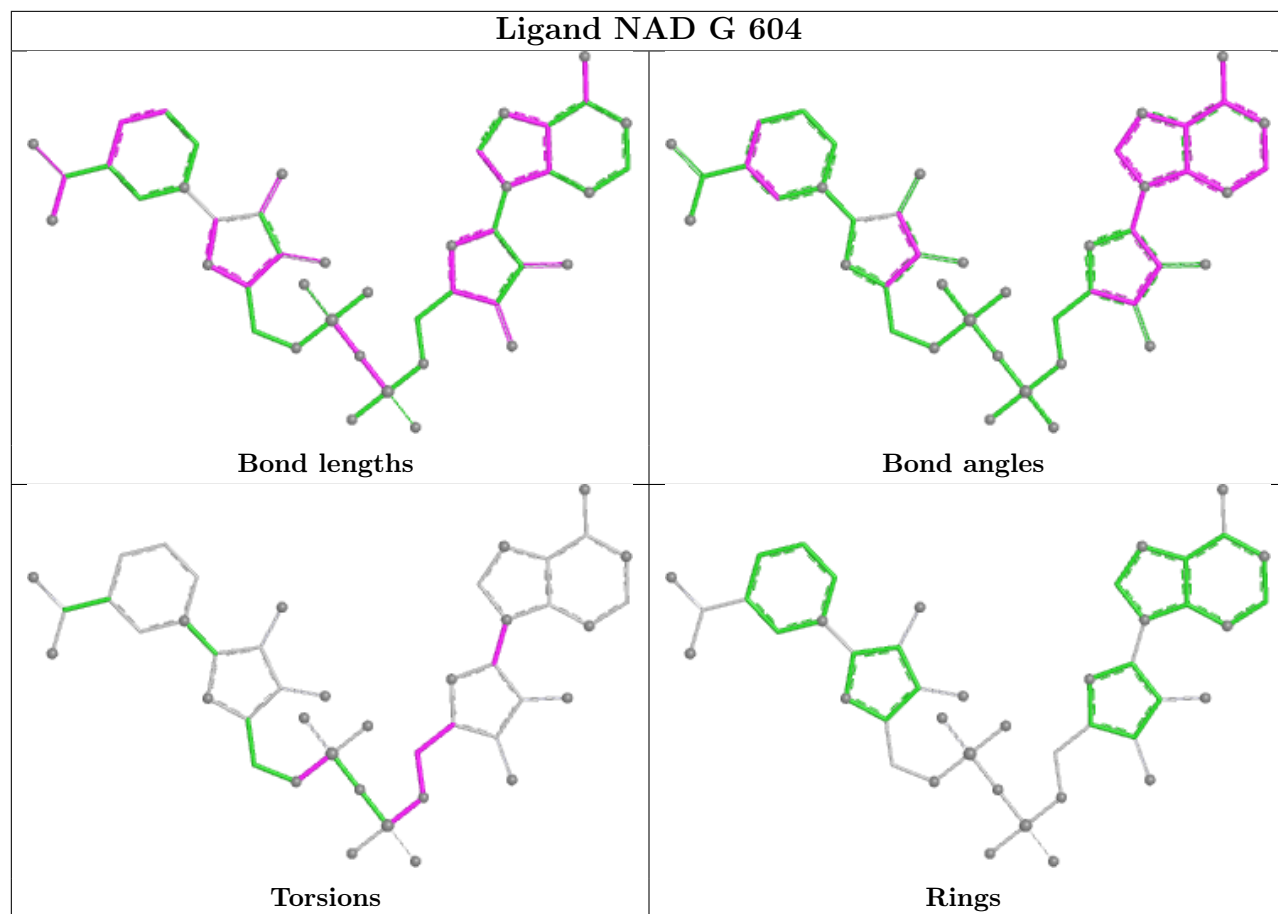


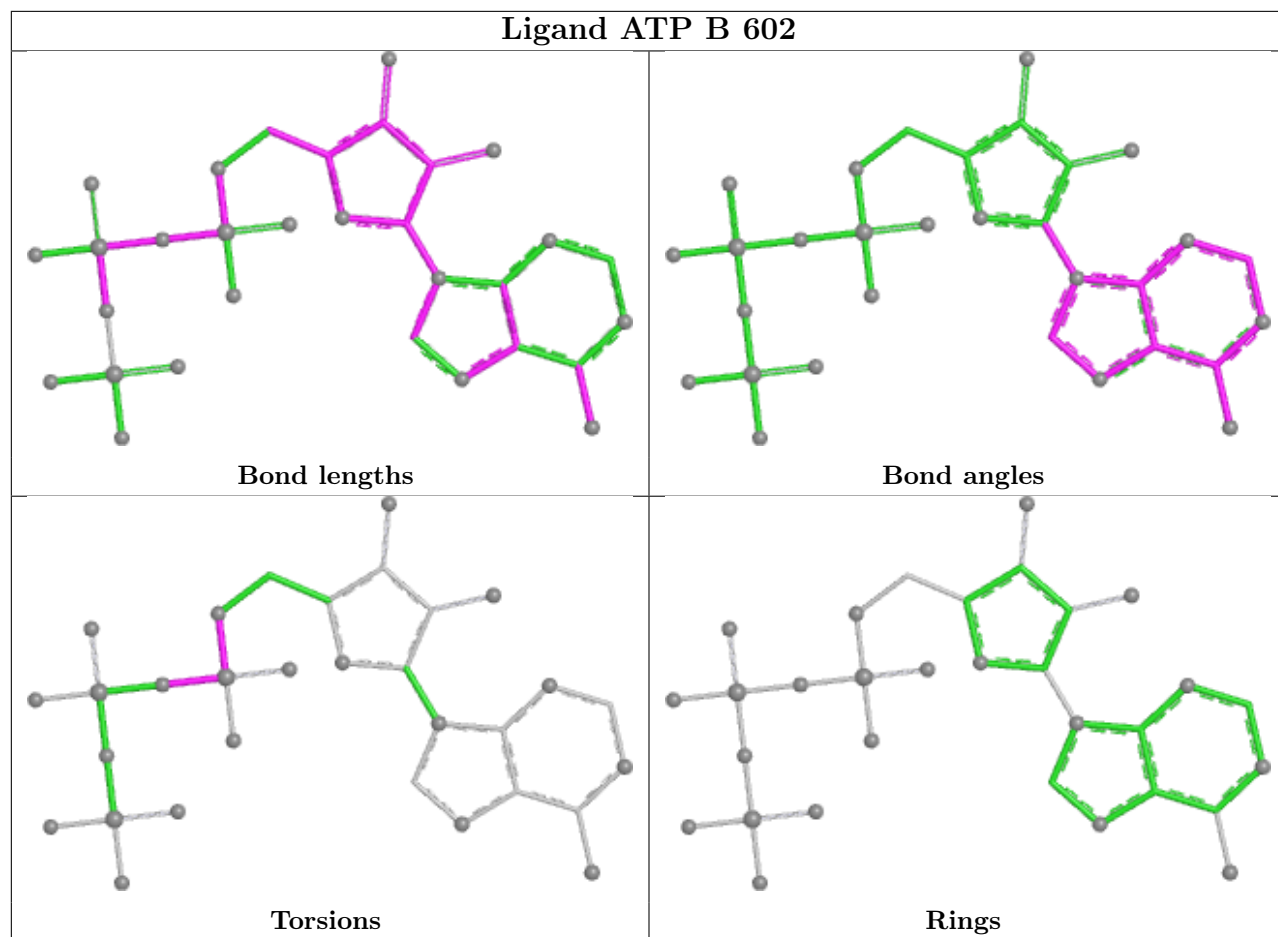
Ligand IMP D 603

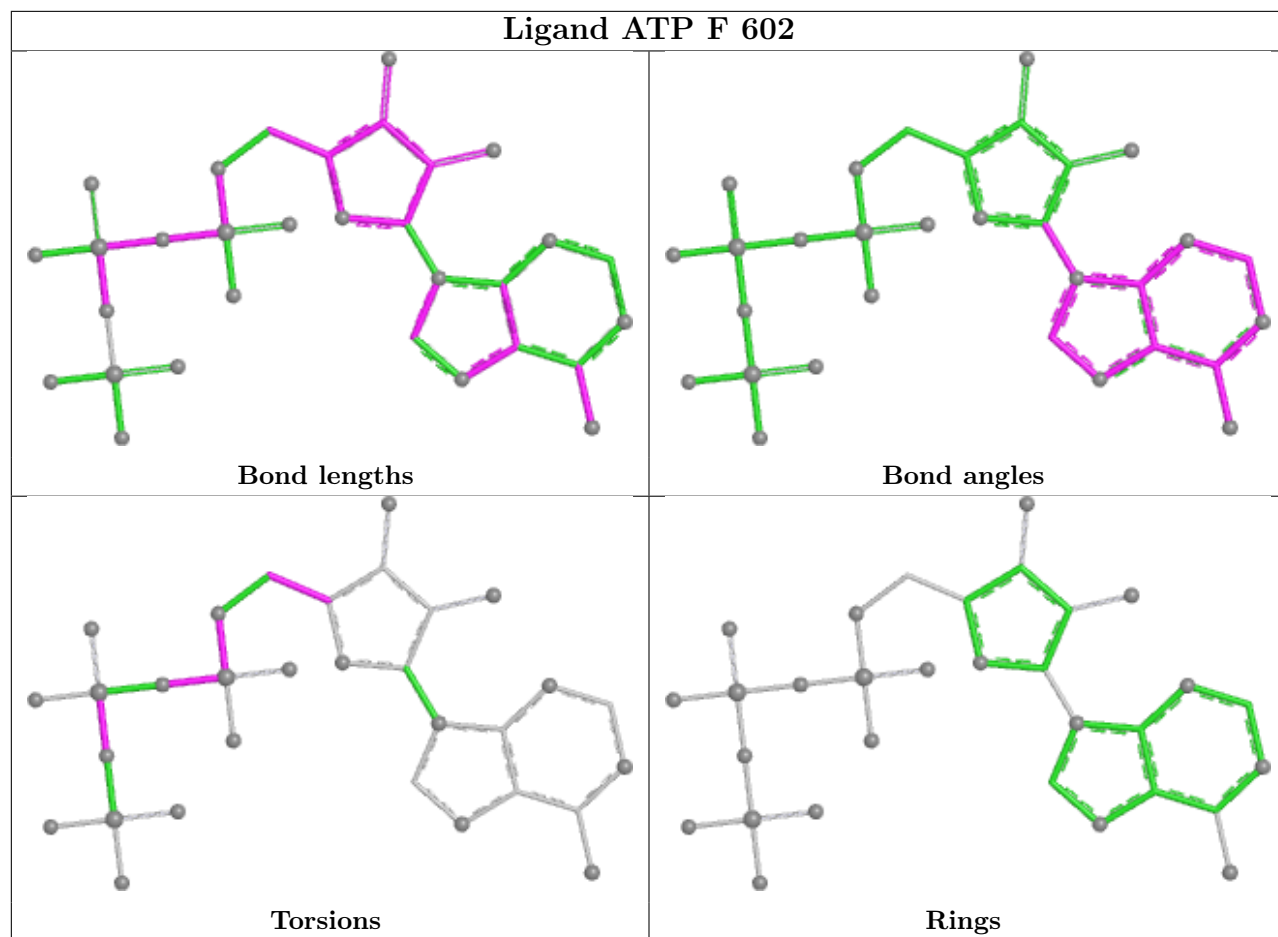


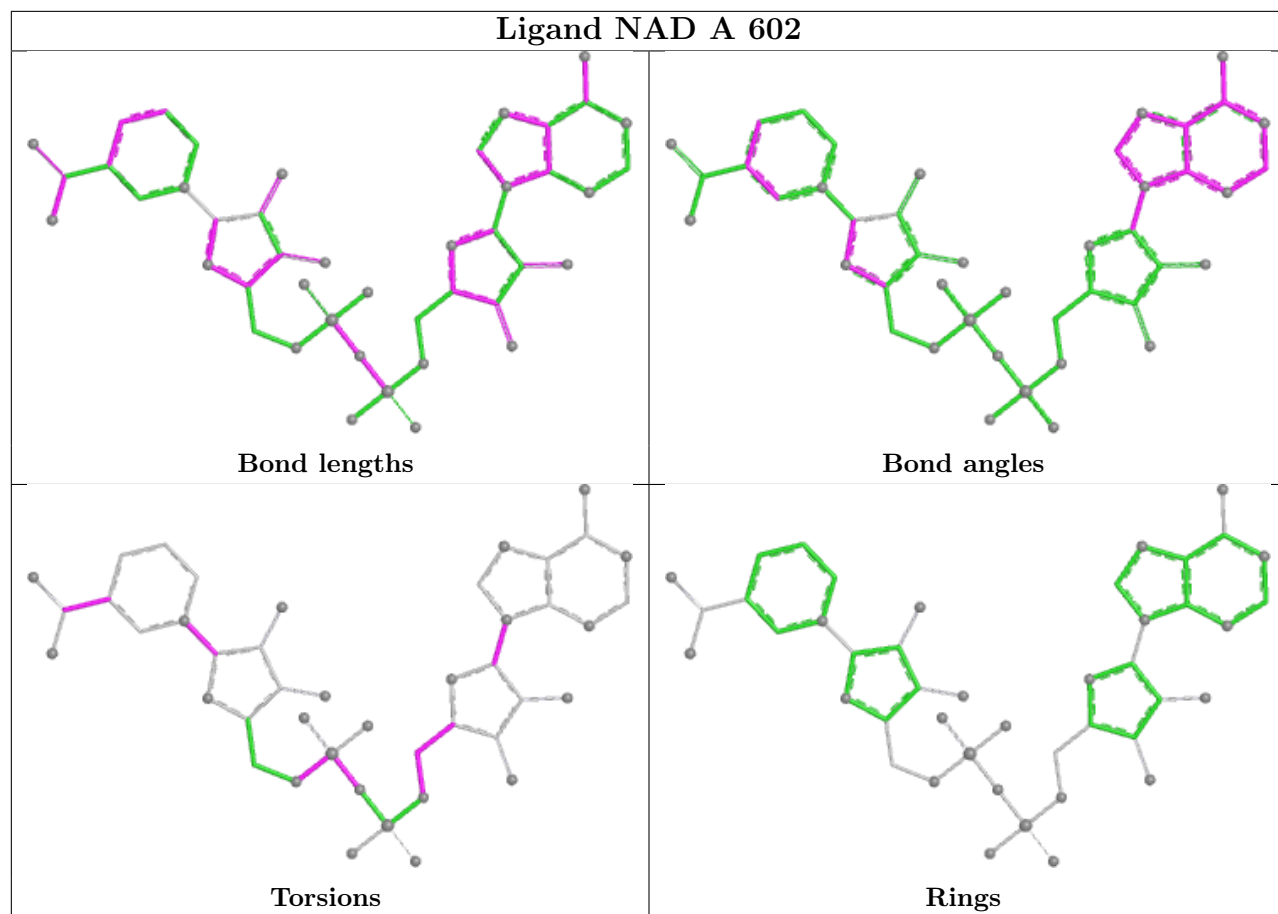


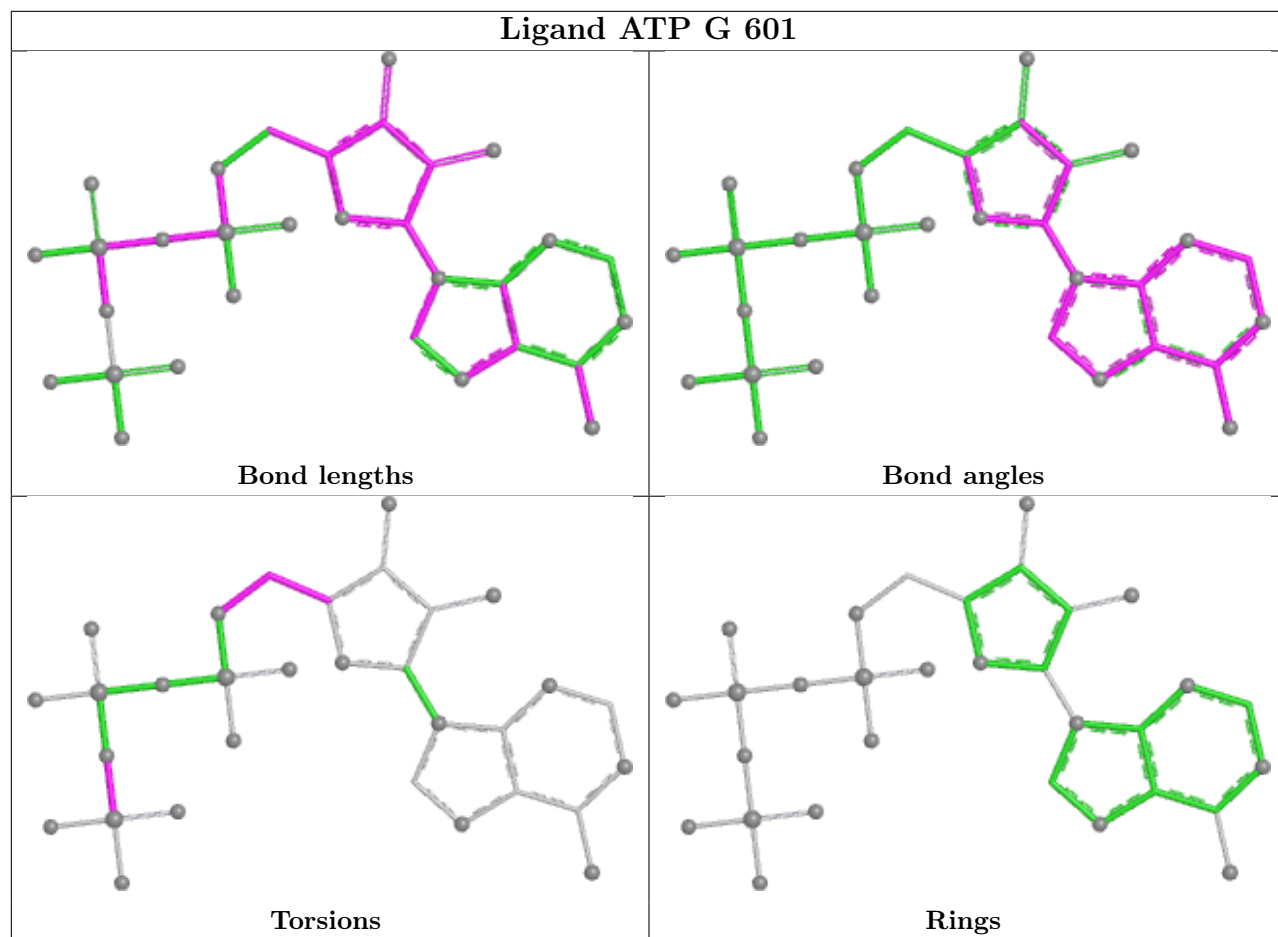


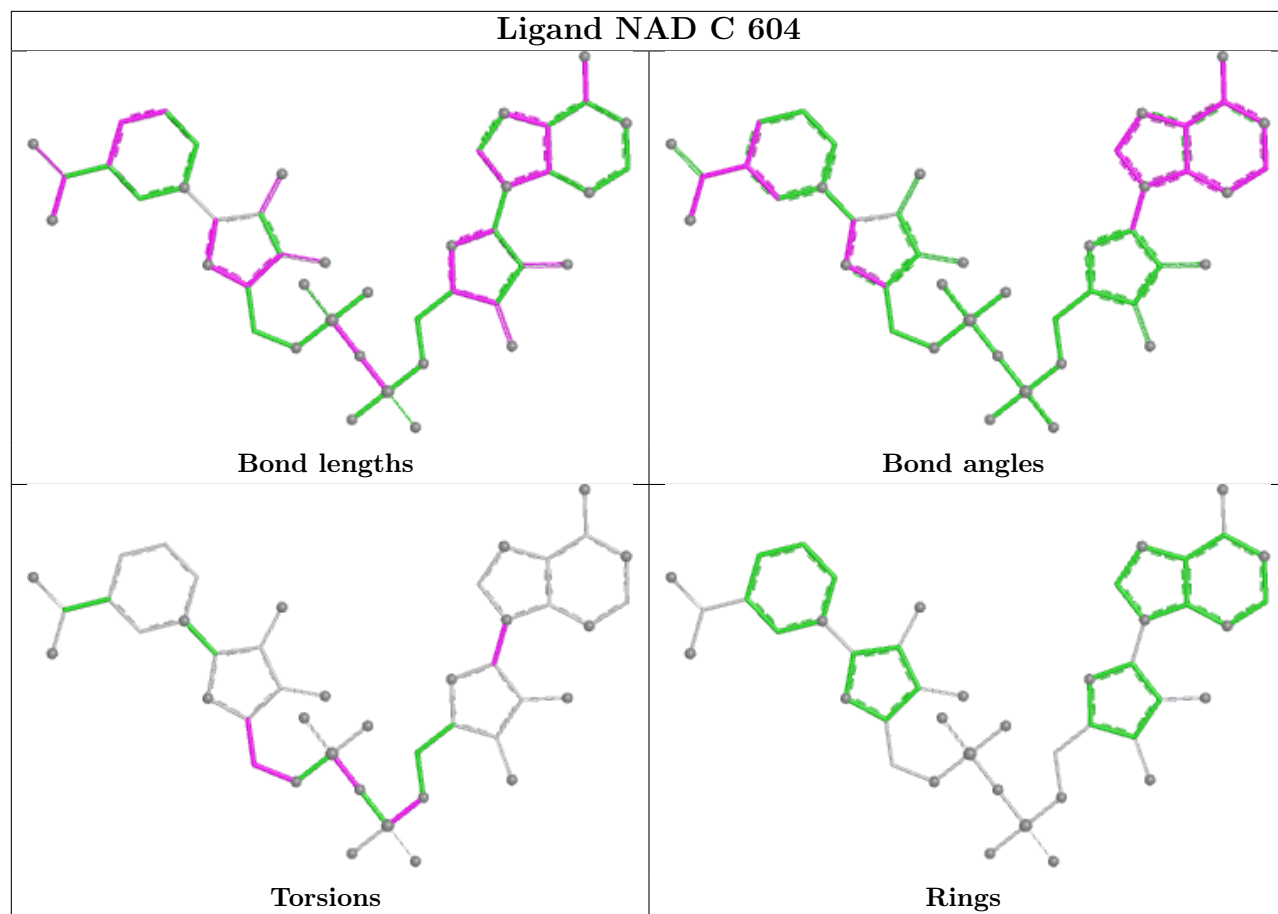


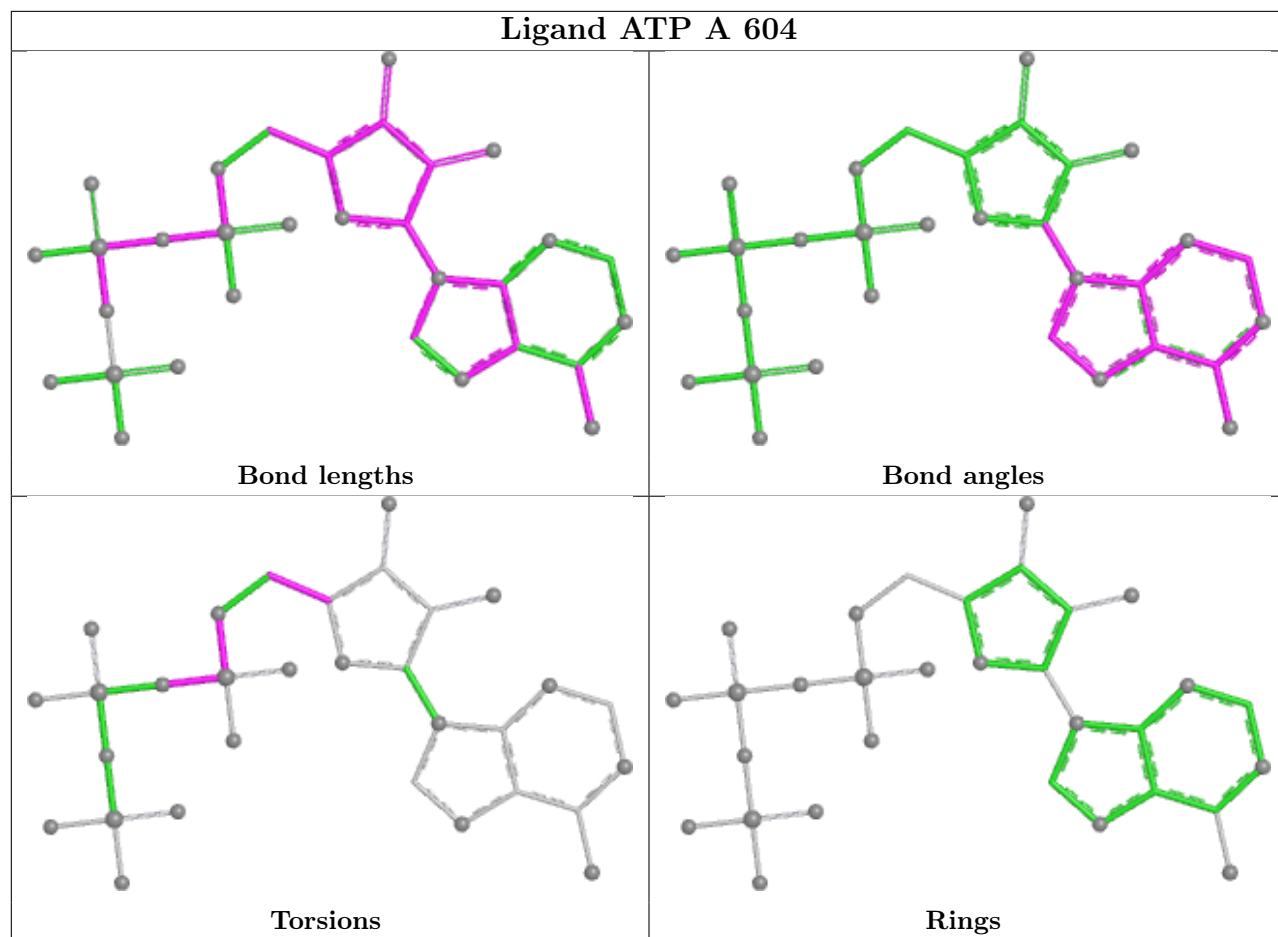


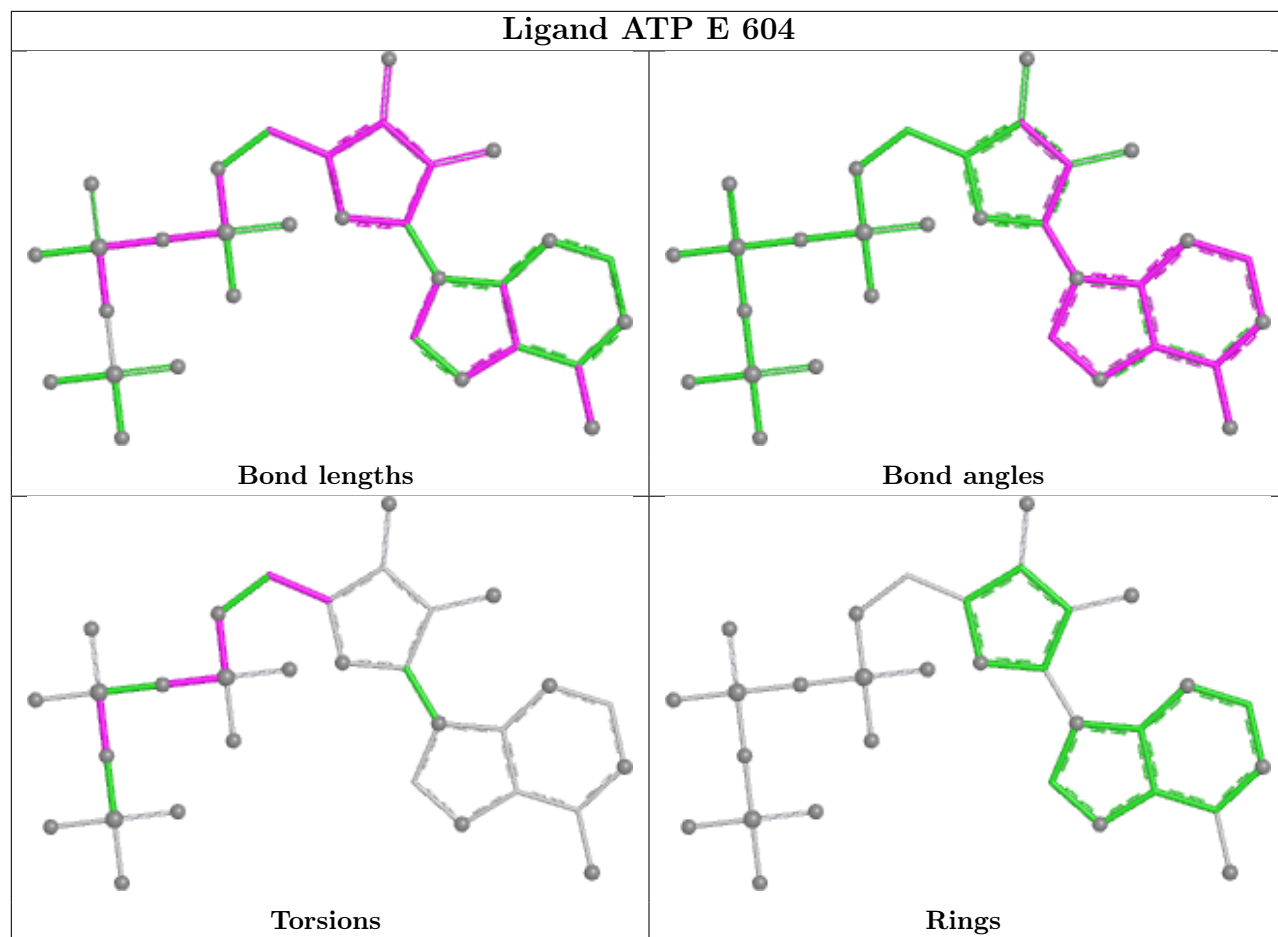




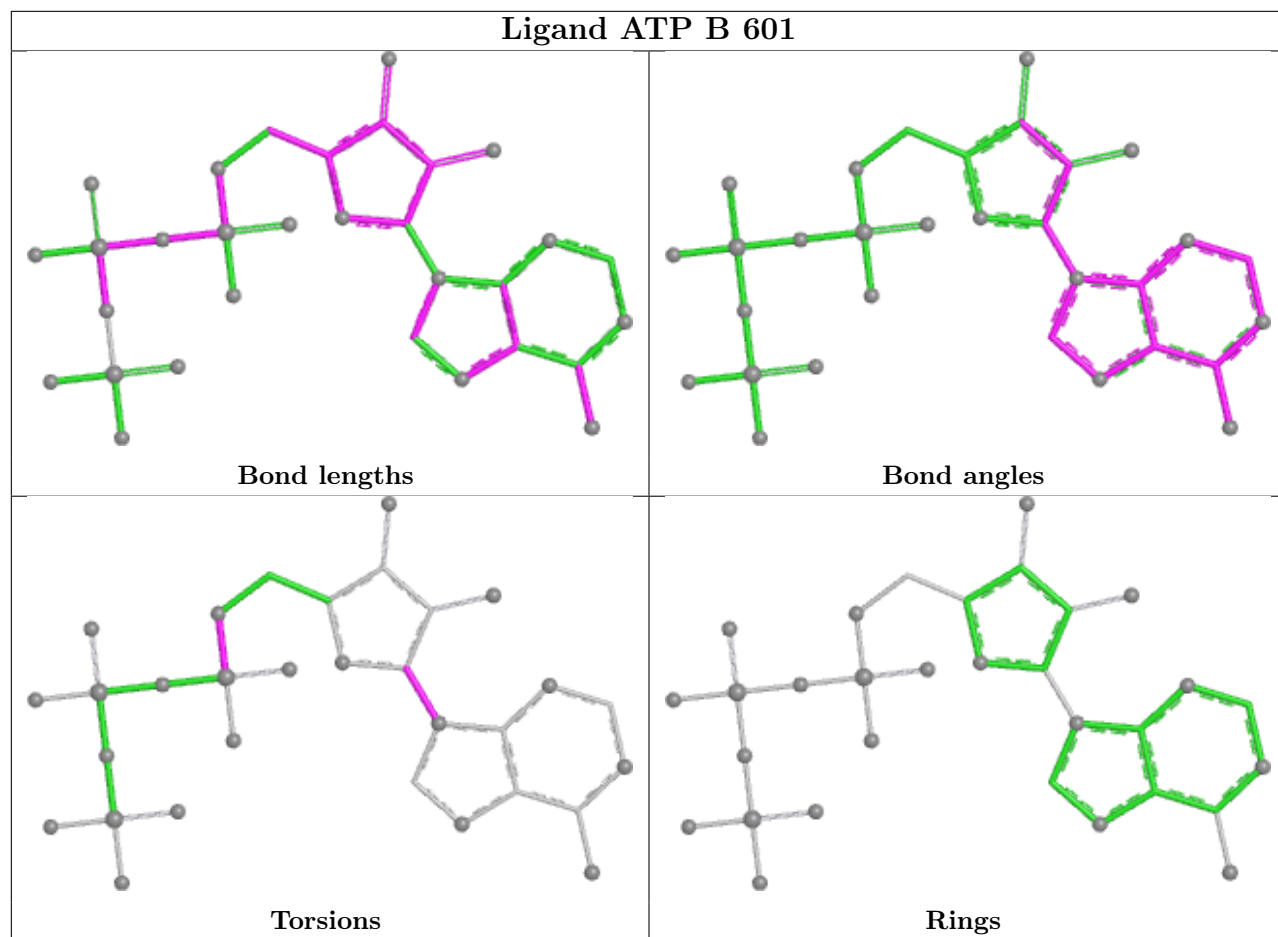




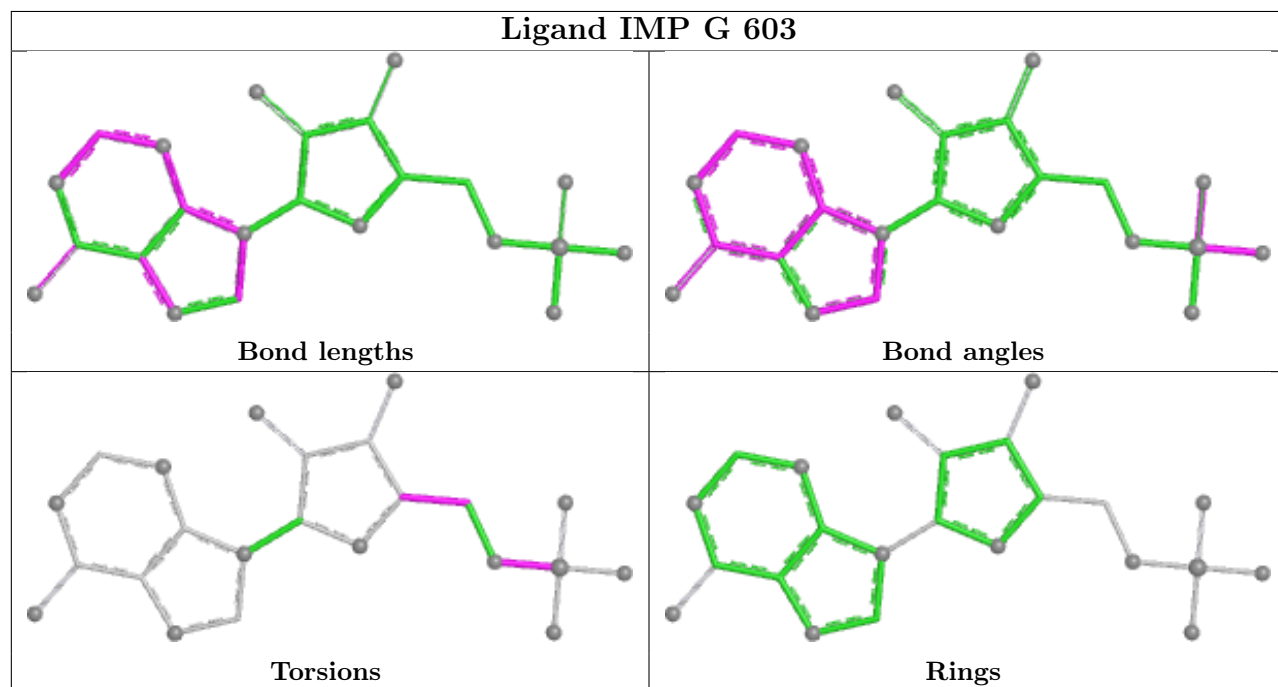


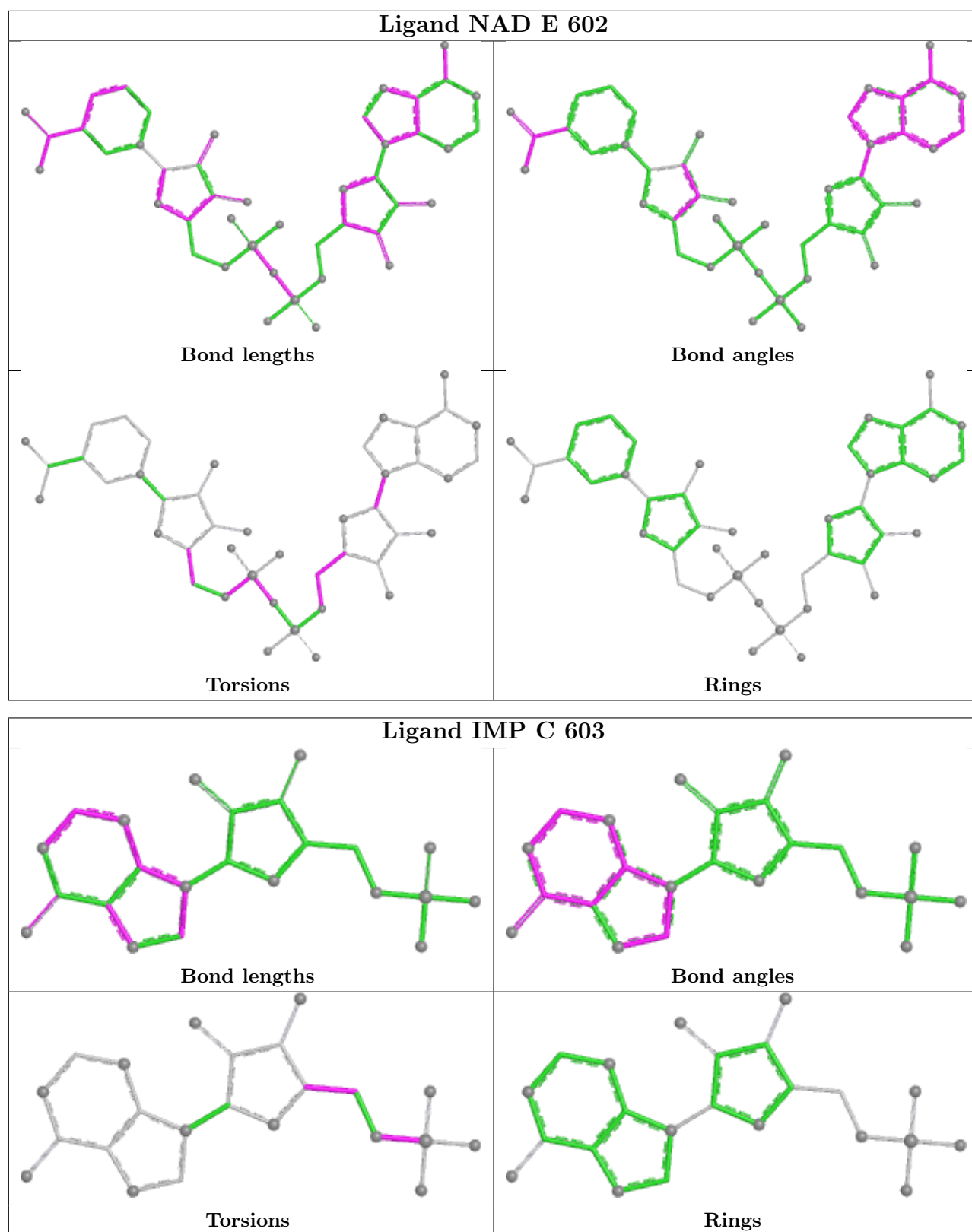


Ligand ATP B 601

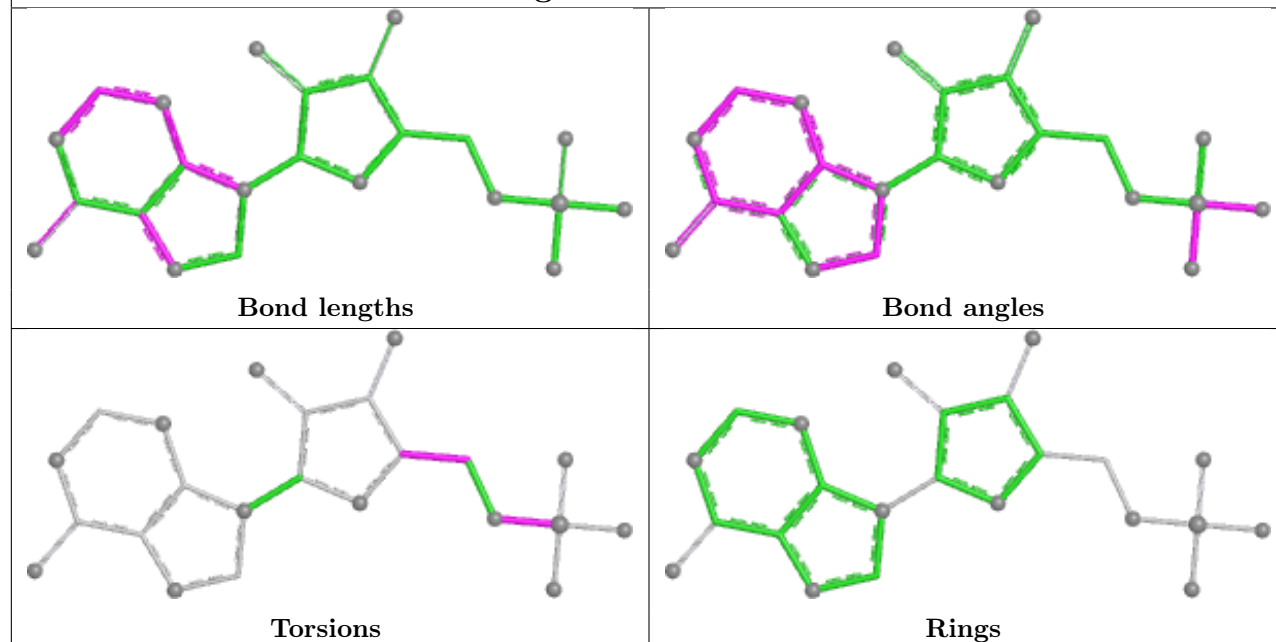


Ligand IMP G 603

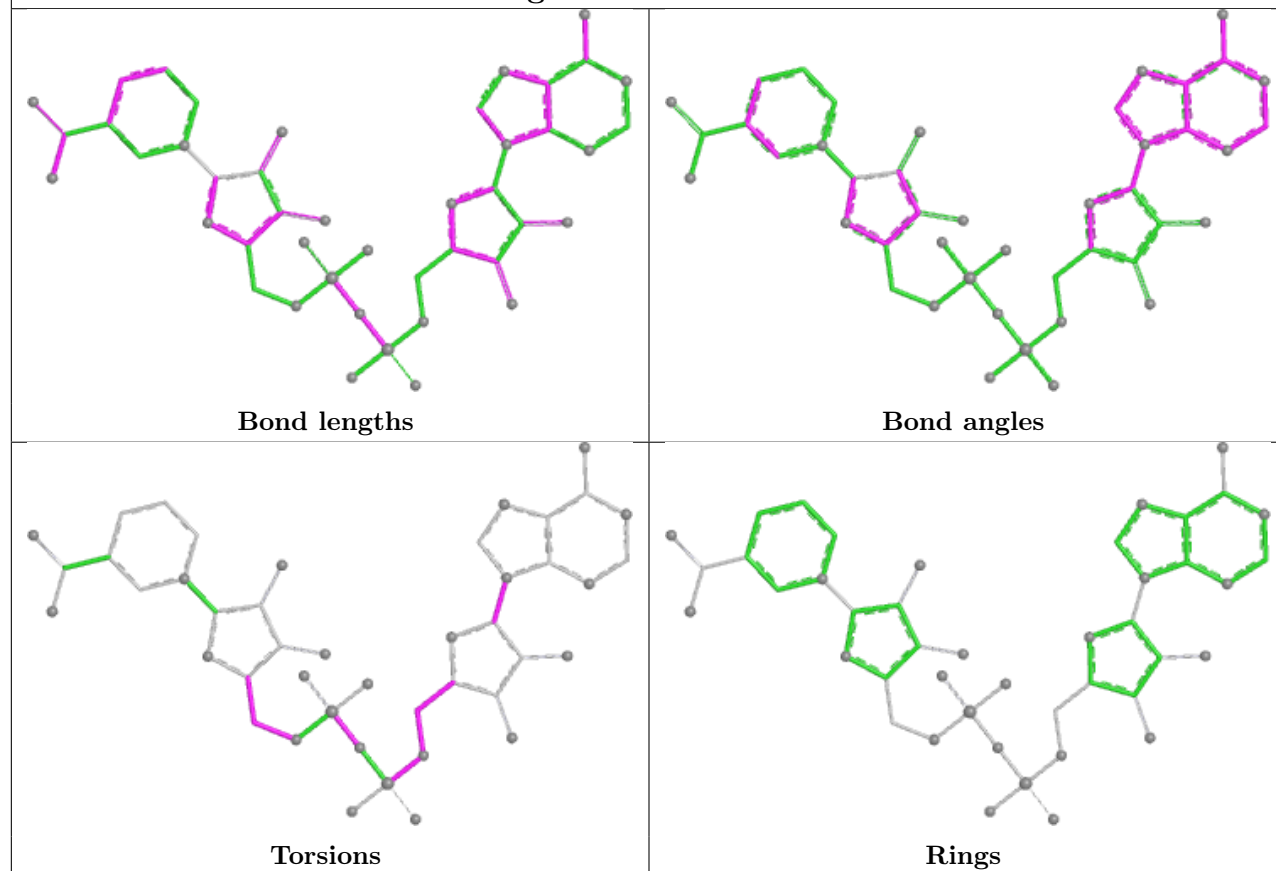


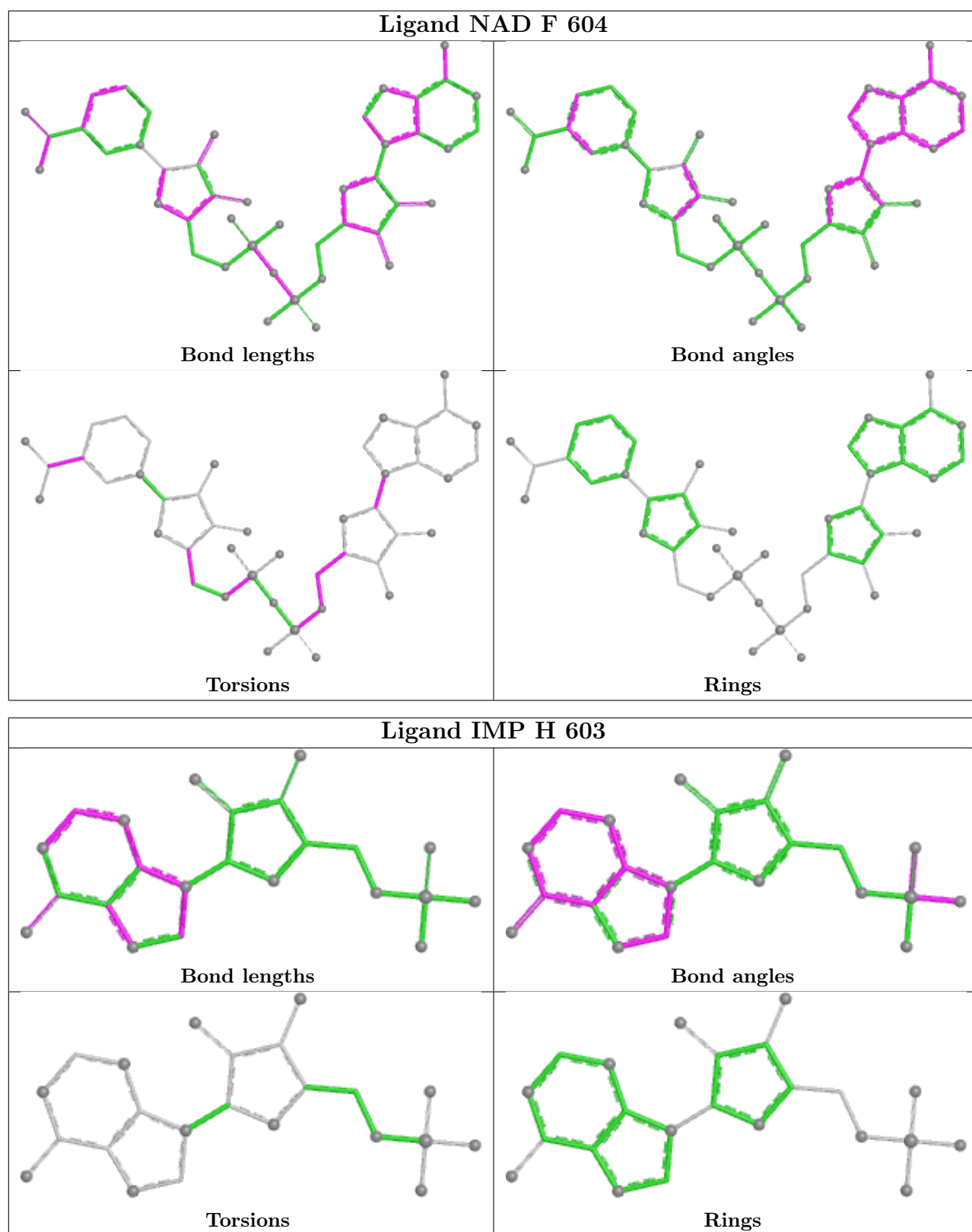


Ligand IMP E 601



Ligand NAD D 604





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

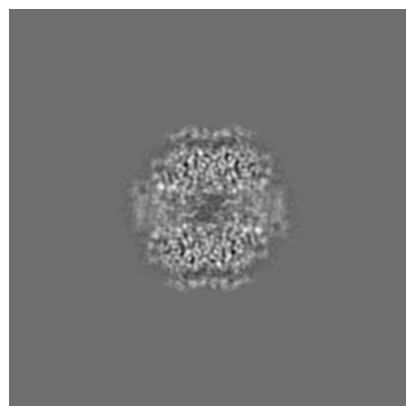
6 Map visualisation [i](#)

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

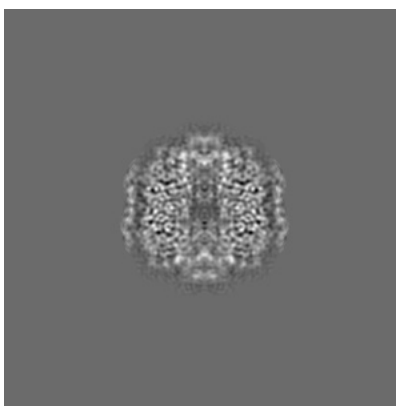
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

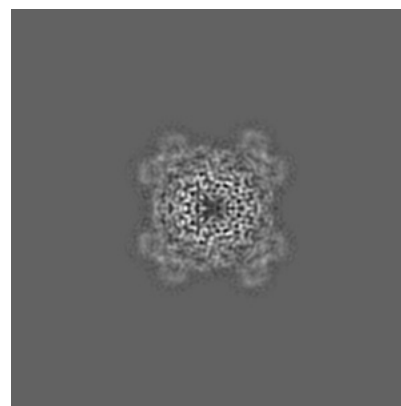
6.1.1 Primary map



X

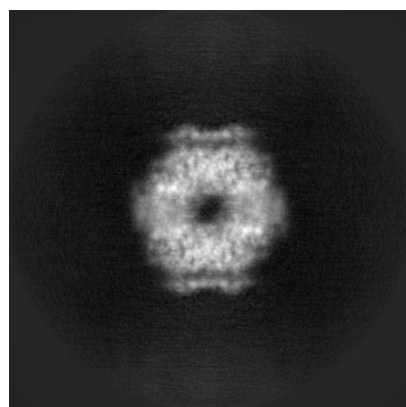


Y

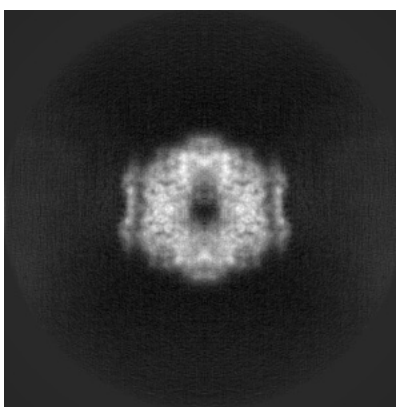


Z

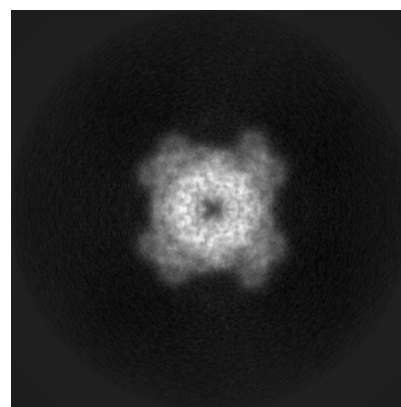
6.1.2 Raw map



X



Y

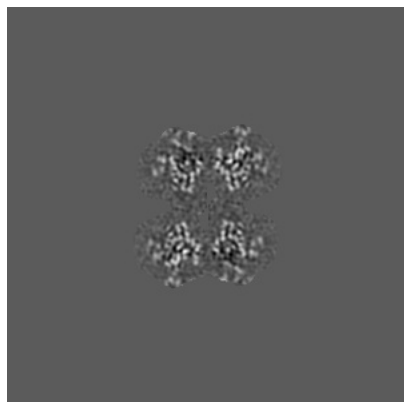


Z

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

6.2 Central slices [i](#)

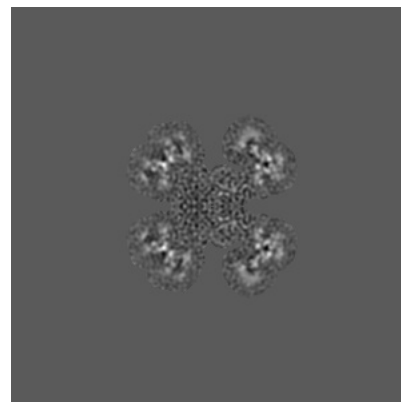
6.2.1 Primary map



X Index: 160

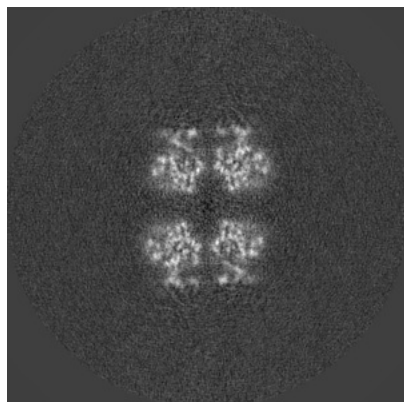


Y Index: 160

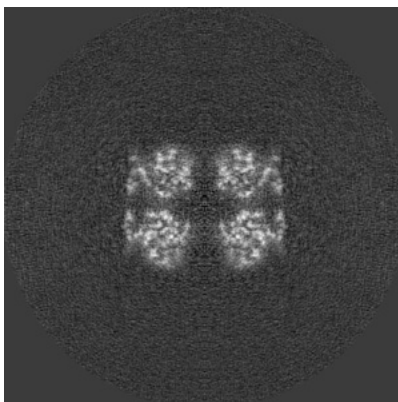


Z Index: 160

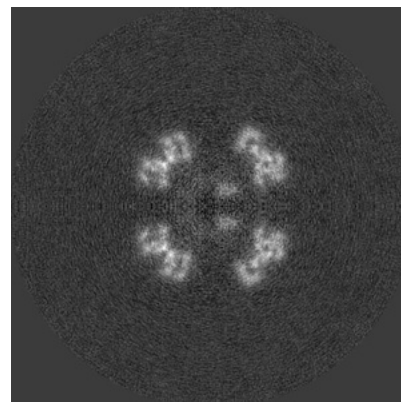
6.2.2 Raw map



X Index: 160



Y Index: 160

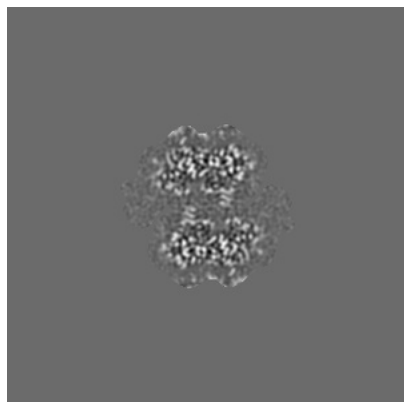


Z Index: 160

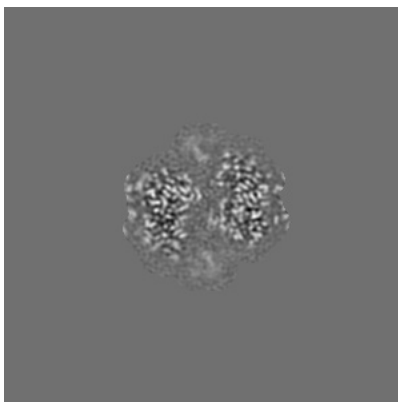
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

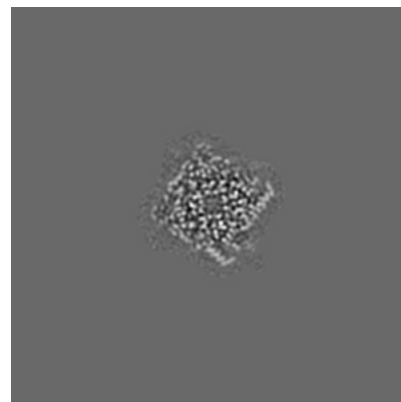
6.3.1 Primary map



X Index: 177

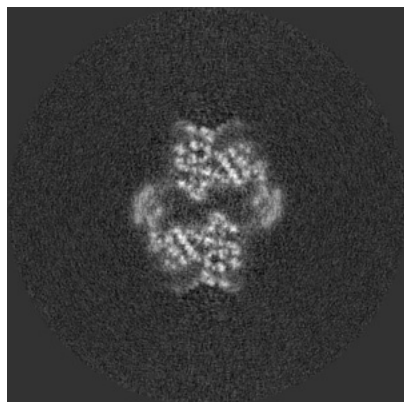


Y Index: 180

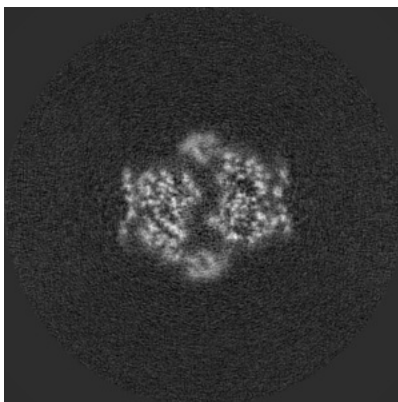


Z Index: 197

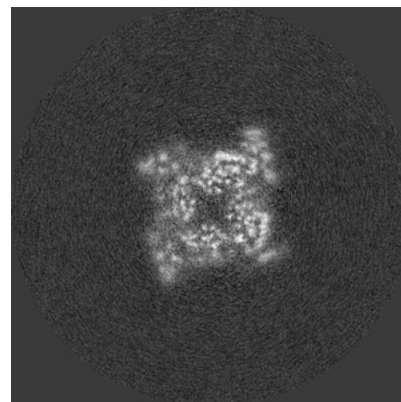
6.3.2 Raw map



X Index: 136



Y Index: 182

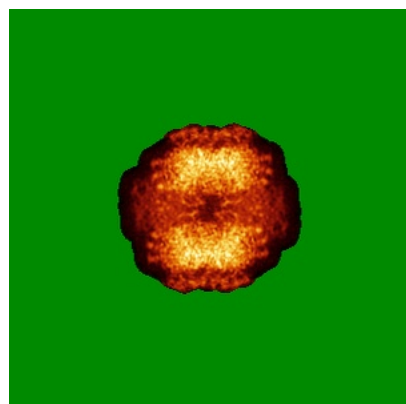


Z Index: 143

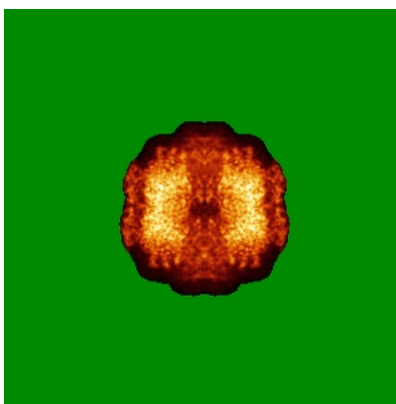
The images above show the largest variance slices of the map in three orthogonal directions.

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

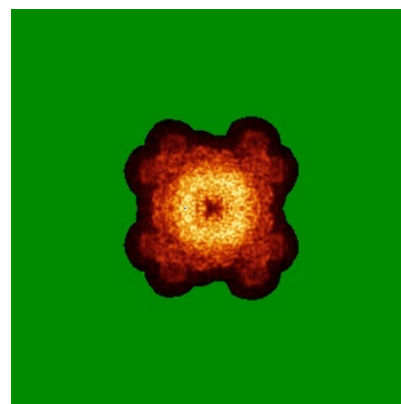
6.4.1 Primary map



X

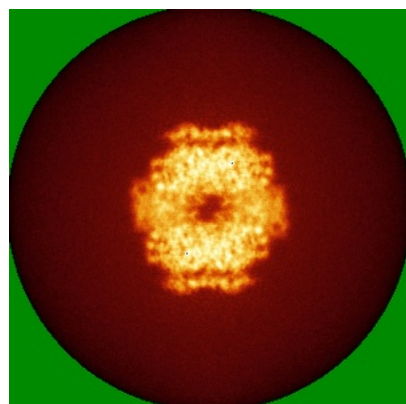


Y

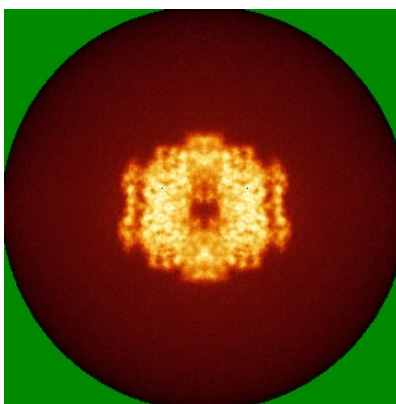


Z

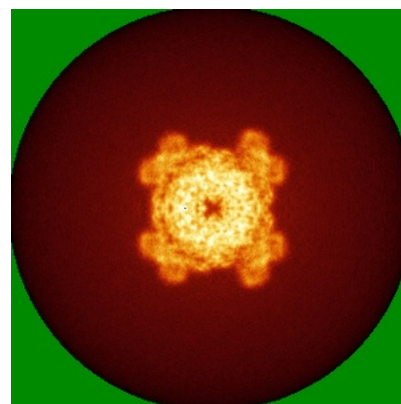
6.4.2 Raw map



X



Y

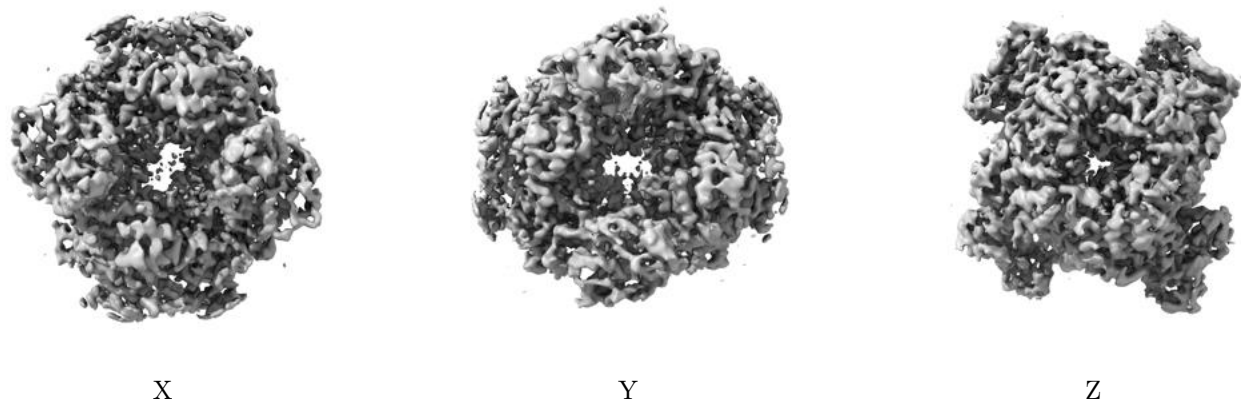


Z

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

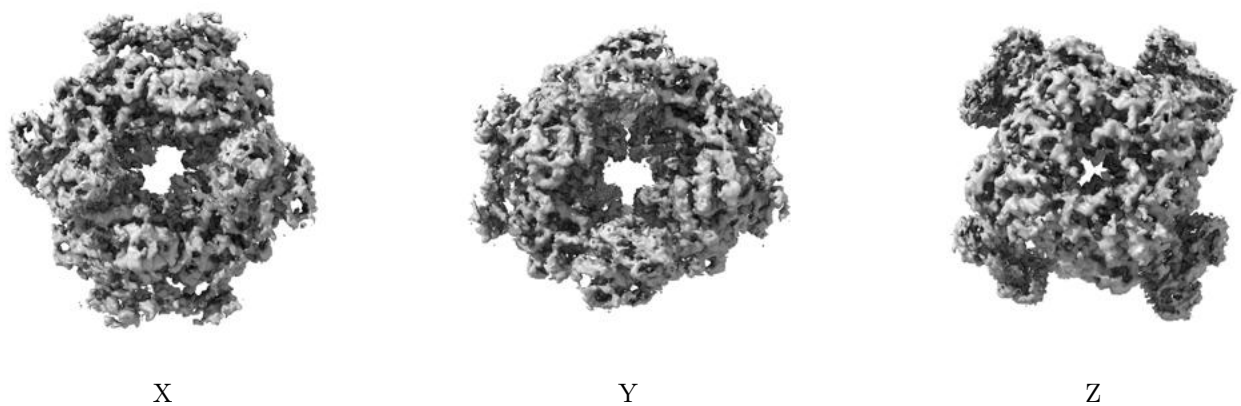
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 17.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

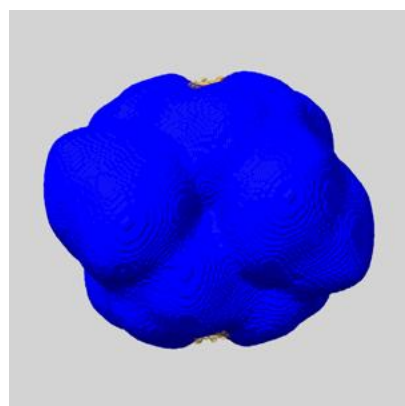
6.6 Mask visualisation [i](#)

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

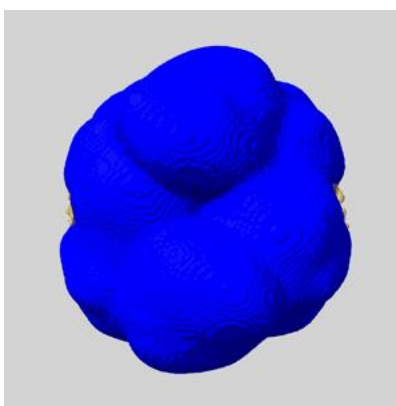
A mask typically either:

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

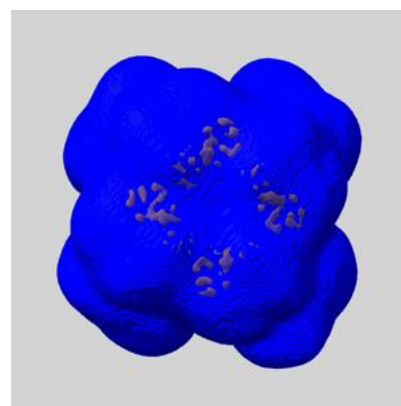
6.6.1 emd_20690_msk_1.map [i](#)



X



Y

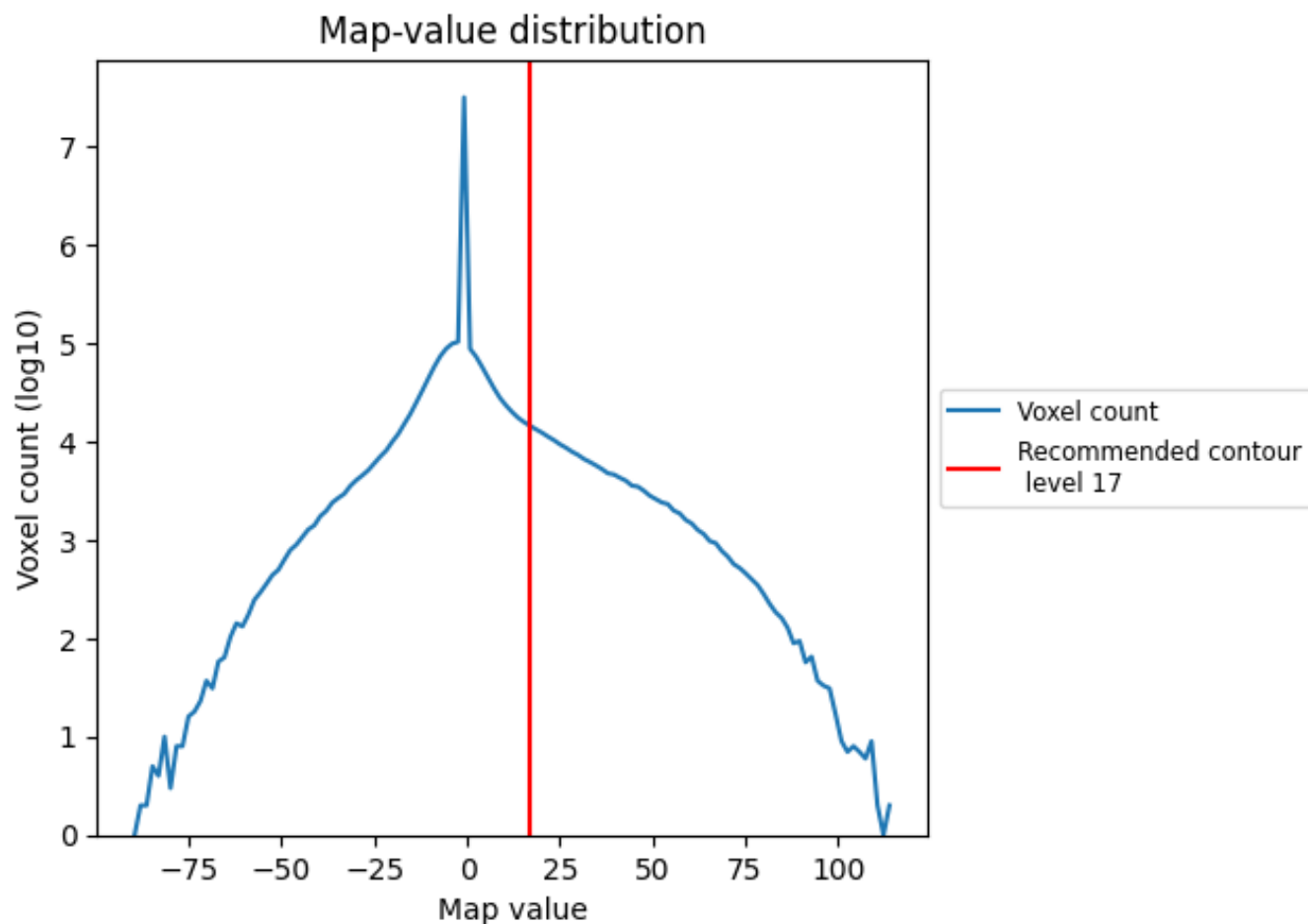


Z

7 Map analysis [i](#)

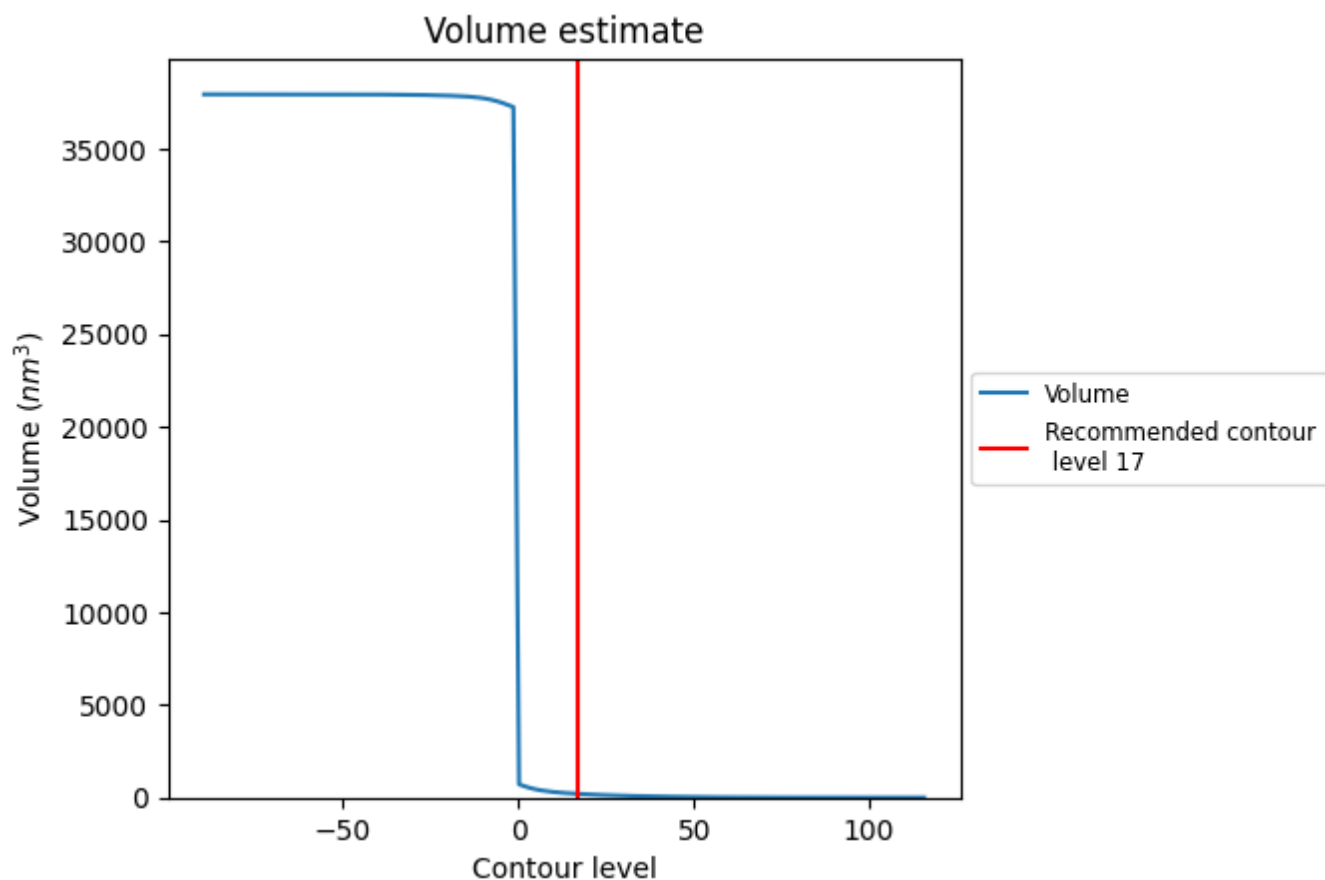
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

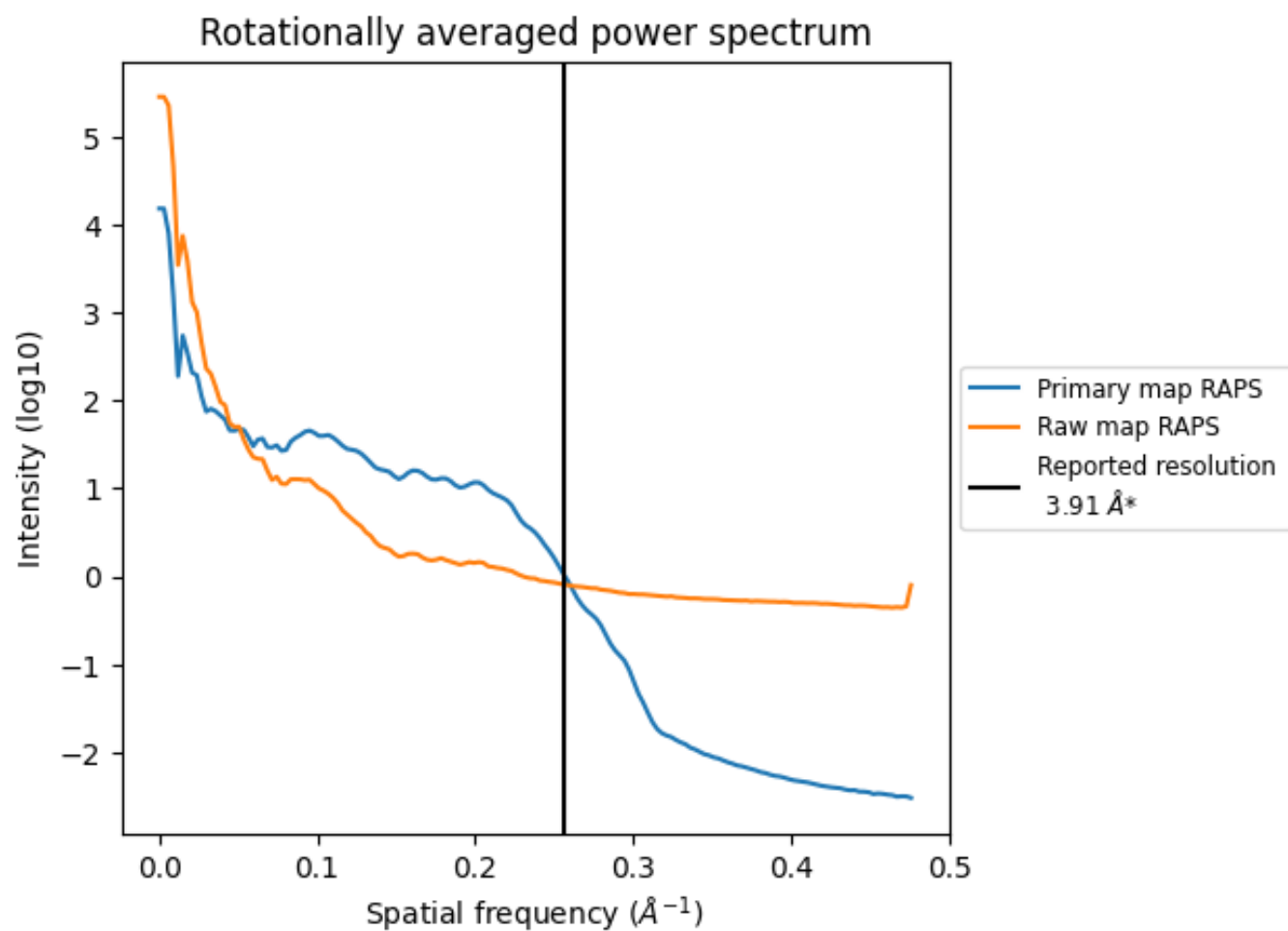
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

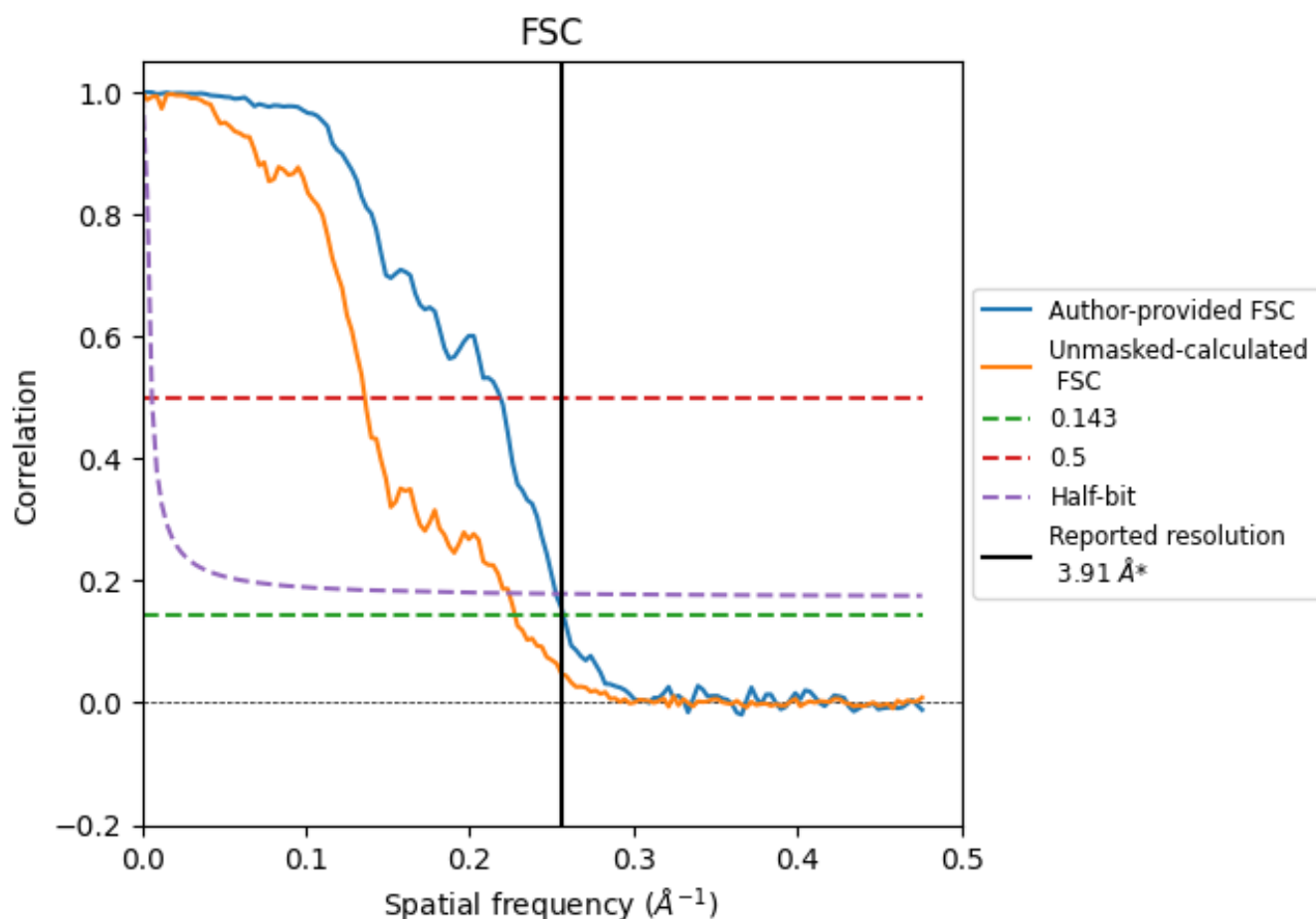


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

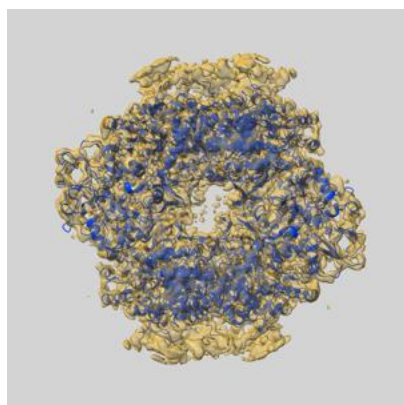
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.89	4.57	3.96
Unmasked-calculated*	4.39	7.36	4.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.39 differs from the reported value 3.91 by more than 10 %

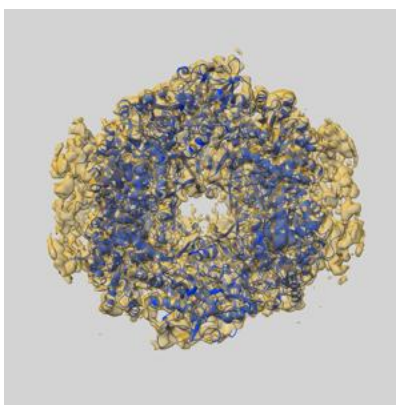
9 Map-model fit [i](#)

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

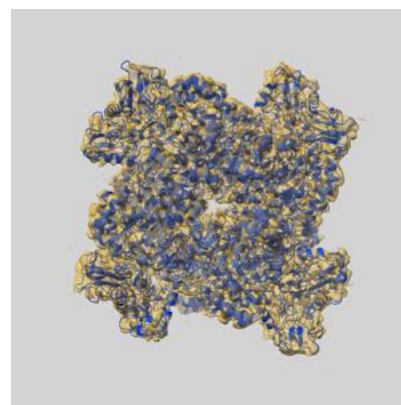
9.1 Map-model overlay [i](#)



X



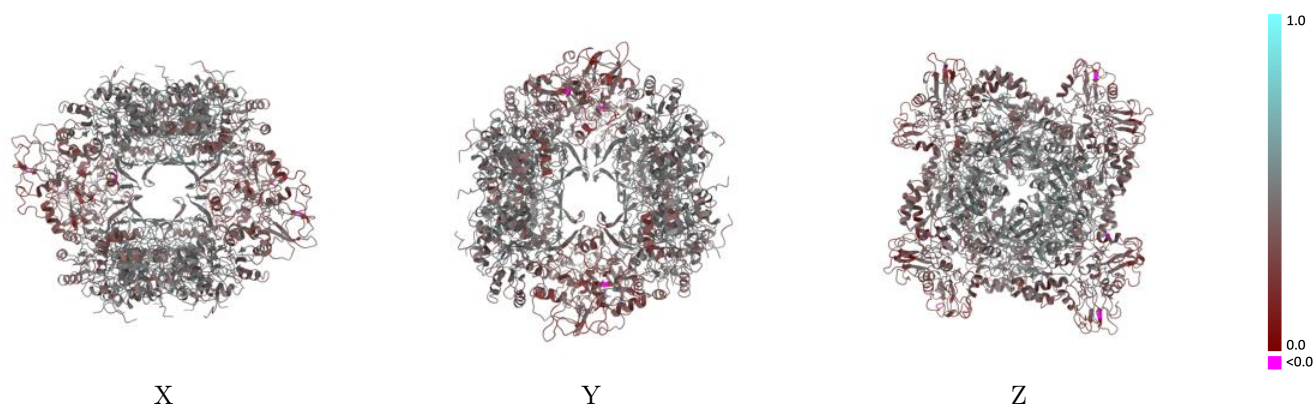
Y



Z

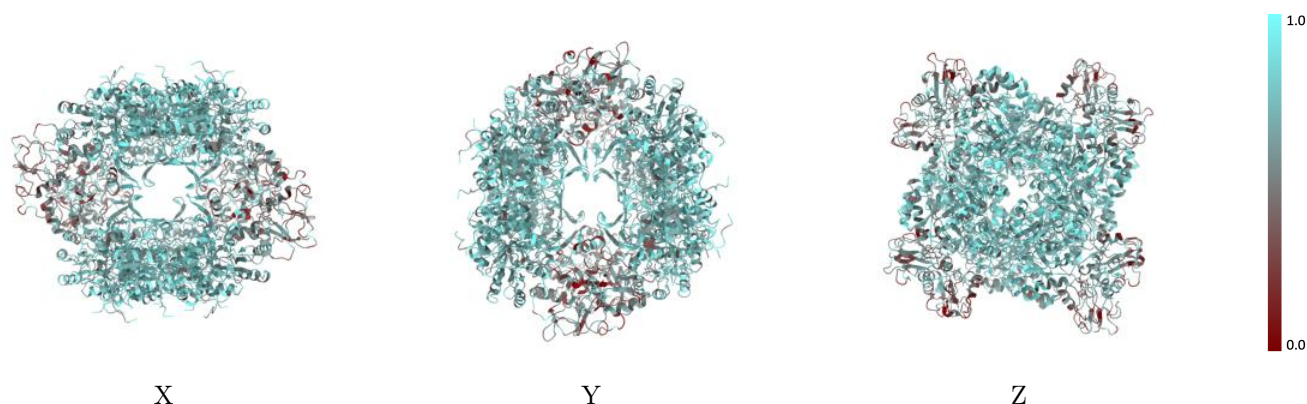
The images above show the 3D surface view of the map at the recommended contour level 17.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



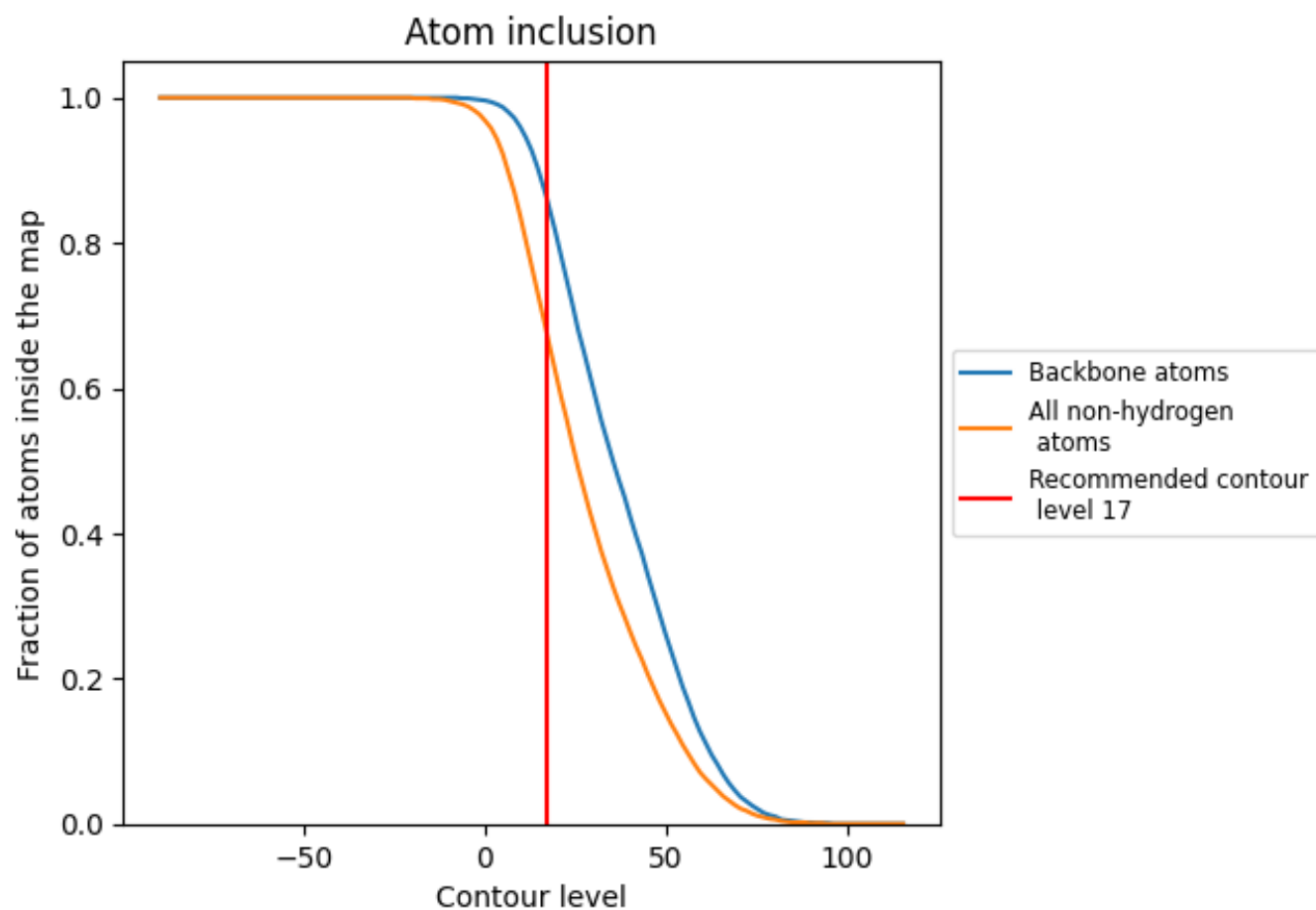
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (17) and Q-score for the entire model and for each chain.

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

