Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 01:26 PM EST

PDB ID	:	7RGM
EMDB ID	:	EMD-24452
Title	:	HUMAN RETINAL VARIANT IMPDH1(546) TREATED WITH ATP, IMP, NAD+, OCTAMER-CENTERED
Authors	:	Burrell, A.L.; Kollman, J.M.
Deposited on	:	2021-07-15
Resolution	:	2.80 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:

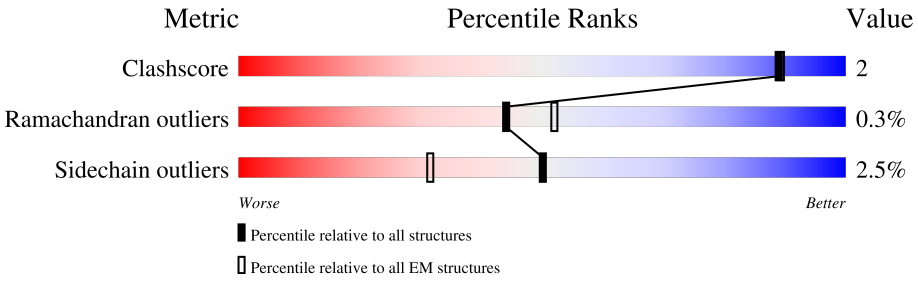
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	546	85% · 11%
1	B	546	84% 5% 11%
1	C	546	83% 5% 11%
1	D	546	81% 8% 11%
1	E	546	82% 7% 11%
1	F	546	82% 6% · 11%
1	G	546	81% 7% · 11%
1	H	546	83% 5% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 60416 atoms, of which 30224 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 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		
1	B	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		
1	C	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		
1	D	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		
1	E	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		
1	F	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		
1	G	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		
1	H	484	Total	C	H	N	O	S	0	0
			7362	2304	3717	624	693	24		

There are 296 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	510	THR	-	expression tag	UNP P20839
A	511	PHE	-	expression tag	UNP P20839
A	512	LEU	-	expression tag	UNP P20839
A	513	PRO	-	expression tag	UNP P20839
A	514	PHE	-	expression tag	UNP P20839
A	515	THR	-	expression tag	UNP P20839
A	516	LYS	-	expression tag	UNP P20839
A	517	SER	-	expression tag	UNP P20839
A	518	GLY	-	expression tag	UNP P20839
A	519	CYS	-	expression tag	UNP P20839
A	520	THR	-	expression tag	UNP P20839
A	521	GLU	-	expression tag	UNP P20839
A	522	ASP	-	expression tag	UNP P20839
A	523	SER	-	expression tag	UNP P20839

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Chain	Residue	Modelled	Actual	Comment	Reference
A	524	GLY	-	expression tag	UNP P20839
A	525	GLY	-	expression tag	UNP P20839
A	526	GLY	-	expression tag	UNP P20839
A	527	ARG	-	expression tag	UNP P20839
A	528	GLY	-	expression tag	UNP P20839
A	529	GLY	-	expression tag	UNP P20839
A	530	GLY	-	expression tag	UNP P20839
A	531	GLY	-	expression tag	UNP P20839
A	532	ASP	-	expression tag	UNP P20839
A	533	ALA	-	expression tag	UNP P20839
A	534	PRO	-	expression tag	UNP P20839
A	535	GLN	-	expression tag	UNP P20839
A	536	CYS	-	expression tag	UNP P20839
A	537	PRO	-	expression tag	UNP P20839
A	538	LEU	-	expression tag	UNP P20839
A	539	LEU	-	expression tag	UNP P20839
A	540	GLY	-	expression tag	UNP P20839
A	541	THR	-	expression tag	UNP P20839
A	542	ALA	-	expression tag	UNP P20839
A	543	SER	-	expression tag	UNP P20839
A	544	LEU	-	expression tag	UNP P20839
A	545	HIS	-	expression tag	UNP P20839
A	546	ASN	-	expression tag	UNP P20839
B	510	THR	-	expression tag	UNP P20839
B	511	PHE	-	expression tag	UNP P20839
B	512	LEU	-	expression tag	UNP P20839
B	513	PRO	-	expression tag	UNP P20839
B	514	PHE	-	expression tag	UNP P20839
B	515	THR	-	expression tag	UNP P20839
B	516	LYS	-	expression tag	UNP P20839
B	517	SER	-	expression tag	UNP P20839
B	518	GLY	-	expression tag	UNP P20839
B	519	CYS	-	expression tag	UNP P20839
B	520	THR	-	expression tag	UNP P20839
B	521	GLU	-	expression tag	UNP P20839
B	522	ASP	-	expression tag	UNP P20839
B	523	SER	-	expression tag	UNP P20839
B	524	GLY	-	expression tag	UNP P20839
B	525	GLY	-	expression tag	UNP P20839
B	526	GLY	-	expression tag	UNP P20839
B	527	ARG	-	expression tag	UNP P20839
B	528	GLY	-	expression tag	UNP P20839

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Chain	Residue	Modelled	Actual	Comment	Reference
B	529	GLY	-	expression tag	UNP P20839
B	530	GLY	-	expression tag	UNP P20839
B	531	GLY	-	expression tag	UNP P20839
B	532	ASP	-	expression tag	UNP P20839
B	533	ALA	-	expression tag	UNP P20839
B	534	PRO	-	expression tag	UNP P20839
B	535	GLN	-	expression tag	UNP P20839
B	536	CYS	-	expression tag	UNP P20839
B	537	PRO	-	expression tag	UNP P20839
B	538	LEU	-	expression tag	UNP P20839
B	539	LEU	-	expression tag	UNP P20839
B	540	GLY	-	expression tag	UNP P20839
B	541	THR	-	expression tag	UNP P20839
B	542	ALA	-	expression tag	UNP P20839
B	543	SER	-	expression tag	UNP P20839
B	544	LEU	-	expression tag	UNP P20839
B	545	HIS	-	expression tag	UNP P20839
B	546	ASN	-	expression tag	UNP P20839
C	510	THR	-	expression tag	UNP P20839
C	511	PHE	-	expression tag	UNP P20839
C	512	LEU	-	expression tag	UNP P20839
C	513	PRO	-	expression tag	UNP P20839
C	514	PHE	-	expression tag	UNP P20839
C	515	THR	-	expression tag	UNP P20839
C	516	LYS	-	expression tag	UNP P20839
C	517	SER	-	expression tag	UNP P20839
C	518	GLY	-	expression tag	UNP P20839
C	519	CYS	-	expression tag	UNP P20839
C	520	THR	-	expression tag	UNP P20839
C	521	GLU	-	expression tag	UNP P20839
C	522	ASP	-	expression tag	UNP P20839
C	523	SER	-	expression tag	UNP P20839
C	524	GLY	-	expression tag	UNP P20839
C	525	GLY	-	expression tag	UNP P20839
C	526	GLY	-	expression tag	UNP P20839
C	527	ARG	-	expression tag	UNP P20839
C	528	GLY	-	expression tag	UNP P20839
C	529	GLY	-	expression tag	UNP P20839
C	530	GLY	-	expression tag	UNP P20839
C	531	GLY	-	expression tag	UNP P20839
C	532	ASP	-	expression tag	UNP P20839
C	533	ALA	-	expression tag	UNP P20839

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Chain	Residue	Modelled	Actual	Comment	Reference
C	534	PRO	-	expression tag	UNP P20839
C	535	GLN	-	expression tag	UNP P20839
C	536	CYS	-	expression tag	UNP P20839
C	537	PRO	-	expression tag	UNP P20839
C	538	LEU	-	expression tag	UNP P20839
C	539	LEU	-	expression tag	UNP P20839
C	540	GLY	-	expression tag	UNP P20839
C	541	THR	-	expression tag	UNP P20839
C	542	ALA	-	expression tag	UNP P20839
C	543	SER	-	expression tag	UNP P20839
C	544	LEU	-	expression tag	UNP P20839
C	545	HIS	-	expression tag	UNP P20839
C	546	ASN	-	expression tag	UNP P20839
D	510	THR	-	expression tag	UNP P20839
D	511	PHE	-	expression tag	UNP P20839
D	512	LEU	-	expression tag	UNP P20839
D	513	PRO	-	expression tag	UNP P20839
D	514	PHE	-	expression tag	UNP P20839
D	515	THR	-	expression tag	UNP P20839
D	516	LYS	-	expression tag	UNP P20839
D	517	SER	-	expression tag	UNP P20839
D	518	GLY	-	expression tag	UNP P20839
D	519	CYS	-	expression tag	UNP P20839
D	520	THR	-	expression tag	UNP P20839
D	521	GLU	-	expression tag	UNP P20839
D	522	ASP	-	expression tag	UNP P20839
D	523	SER	-	expression tag	UNP P20839
D	524	GLY	-	expression tag	UNP P20839
D	525	GLY	-	expression tag	UNP P20839
D	526	GLY	-	expression tag	UNP P20839
D	527	ARG	-	expression tag	UNP P20839
D	528	GLY	-	expression tag	UNP P20839
D	529	GLY	-	expression tag	UNP P20839
D	530	GLY	-	expression tag	UNP P20839
D	531	GLY	-	expression tag	UNP P20839
D	532	ASP	-	expression tag	UNP P20839
D	533	ALA	-	expression tag	UNP P20839
D	534	PRO	-	expression tag	UNP P20839
D	535	GLN	-	expression tag	UNP P20839
D	536	CYS	-	expression tag	UNP P20839
D	537	PRO	-	expression tag	UNP P20839
D	538	LEU	-	expression tag	UNP P20839

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Chain	Residue	Modelled	Actual	Comment	Reference
D	539	LEU	-	expression tag	UNP P20839
D	540	GLY	-	expression tag	UNP P20839
D	541	THR	-	expression tag	UNP P20839
D	542	ALA	-	expression tag	UNP P20839
D	543	SER	-	expression tag	UNP P20839
D	544	LEU	-	expression tag	UNP P20839
D	545	HIS	-	expression tag	UNP P20839
D	546	ASN	-	expression tag	UNP P20839
E	510	THR	-	expression tag	UNP P20839
E	511	PHE	-	expression tag	UNP P20839
E	512	LEU	-	expression tag	UNP P20839
E	513	PRO	-	expression tag	UNP P20839
E	514	PHE	-	expression tag	UNP P20839
E	515	THR	-	expression tag	UNP P20839
E	516	LYS	-	expression tag	UNP P20839
E	517	SER	-	expression tag	UNP P20839
E	518	GLY	-	expression tag	UNP P20839
E	519	CYS	-	expression tag	UNP P20839
E	520	THR	-	expression tag	UNP P20839
E	521	GLU	-	expression tag	UNP P20839
E	522	ASP	-	expression tag	UNP P20839
E	523	SER	-	expression tag	UNP P20839
E	524	GLY	-	expression tag	UNP P20839
E	525	GLY	-	expression tag	UNP P20839
E	526	GLY	-	expression tag	UNP P20839
E	527	ARG	-	expression tag	UNP P20839
E	528	GLY	-	expression tag	UNP P20839
E	529	GLY	-	expression tag	UNP P20839
E	530	GLY	-	expression tag	UNP P20839
E	531	GLY	-	expression tag	UNP P20839
E	532	ASP	-	expression tag	UNP P20839
E	533	ALA	-	expression tag	UNP P20839
E	534	PRO	-	expression tag	UNP P20839
E	535	GLN	-	expression tag	UNP P20839
E	536	CYS	-	expression tag	UNP P20839
E	537	PRO	-	expression tag	UNP P20839
E	538	LEU	-	expression tag	UNP P20839
E	539	LEU	-	expression tag	UNP P20839
E	540	GLY	-	expression tag	UNP P20839
E	541	THR	-	expression tag	UNP P20839
E	542	ALA	-	expression tag	UNP P20839
E	543	SER	-	expression tag	UNP P20839

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Chain	Residue	Modelled	Actual	Comment	Reference
E	544	LEU	-	expression tag	UNP P20839
E	545	HIS	-	expression tag	UNP P20839
E	546	ASN	-	expression tag	UNP P20839
F	510	THR	-	expression tag	UNP P20839
F	511	PHE	-	expression tag	UNP P20839
F	512	LEU	-	expression tag	UNP P20839
F	513	PRO	-	expression tag	UNP P20839
F	514	PHE	-	expression tag	UNP P20839
F	515	THR	-	expression tag	UNP P20839
F	516	LYS	-	expression tag	UNP P20839
F	517	SER	-	expression tag	UNP P20839
F	518	GLY	-	expression tag	UNP P20839
F	519	CYS	-	expression tag	UNP P20839
F	520	THR	-	expression tag	UNP P20839
F	521	GLU	-	expression tag	UNP P20839
F	522	ASP	-	expression tag	UNP P20839
F	523	SER	-	expression tag	UNP P20839
F	524	GLY	-	expression tag	UNP P20839
F	525	GLY	-	expression tag	UNP P20839
F	526	GLY	-	expression tag	UNP P20839
F	527	ARG	-	expression tag	UNP P20839
F	528	GLY	-	expression tag	UNP P20839
F	529	GLY	-	expression tag	UNP P20839
F	530	GLY	-	expression tag	UNP P20839
F	531	GLY	-	expression tag	UNP P20839
F	532	ASP	-	expression tag	UNP P20839
F	533	ALA	-	expression tag	UNP P20839
F	534	PRO	-	expression tag	UNP P20839
F	535	GLN	-	expression tag	UNP P20839
F	536	CYS	-	expression tag	UNP P20839
F	537	PRO	-	expression tag	UNP P20839
F	538	LEU	-	expression tag	UNP P20839
F	539	LEU	-	expression tag	UNP P20839
F	540	GLY	-	expression tag	UNP P20839
F	541	THR	-	expression tag	UNP P20839
F	542	ALA	-	expression tag	UNP P20839
F	543	SER	-	expression tag	UNP P20839
F	544	LEU	-	expression tag	UNP P20839
F	545	HIS	-	expression tag	UNP P20839
F	546	ASN	-	expression tag	UNP P20839
G	510	THR	-	expression tag	UNP P20839
G	511	PHE	-	expression tag	UNP P20839

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Chain	Residue	Modelled	Actual	Comment	Reference
G	512	LEU	-	expression tag	UNP P20839
G	513	PRO	-	expression tag	UNP P20839
G	514	PHE	-	expression tag	UNP P20839
G	515	THR	-	expression tag	UNP P20839
G	516	LYS	-	expression tag	UNP P20839
G	517	SER	-	expression tag	UNP P20839
G	518	GLY	-	expression tag	UNP P20839
G	519	CYS	-	expression tag	UNP P20839
G	520	THR	-	expression tag	UNP P20839
G	521	GLU	-	expression tag	UNP P20839
G	522	ASP	-	expression tag	UNP P20839
G	523	SER	-	expression tag	UNP P20839
G	524	GLY	-	expression tag	UNP P20839
G	525	GLY	-	expression tag	UNP P20839
G	526	GLY	-	expression tag	UNP P20839
G	527	ARG	-	expression tag	UNP P20839
G	528	GLY	-	expression tag	UNP P20839
G	529	GLY	-	expression tag	UNP P20839
G	530	GLY	-	expression tag	UNP P20839
G	531	GLY	-	expression tag	UNP P20839
G	532	ASP	-	expression tag	UNP P20839
G	533	ALA	-	expression tag	UNP P20839
G	534	PRO	-	expression tag	UNP P20839
G	535	GLN	-	expression tag	UNP P20839
G	536	CYS	-	expression tag	UNP P20839
G	537	PRO	-	expression tag	UNP P20839
G	538	LEU	-	expression tag	UNP P20839
G	539	LEU	-	expression tag	UNP P20839
G	540	GLY	-	expression tag	UNP P20839
G	541	THR	-	expression tag	UNP P20839
G	542	ALA	-	expression tag	UNP P20839
G	543	SER	-	expression tag	UNP P20839
G	544	LEU	-	expression tag	UNP P20839
G	545	HIS	-	expression tag	UNP P20839
G	546	ASN	-	expression tag	UNP P20839
H	510	THR	-	expression tag	UNP P20839
H	511	PHE	-	expression tag	UNP P20839
H	512	LEU	-	expression tag	UNP P20839
H	513	PRO	-	expression tag	UNP P20839
H	514	PHE	-	expression tag	UNP P20839
H	515	THR	-	expression tag	UNP P20839
H	516	LYS	-	expression tag	UNP P20839

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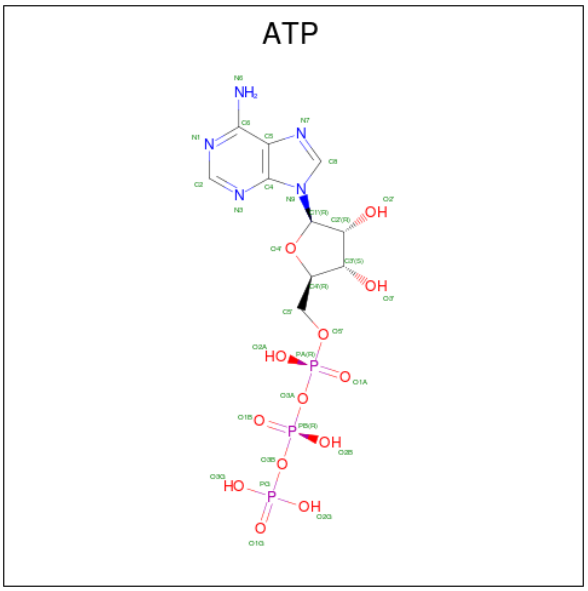
Chain	Residue	Modelled	Actual	Comment	Reference
H	517	SER	-	expression tag	UNP P20839
H	518	GLY	-	expression tag	UNP P20839
H	519	CYS	-	expression tag	UNP P20839
H	520	THR	-	expression tag	UNP P20839
H	521	GLU	-	expression tag	UNP P20839
H	522	ASP	-	expression tag	UNP P20839
H	523	SER	-	expression tag	UNP P20839
H	524	GLY	-	expression tag	UNP P20839
H	525	GLY	-	expression tag	UNP P20839
H	526	GLY	-	expression tag	UNP P20839
H	527	ARG	-	expression tag	UNP P20839
H	528	GLY	-	expression tag	UNP P20839
H	529	GLY	-	expression tag	UNP P20839
H	530	GLY	-	expression tag	UNP P20839
H	531	GLY	-	expression tag	UNP P20839
H	532	ASP	-	expression tag	UNP P20839
H	533	ALA	-	expression tag	UNP P20839
H	534	PRO	-	expression tag	UNP P20839
H	535	GLN	-	expression tag	UNP P20839
H	536	CYS	-	expression tag	UNP P20839
H	537	PRO	-	expression tag	UNP P20839
H	538	LEU	-	expression tag	UNP P20839
H	539	LEU	-	expression tag	UNP P20839
H	540	GLY	-	expression tag	UNP P20839
H	541	THR	-	expression tag	UNP P20839
H	542	ALA	-	expression tag	UNP P20839
H	543	SER	-	expression tag	UNP P20839
H	544	LEU	-	expression tag	UNP P20839
H	545	HIS	-	expression tag	UNP P20839
H	546	ASN	-	expression tag	UNP P20839

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	A	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	B	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	B	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	C	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	C	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	D	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	D	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	E	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	E	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	F	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	F	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	G	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	G	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	

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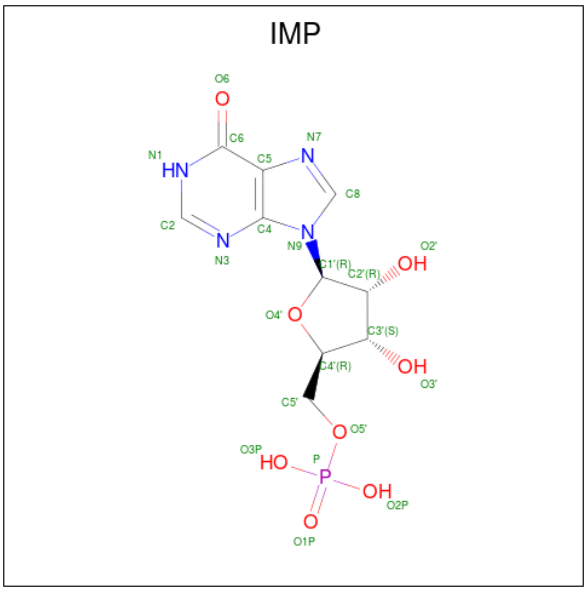
Mol	Chain	Residues	Atoms						AltConf
2	H	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	
2	H	1	Total	C	H	N	O	P	0
			86	20	24	10	26	6	

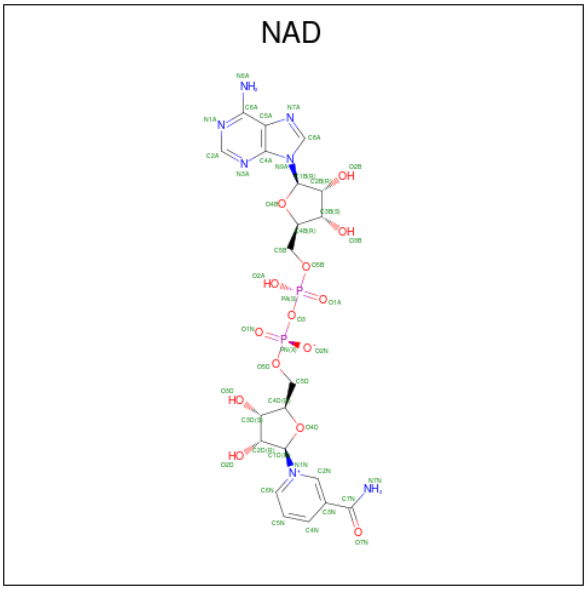
- Molecule 3 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD)

(formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



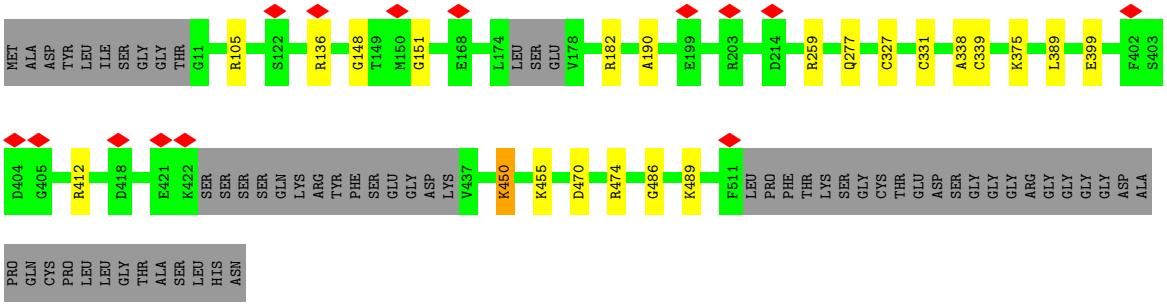
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
4	B	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
4	C	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
4	D	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
4	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
4	F	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2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

3 Residue-property plots (i)

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.

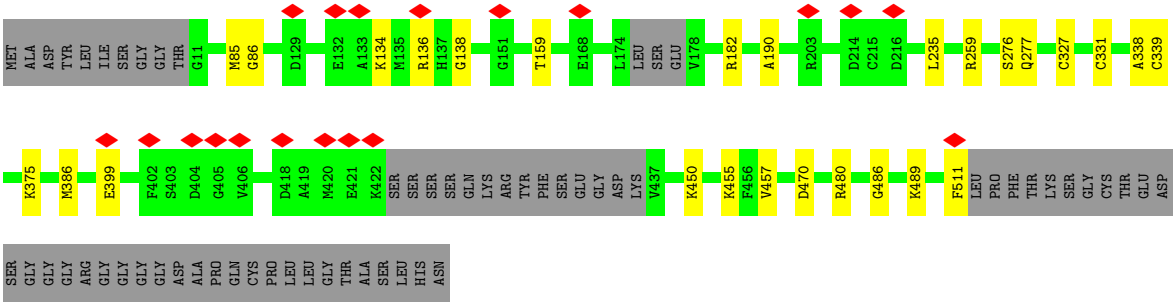
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 1

Chain A:



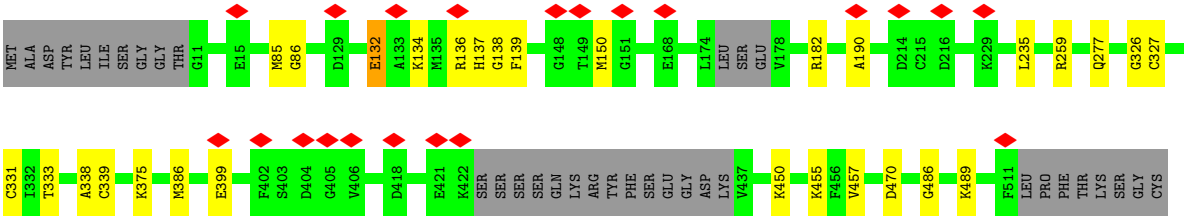
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 1

Chain B:



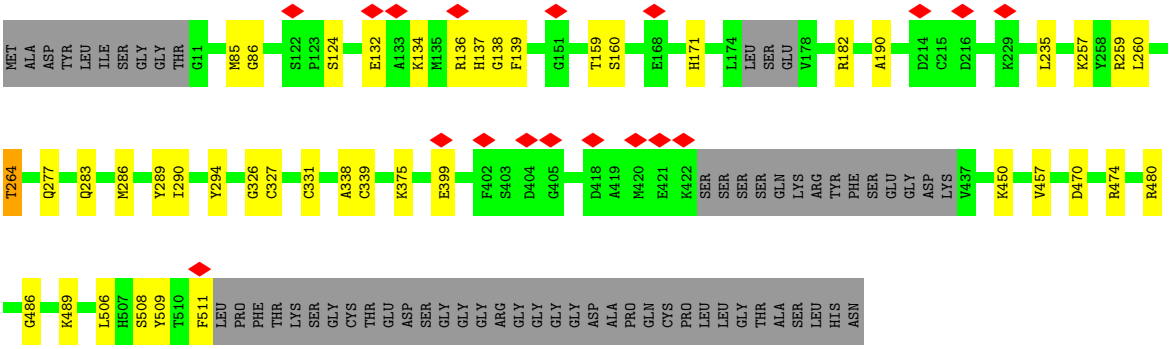
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 1

Chain C:



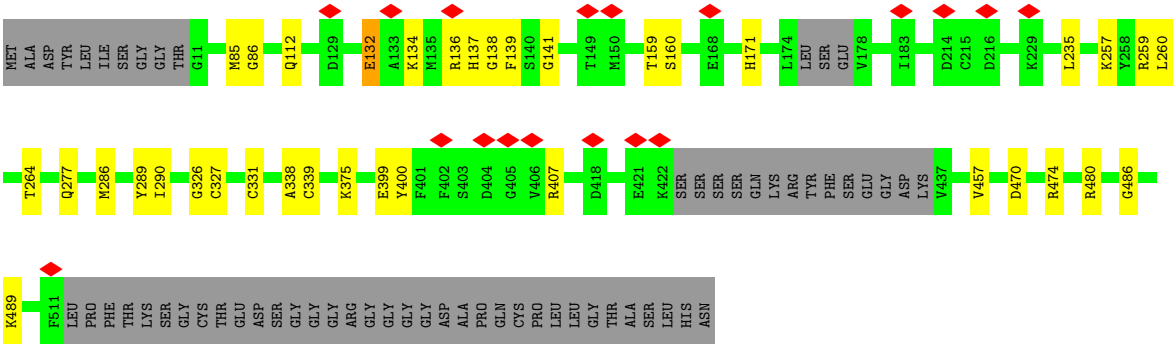
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 1

Chain D:



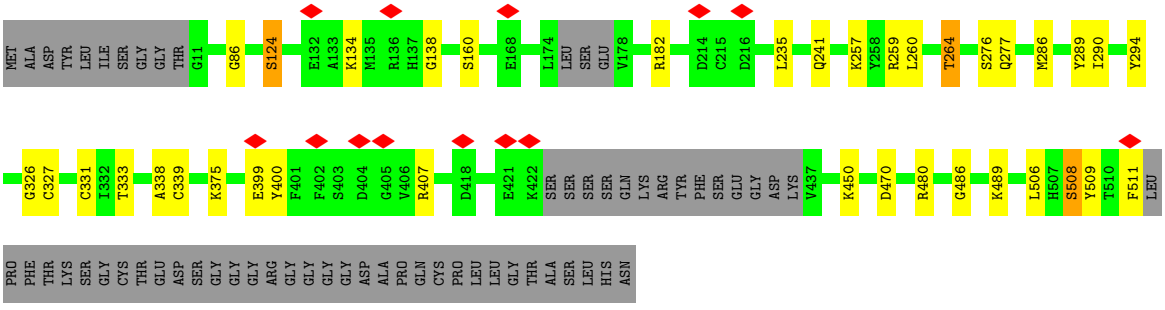
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 1

Chain E:



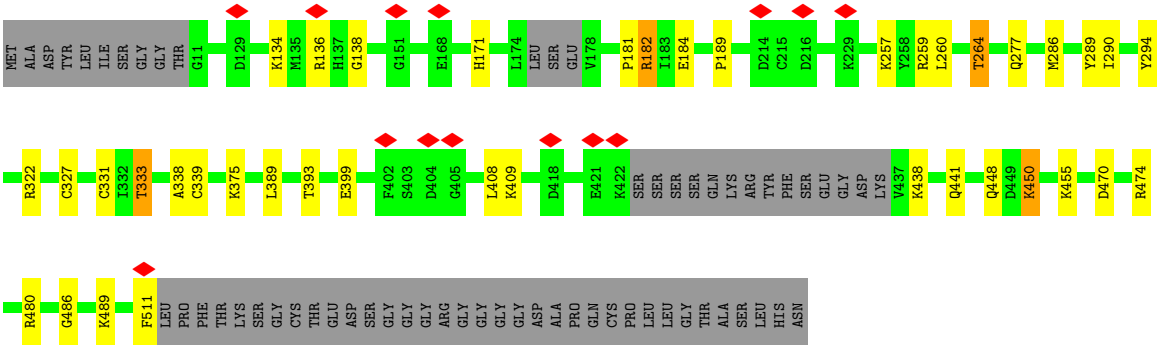
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 1

Chain F:



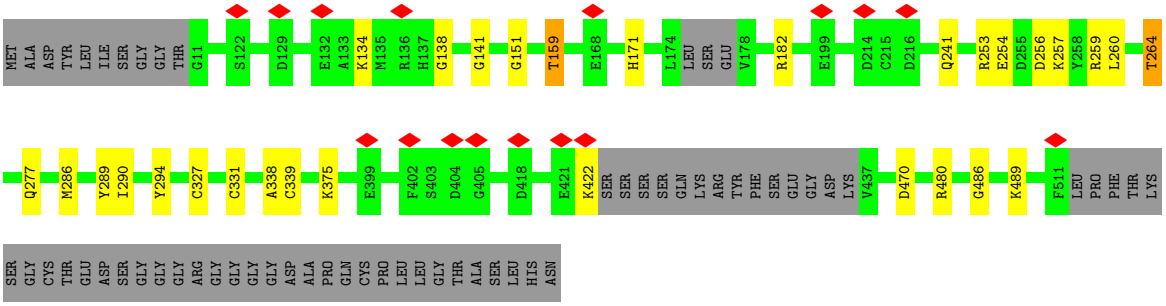
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 1

Chain G:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18885	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.852	Depositor
Minimum map value	-6.242	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.278	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	337.2, 337.2, 337.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84300005, 0.84300005, 0.84300005	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/3700	0.83	6/4995 (0.1%)
1	B	0.63	0/3700	0.82	3/4995 (0.1%)
1	C	0.64	0/3700	0.84	2/4995 (0.0%)
1	D	0.62	0/3700	0.82	4/4995 (0.1%)
1	E	0.63	0/3700	0.84	4/4995 (0.1%)
1	F	0.62	0/3700	0.82	4/4995 (0.1%)
1	G	0.61	0/3700	0.82	4/4995 (0.1%)
1	H	0.63	0/3700	0.83	2/4995 (0.0%)
All	All	0.62	0/29600	0.83	29/39960 (0.1%)

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	E	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	259	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	G	322	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	D	259	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	E	259	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	F	407	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	A	259	ARG	NE-CZ-NH1	6.48	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	259	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	F	259	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	259	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	H	259	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	E	407	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	F	182	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	182	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	136	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	105	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	412	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	A	182	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	B	182	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	H	480	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	480	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	474	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	E	480	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	474	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	480	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	474	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	F	480	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	182	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	G	474	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	G	480	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	400	TYR	Sidechain
1	F	400	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3645	3717	3714	8	0
1	B	3645	3717	3714	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3645	3717	3714	13	0
1	D	3645	3717	3714	17	0
1	E	3645	3717	3714	14	0
1	F	3645	3717	3714	15	0
1	G	3645	3717	3714	20	0
1	H	3645	3717	3714	13	0
2	A	62	24	24	0	0
2	B	62	24	24	0	0
2	C	62	24	24	0	0
2	D	62	24	24	0	0
2	E	62	24	24	0	0
2	F	62	24	24	0	0
2	G	62	24	24	0	0
2	H	62	24	24	0	0
3	A	23	11	11	2	0
3	B	23	11	11	4	0
3	C	23	11	11	2	0
3	D	23	11	11	1	0
3	E	23	11	11	1	0
3	F	23	11	11	1	0
3	G	23	11	11	3	0
3	H	23	11	11	4	0
4	A	44	26	26	0	0
4	B	44	26	26	3	0
4	C	44	26	26	0	0
4	D	44	26	26	0	0
4	E	44	26	26	0	0
4	F	44	26	26	1	0
4	G	44	26	26	0	0
4	H	44	26	26	2	0
All	All	30192	30224	30200	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:CYS:SG	3:A:603:IMP:H2	2.29	0.72
1:D:260:LEU:HD21	1:D:290:ILE:HG12	1.78	0.66
1:H:260:LEU:HD21	1:H:290:ILE:HG12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:LEU:HD21	1:G:290:ILE:HG12	1.78	0.65
1:F:260:LEU:HD21	1:F:290:ILE:HG12	1.78	0.64
1:H:331:CYS:SG	3:H:603:IMP:H2	2.38	0.63
1:E:260:LEU:HD21	1:E:290:ILE:HG12	1.78	0.63
1:A:331:CYS:SG	3:A:603:IMP:C2	2.86	0.62
1:G:331:CYS:CB	3:G:603:IMP:H2	2.29	0.62
1:B:331:CYS:SG	3:B:603:IMP:C2	2.88	0.61
1:H:331:CYS:SG	3:H:603:IMP:C2	2.89	0.61
1:F:506:LEU:HD12	1:F:509:TYR:HB3	1.83	0.61
1:B:331:CYS:SG	3:B:603:IMP:H2	2.40	0.60
1:D:506:LEU:HD12	1:D:509:TYR:HB3	1.83	0.59
1:A:389:LEU:O	1:A:450:LYS:NZ	2.36	0.58
1:C:331:CYS:SG	3:C:603:IMP:H2	2.44	0.58
1:G:331:CYS:HB2	3:G:603:IMP:H2	1.87	0.56
1:B:375:LYS:HE3	1:C:338:ALA:HB1	1.88	0.56
1:B:136:ARG:HH21	1:B:136:ARG:HG3	1.72	0.55
1:C:375:LYS:HE3	1:D:338:ALA:HB1	1.89	0.55
1:G:375:LYS:HE3	1:H:338:ALA:HB1	1.90	0.54
1:A:338:ALA:HB1	1:D:375:LYS:HE3	1.90	0.54
1:E:338:ALA:HB1	1:H:375:LYS:HE3	1.90	0.54
1:A:375:LYS:HE3	1:B:338:ALA:HB1	1.89	0.54
1:F:375:LYS:HE3	1:G:338:ALA:HB1	1.89	0.53
1:G:389:LEU:O	1:G:450:LYS:NZ	2.41	0.53
1:E:132:GLU:O	1:E:136:ARG:HG2	2.10	0.52
1:E:331:CYS:SG	3:E:603:IMP:H2	2.50	0.52
1:C:132:GLU:O	1:C:136:ARG:HG2	2.10	0.51
1:D:331:CYS:SG	3:D:603:IMP:H2	2.51	0.51
1:D:86:GLY:HA2	1:D:235:LEU:O	2.11	0.50
1:B:486:GLY:O	1:B:489:LYS:NZ	2.45	0.50
1:G:257:LYS:HD3	1:G:289:TYR:CZ	2.47	0.50
1:C:86:GLY:HA2	1:C:235:LEU:O	2.11	0.50
1:B:86:GLY:HA2	1:B:235:LEU:O	2.11	0.50
1:F:86:GLY:HA2	1:F:235:LEU:O	2.11	0.50
1:F:257:LYS:HD3	1:F:289:TYR:CZ	2.46	0.50
1:E:86:GLY:HA2	1:E:235:LEU:O	2.11	0.50
1:E:257:LYS:HD3	1:E:289:TYR:CZ	2.47	0.50
1:E:375:LYS:HE3	1:F:338:ALA:HB1	1.93	0.49
1:H:257:LYS:HD3	1:H:289:TYR:CZ	2.47	0.49
1:E:486:GLY:O	1:E:489:LYS:NZ	2.44	0.49
1:H:486:GLY:O	1:H:489:LYS:NZ	2.44	0.49
1:F:486:GLY:O	1:F:489:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:GLU:N	1:G:184:GLU:OE2	2.42	0.49
1:D:257:LYS:HD3	1:D:289:TYR:CZ	2.47	0.49
1:B:276:SER:HB3	4:B:604:NAD:C5N	2.43	0.48
1:A:486:GLY:O	1:A:489:LYS:NZ	2.45	0.48
1:C:486:GLY:O	1:C:489:LYS:NZ	2.46	0.48
1:D:486:GLY:O	1:D:489:LYS:NZ	2.46	0.48
1:G:455:LYS:HD3	1:G:455:LYS:HA	1.59	0.47
1:C:326:GLY:HA2	1:C:331:CYS:SG	2.53	0.47
1:F:134:LYS:O	1:F:138:GLY:N	2.48	0.47
1:G:486:GLY:O	1:G:489:LYS:NZ	2.46	0.47
1:H:134:LYS:O	1:H:138:GLY:N	2.47	0.47
1:F:508:SER:O	1:F:508:SER:OG	2.33	0.46
1:D:326:GLY:HA2	1:D:331:CYS:SG	2.55	0.46
1:G:134:LYS:O	1:G:138:GLY:N	2.49	0.46
1:G:331:CYS:SG	3:G:603:IMP:C2	3.04	0.46
1:B:134:LYS:O	1:B:138:GLY:N	2.50	0.45
1:C:134:LYS:O	1:C:138:GLY:N	2.49	0.45
1:E:134:LYS:O	1:E:138:GLY:N	2.49	0.45
1:D:134:LYS:O	1:D:138:GLY:N	2.49	0.45
1:F:331:CYS:SG	3:F:603:IMP:H2	2.56	0.45
1:G:389:LEU:HD12	1:G:389:LEU:HA	1.74	0.45
1:C:85:MET:HB3	1:C:457:VAL:HG11	1.99	0.45
1:G:333:THR:OG1	1:G:441:GLN:OE1	2.35	0.45
1:E:85:MET:HB3	1:E:457:VAL:HG11	1.99	0.45
1:D:85:MET:HB3	1:D:457:VAL:HG11	1.99	0.44
1:F:276:SER:HB3	4:F:604:NAD:C5N	2.47	0.44
1:C:386:MET:HB2	1:C:386:MET:HE2	1.73	0.44
1:A:450:LYS:HE3	1:A:450:LYS:HB2	1.82	0.44
1:C:455:LYS:HA	1:C:455:LYS:HD3	1.59	0.44
1:G:393:THR:O	1:G:409:LYS:NZ	2.50	0.44
1:H:141:GLY:HA2	1:H:159:THR:HG23	2.00	0.44
1:E:326:GLY:HA2	1:E:331:CYS:SG	2.58	0.43
1:F:326:GLY:HA2	1:F:331:CYS:SG	2.58	0.43
1:F:124:SER:O	1:F:124:SER:OG	2.37	0.43
1:B:85:MET:HB3	1:B:457:VAL:HG11	2.01	0.43
1:B:386:MET:HE2	1:B:386:MET:HB2	1.78	0.43
1:D:283:GLN:HE21	1:D:283:GLN:HB2	1.64	0.43
3:B:603:IMP:H2	4:B:604:NAD:C4N	2.49	0.43
1:G:136:ARG:HH21	1:G:136:ARG:HG3	1.83	0.43
3:H:603:IMP:H2	4:H:604:NAD:C4N	2.48	0.43
1:G:438:LYS:H	1:G:438:LYS:HG2	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:CYS:SG	3:C:603:IMP:C2	3.08	0.42
3:H:603:IMP:H2	4:H:604:NAD:C5N	2.49	0.42
1:D:136:ARG:HH21	1:D:136:ARG:HB3	1.85	0.42
1:D:286:MET:O	1:D:290:ILE:HG13	2.20	0.42
1:E:286:MET:O	1:E:290:ILE:HG13	2.20	0.42
1:F:286:MET:O	1:F:290:ILE:HG13	2.20	0.42
1:E:141:GLY:HA2	1:E:159:THR:HG22	2.00	0.42
1:H:286:MET:O	1:H:290:ILE:HG13	2.20	0.42
1:F:264:THR:HG21	1:F:294:TYR:CE1	2.55	0.41
3:B:603:IMP:H2	4:B:604:NAD:C5N	2.50	0.41
1:G:286:MET:O	1:G:290:ILE:HG13	2.20	0.41
1:H:253:ARG:O	1:H:256:ASP:HB2	2.20	0.41
1:G:408:LEU:HD23	1:G:448:GLN:HA	2.02	0.41
1:D:264:THR:HG21	1:D:294:TYR:CE1	2.56	0.41
1:G:264:THR:HG21	1:G:294:TYR:CE1	2.55	0.41
1:H:254:GLU:C	1:H:256:ASP:H	2.23	0.41
1:A:455:LYS:HD3	1:A:455:LYS:HA	1.60	0.41
1:B:136:ARG:HG3	1:B:136:ARG:NH2	2.35	0.41
1:D:159:THR:HG22	1:D:160:SER:H	1.86	0.41
1:E:137:HIS:HB3	1:E:139:PHE:CE2	2.56	0.41
1:C:137:HIS:HB3	1:C:139:PHE:CE2	2.56	0.40
1:D:137:HIS:HB3	1:D:139:PHE:CE2	2.56	0.40
1:H:264:THR:HG21	1:H:294:TYR:CE1	2.56	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	478/546 (88%)	452 (95%)	23 (5%)	3 (1%)	25 56
1	B	478/546 (88%)	454 (95%)	23 (5%)	1 (0%)	47 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	478/546 (88%)	450 (94%)	27 (6%)	1 (0%)	47 78
1	D	478/546 (88%)	454 (95%)	23 (5%)	1 (0%)	47 78
1	E	478/546 (88%)	449 (94%)	29 (6%)	0	100 100
1	F	478/546 (88%)	457 (96%)	21 (4%)	0	100 100
1	G	478/546 (88%)	448 (94%)	27 (6%)	3 (1%)	25 56
1	H	478/546 (88%)	452 (95%)	25 (5%)	1 (0%)	47 78
All	All	3824/4368 (88%)	3616 (95%)	198 (5%)	10 (0%)	44 72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	GLY
1	B	190	ALA
1	A	151	GLY
1	A	190	ALA
1	D	190	ALA
1	G	181	PRO
1	H	151	GLY
1	C	190	ALA
1	G	182	ARG
1	G	189	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	393/440 (89%)	387 (98%)	6 (2%)	65 89
1	B	393/440 (89%)	384 (98%)	9 (2%)	50 82
1	C	393/440 (89%)	384 (98%)	9 (2%)	50 82
1	D	393/440 (89%)	381 (97%)	12 (3%)	40 74
1	E	393/440 (89%)	383 (98%)	10 (2%)	47 80
1	F	393/440 (89%)	380 (97%)	13 (3%)	38 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	393/440 (89%)	382 (97%)	11 (3%)	43 77
1	H	393/440 (89%)	383 (98%)	10 (2%)	47 80
All	All	3144/3520 (89%)	3064 (98%)	80 (2%)	50 80

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	A	327	CYS
1	A	339	CYS
1	A	399	GLU
1	A	450	LYS
1	A	470	ASP
1	B	159	THR
1	B	277	GLN
1	B	327	CYS
1	B	339	CYS
1	B	399	GLU
1	B	450	LYS
1	B	455	LYS
1	B	470	ASP
1	B	511	PHE
1	C	132	GLU
1	C	150	MET
1	C	277	GLN
1	C	327	CYS
1	C	333	THR
1	C	339	CYS
1	C	399	GLU
1	C	450	LYS
1	C	470	ASP
1	D	124	SER
1	D	132	GLU
1	D	171	HIS
1	D	264	THR
1	D	277	GLN
1	D	327	CYS
1	D	339	CYS
1	D	399	GLU
1	D	450	LYS
1	D	470	ASP

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Mol	Chain	Res	Type
1	D	508	SER
1	D	511	PHE
1	E	112	GLN
1	E	132	GLU
1	E	160	SER
1	E	171	HIS
1	E	264	THR
1	E	277	GLN
1	E	327	CYS
1	E	339	CYS
1	E	399	GLU
1	E	470	ASP
1	F	124	SER
1	F	160	SER
1	F	241	GLN
1	F	264	THR
1	F	277	GLN
1	F	327	CYS
1	F	333	THR
1	F	339	CYS
1	F	399	GLU
1	F	450	LYS
1	F	470	ASP
1	F	508	SER
1	F	511	PHE
1	G	171	HIS
1	G	182	ARG
1	G	264	THR
1	G	277	GLN
1	G	327	CYS
1	G	333	THR
1	G	339	CYS
1	G	399	GLU
1	G	450	LYS
1	G	470	ASP
1	G	511	PHE
1	H	159	THR
1	H	171	HIS
1	H	182	ARG
1	H	241	GLN
1	H	264	THR
1	H	277	GLN

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Mol	Chain	Res	Type
1	H	327	CYS
1	H	339	CYS
1	H	422	LYS
1	H	470	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	GLN
1	A	498	GLN
1	B	277	GLN
1	B	498	GLN
1	C	277	GLN
1	C	498	GLN
1	D	265	GLN
1	D	277	GLN
1	D	498	GLN
1	E	265	GLN
1	E	277	GLN
1	E	498	GLN
1	F	265	GLN
1	F	277	GLN
1	F	498	GLN
1	G	265	GLN
1	G	277	GLN
1	G	498	GLN
1	H	265	GLN
1	H	277	GLN
1	H	498	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IMP	F	603	-	21,25,25	1.19	2 (9%)	24,38,38	0.92	1 (4%)
4	NAD	G	604	-	42,48,48	1.25	1 (2%)	50,73,73	1.43	5 (10%)
2	ATP	H	602	-	26,33,33	1.04	1 (3%)	31,52,52	1.45	5 (16%)
2	ATP	E	601	-	26,33,33	1.08	2 (7%)	31,52,52	1.50	6 (19%)
3	IMP	D	603	-	21,25,25	1.13	1 (4%)	24,38,38	0.91	1 (4%)
2	ATP	B	601	-	26,33,33	1.10	2 (7%)	31,52,52	1.45	5 (16%)
2	ATP	A	602	-	26,33,33	1.06	1 (3%)	31,52,52	1.46	5 (16%)
2	ATP	E	602	-	26,33,33	1.16	1 (3%)	31,52,52	1.48	6 (19%)
2	ATP	G	602	-	26,33,33	1.06	1 (3%)	31,52,52	1.48	5 (16%)
4	NAD	D	604	-	42,48,48	1.26	1 (2%)	50,73,73	1.29	5 (10%)
3	IMP	C	603	-	21,25,25	1.16	2 (9%)	24,38,38	0.94	1 (4%)
3	IMP	H	603	-	21,25,25	1.30	3 (14%)	24,38,38	1.02	2 (8%)
2	ATP	A	601	-	26,33,33	1.06	2 (7%)	31,52,52	1.52	7 (22%)
2	ATP	F	602	-	26,33,33	1.09	1 (3%)	31,52,52	1.45	4 (12%)
2	ATP	B	602	-	26,33,33	1.06	1 (3%)	31,52,52	1.49	5 (16%)
4	NAD	A	604	-	42,48,48	1.25	1 (2%)	50,73,73	1.32	5 (10%)
3	IMP	E	603	-	21,25,25	1.16	3 (14%)	24,38,38	0.93	1 (4%)
4	NAD	E	604	-	42,48,48	1.27	1 (2%)	50,73,73	1.29	4 (8%)
2	ATP	G	601	-	26,33,33	1.08	2 (7%)	31,52,52	1.49	6 (19%)
2	ATP	C	602	-	26,33,33	1.04	1 (3%)	31,52,52	1.46	6 (19%)
4	NAD	F	604	-	42,48,48	1.33	1 (2%)	50,73,73	1.23	4 (8%)
2	ATP	D	601	-	26,33,33	1.07	1 (3%)	31,52,52	1.51	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAD	B	604	-	42,48,48	1.31	1 (2%)	50,73,73	1.24	4 (8%)
2	ATP	F	601	-	26,33,33	1.05	2 (7%)	31,52,52	1.52	7 (22%)
3	IMP	B	603	-	21,25,25	1.25	3 (14%)	24,38,38	1.04	2 (8%)
2	ATP	C	601	-	26,33,33	1.04	2 (7%)	31,52,52	1.43	6 (19%)
4	NAD	C	604	-	42,48,48	1.32	1 (2%)	50,73,73	1.23	4 (8%)
4	NAD	H	604	-	42,48,48	1.31	1 (2%)	50,73,73	1.25	4 (8%)
3	IMP	A	603	-	21,25,25	1.36	3 (14%)	24,38,38	1.10	2 (8%)
2	ATP	H	601	-	26,33,33	1.02	2 (7%)	31,52,52	1.47	6 (19%)
2	ATP	D	602	-	26,33,33	1.04	1 (3%)	31,52,52	1.49	5 (16%)
3	IMP	G	603	-	21,25,25	1.25	2 (9%)	24,38,38	0.94	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMP	F	603	-	-	0/6/26/26	0/3/3/3
4	NAD	G	604	-	-	1/26/62/62	0/5/5/5
2	ATP	H	602	-	-	3/18/38/38	0/3/3/3
2	ATP	E	601	-	-	0/18/38/38	0/3/3/3
3	IMP	D	603	-	-	0/6/26/26	0/3/3/3
2	ATP	B	601	-	-	2/18/38/38	0/3/3/3
2	ATP	A	602	-	-	2/18/38/38	0/3/3/3
2	ATP	E	602	-	-	5/18/38/38	0/3/3/3
2	ATP	G	602	-	-	1/18/38/38	0/3/3/3
4	NAD	D	604	-	-	7/26/62/62	0/5/5/5
3	IMP	C	603	-	-	0/6/26/26	0/3/3/3
3	IMP	H	603	-	-	0/6/26/26	0/3/3/3
2	ATP	A	601	-	-	0/18/38/38	0/3/3/3
2	ATP	F	602	-	-	0/18/38/38	0/3/3/3
2	ATP	B	602	-	-	2/18/38/38	0/3/3/3
4	NAD	A	604	-	-	6/26/62/62	0/5/5/5
3	IMP	E	603	-	-	0/6/26/26	0/3/3/3
4	NAD	E	604	-	-	4/26/62/62	0/5/5/5
2	ATP	G	601	-	-	1/18/38/38	0/3/3/3
2	ATP	C	602	-	-	1/18/38/38	0/3/3/3
4	NAD	F	604	-	-	5/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	601	-	-	4/18/38/38	0/3/3/3
4	NAD	B	604	-	-	8/26/62/62	0/5/5/5
2	ATP	F	601	-	-	1/18/38/38	0/3/3/3
3	IMP	B	603	-	-	0/6/26/26	0/3/3/3
2	ATP	C	601	-	-	1/18/38/38	0/3/3/3
4	NAD	C	604	-	-	9/26/62/62	0/5/5/5
4	NAD	H	604	-	-	11/26/62/62	0/5/5/5
3	IMP	A	603	-	-	0/6/26/26	0/3/3/3
2	ATP	H	601	-	-	0/18/38/38	0/3/3/3
2	ATP	D	602	-	-	2/18/38/38	0/3/3/3
3	IMP	G	603	-	-	0/6/26/26	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	604	NAD	C3N-C7N	-6.51	1.40	1.50
4	C	604	NAD	C3N-C7N	-6.41	1.40	1.50
4	H	604	NAD	C3N-C7N	-6.37	1.41	1.50
4	B	604	NAD	C3N-C7N	-6.29	1.41	1.50
4	E	604	NAD	C3N-C7N	-6.10	1.41	1.50
4	D	604	NAD	C3N-C7N	-5.84	1.41	1.50
4	G	604	NAD	C3N-C7N	-5.71	1.42	1.50
4	A	604	NAD	C3N-C7N	-5.68	1.42	1.50
3	A	603	IMP	C6-N1	-3.31	1.32	1.38
2	E	602	ATP	O4'-C1'	3.00	1.45	1.41
3	G	603	IMP	C5-C4	-2.98	1.35	1.43
3	H	603	IMP	C6-N1	-2.97	1.32	1.38
2	B	601	ATP	O4'-C1'	2.86	1.45	1.41
3	A	603	IMP	C5-C4	-2.86	1.35	1.43
3	H	603	IMP	C5-C4	-2.78	1.36	1.43
3	G	603	IMP	C6-N1	-2.78	1.33	1.38
3	B	603	IMP	C5-C4	-2.76	1.36	1.43
3	D	603	IMP	C5-C4	-2.74	1.36	1.43
3	E	603	IMP	C5-C4	-2.72	1.36	1.43
3	C	603	IMP	C5-C4	-2.71	1.36	1.43
3	F	603	IMP	C5-C4	-2.71	1.36	1.43
3	B	603	IMP	C6-N1	-2.68	1.33	1.38
2	F	602	ATP	O4'-C1'	2.60	1.44	1.41
2	G	601	ATP	O4'-C1'	2.58	1.44	1.41
2	A	602	ATP	O4'-C1'	2.51	1.44	1.41
2	D	602	ATP	O4'-C1'	2.49	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	602	ATP	O4'-C1'	2.48	1.44	1.41
2	H	602	ATP	O4'-C1'	2.48	1.44	1.41
2	B	602	ATP	O4'-C1'	2.48	1.44	1.41
2	D	601	ATP	O4'-C1'	2.40	1.44	1.41
2	F	601	ATP	O4'-C1'	2.37	1.44	1.41
2	C	602	ATP	O4'-C1'	2.32	1.44	1.41
2	A	601	ATP	O4'-C1'	2.31	1.44	1.41
2	C	601	ATP	O4'-C1'	2.26	1.44	1.41
2	H	601	ATP	O4'-C1'	2.26	1.44	1.41
3	H	603	IMP	O4'-C1'	2.26	1.44	1.41
2	E	601	ATP	O4'-C1'	2.25	1.44	1.41
3	A	603	IMP	O4'-C1'	2.16	1.44	1.41
2	E	601	ATP	C5-C4	-2.13	1.35	1.40
2	H	601	ATP	C5-C4	-2.11	1.35	1.40
3	B	603	IMP	O4'-C1'	2.11	1.44	1.41
3	F	603	IMP	C2-N3	2.10	1.33	1.29
3	C	603	IMP	C2-N3	2.08	1.33	1.29
2	B	601	ATP	C5-C4	-2.05	1.35	1.40
2	F	601	ATP	C5-C4	-2.05	1.35	1.40
3	E	603	IMP	C2-N3	2.05	1.33	1.29
2	A	601	ATP	C5-C4	-2.05	1.35	1.40
3	E	603	IMP	O4'-C1'	2.02	1.43	1.41
2	C	601	ATP	C5-C4	-2.02	1.35	1.40
2	G	601	ATP	C5-C4	-2.01	1.35	1.40

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	604	NAD	PN-O3-PA	-5.51	113.94	132.83
4	F	604	NAD	PN-O3-PA	-4.59	117.08	132.83
4	D	604	NAD	PN-O3-PA	-4.51	117.36	132.83
4	H	604	NAD	PN-O3-PA	-4.50	117.39	132.83
4	B	604	NAD	PN-O3-PA	-4.48	117.47	132.83
4	A	604	NAD	PN-O3-PA	-4.40	117.74	132.83
4	E	604	NAD	PN-O3-PA	-4.36	117.88	132.83
2	G	602	ATP	C4-C5-N7	4.20	113.78	109.40
2	A	602	ATP	C4-C5-N7	4.19	113.76	109.40
4	C	604	NAD	PN-O3-PA	-4.16	118.56	132.83
2	C	602	ATP	C4-C5-N7	4.15	113.72	109.40
2	D	602	ATP	C4-C5-N7	4.14	113.71	109.40
2	H	602	ATP	C4-C5-N7	4.08	113.65	109.40
2	B	602	ATP	C4-C5-N7	4.07	113.64	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	602	ATP	C4-C5-N7	4.06	113.63	109.40
2	E	602	ATP	C4-C5-N7	4.04	113.61	109.40
2	G	601	ATP	C4-C5-N7	3.97	113.54	109.40
2	B	601	ATP	C4-C5-N7	3.93	113.50	109.40
2	A	601	ATP	C4-C5-N7	3.89	113.45	109.40
2	D	601	ATP	C4-C5-N7	3.88	113.44	109.40
2	F	601	ATP	C4-C5-N7	3.85	113.41	109.40
2	E	601	ATP	C4-C5-N7	3.83	113.39	109.40
2	H	601	ATP	C4-C5-N7	3.82	113.38	109.40
4	G	604	NAD	C5A-C6A-N6A	3.81	126.15	120.35
4	A	604	NAD	C5A-C6A-N6A	3.76	126.07	120.35
2	C	601	ATP	C4-C5-N7	3.75	113.30	109.40
4	C	604	NAD	C5A-C6A-N6A	3.66	125.92	120.35
4	E	604	NAD	C5A-C6A-N6A	3.66	125.92	120.35
4	B	604	NAD	C5A-C6A-N6A	3.58	125.79	120.35
4	H	604	NAD	C5A-C6A-N6A	3.55	125.75	120.35
4	D	604	NAD	C5A-C6A-N6A	3.52	125.70	120.35
4	F	604	NAD	C5A-C6A-N6A	3.51	125.68	120.35
2	D	601	ATP	PB-O3B-PG	-3.44	121.01	132.83
2	E	602	ATP	PB-O3B-PG	-3.42	121.09	132.83
2	G	601	ATP	PA-O3A-PB	-3.32	121.44	132.83
2	C	601	ATP	PA-O3A-PB	-3.28	121.56	132.83
2	F	602	ATP	PB-O3B-PG	-3.25	121.66	132.83
2	H	602	ATP	PB-O3B-PG	-3.17	121.96	132.83
2	D	602	ATP	PB-O3B-PG	-3.13	122.08	132.83
2	A	601	ATP	PA-O3A-PB	-3.12	122.11	132.83
2	G	602	ATP	PB-O3B-PG	-3.12	122.13	132.83
2	C	602	ATP	PB-O3B-PG	-3.11	122.17	132.83
2	A	602	ATP	PB-O3B-PG	-3.09	122.24	132.83
2	F	601	ATP	PA-O3A-PB	-3.08	122.25	132.83
2	G	601	ATP	C5-C6-N6	3.06	125.01	120.35
2	G	602	ATP	PA-O3A-PB	-3.00	122.52	132.83
2	C	602	ATP	PA-O3A-PB	-2.98	122.61	132.83
2	B	601	ATP	PB-O3B-PG	-2.97	122.65	132.83
4	H	604	NAD	C6N-N1N-C2N	-2.96	119.27	121.97
2	D	602	ATP	PA-O3A-PB	-2.94	122.73	132.83
4	A	604	NAD	N6A-C6A-N1A	-2.93	112.49	118.57
2	B	602	ATP	PB-O3B-PG	-2.92	122.80	132.83
2	H	601	ATP	PA-O3A-PB	-2.92	122.82	132.83
2	A	602	ATP	PA-O3A-PB	-2.89	122.89	132.83
2	F	601	ATP	PB-O3B-PG	-2.89	122.92	132.83
2	H	602	ATP	PA-O3A-PB	-2.89	122.92	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	604	NAD	C6N-N1N-C2N	-2.88	119.35	121.97
2	E	601	ATP	PA-O3A-PB	-2.87	122.97	132.83
4	G	604	NAD	N6A-C6A-N1A	-2.87	112.61	118.57
4	C	604	NAD	N6A-C6A-N1A	-2.85	112.66	118.57
2	E	601	ATP	O3G-PG-O3B	2.82	114.10	104.64
4	B	604	NAD	N6A-C6A-N1A	-2.82	112.71	118.57
2	F	602	ATP	PA-O3A-PB	-2.82	123.14	132.83
2	G	601	ATP	N6-C6-N1	-2.78	112.81	118.57
4	E	604	NAD	N6A-C6A-N1A	-2.77	112.82	118.57
4	B	604	NAD	C6N-N1N-C2N	-2.77	119.45	121.97
4	D	604	NAD	C6N-N1N-C2N	-2.77	119.45	121.97
2	D	601	ATP	O3G-PG-O3B	2.74	113.83	104.64
4	H	604	NAD	N6A-C6A-N1A	-2.73	112.91	118.57
4	D	604	NAD	N6A-C6A-N1A	-2.72	112.93	118.57
2	H	601	ATP	O3G-PG-O3B	2.72	113.74	104.64
4	F	604	NAD	N6A-C6A-N1A	-2.71	112.95	118.57
2	E	602	ATP	PA-O3A-PB	-2.70	123.58	132.83
4	A	604	NAD	C6N-N1N-C2N	-2.69	119.52	121.97
2	D	601	ATP	PA-O3A-PB	-2.67	123.68	132.83
3	A	603	IMP	O6-C6-C5	2.64	129.53	124.37
4	G	604	NAD	C6N-N1N-C2N	-2.63	119.58	121.97
2	H	601	ATP	C5-C6-N6	2.63	124.34	120.35
2	E	601	ATP	C5-C6-N6	2.61	124.31	120.35
2	B	602	ATP	PA-O3A-PB	-2.61	123.88	132.83
2	D	602	ATP	O3G-PG-O3B	2.60	113.36	104.64
2	A	601	ATP	PB-O3B-PG	-2.60	123.90	132.83
2	C	601	ATP	C5-C6-N6	2.58	124.28	120.35
4	G	604	NAD	O7N-C7N-N7N	-2.58	118.91	122.58
2	A	601	ATP	O2G-PG-O3B	2.56	113.24	104.64
3	A	603	IMP	O6-C6-N1	-2.56	117.21	120.32
2	F	601	ATP	O3G-PG-O3B	2.54	113.16	104.64
2	A	601	ATP	O3G-PG-O3B	2.50	113.03	104.64
2	H	601	ATP	PB-O3B-PG	-2.48	124.31	132.83
2	C	601	ATP	N6-C6-N1	-2.48	113.43	118.57
2	E	601	ATP	N6-C6-N1	-2.46	113.46	118.57
2	A	601	ATP	C5-C6-N6	2.46	124.09	120.35
3	D	603	IMP	O4'-C4'-C3'	-2.44	100.28	105.11
2	H	601	ATP	N6-C6-N1	-2.43	113.52	118.57
2	E	601	ATP	O2G-PG-O3B	2.41	112.71	104.64
3	E	603	IMP	O4'-C4'-C3'	-2.40	100.37	105.11
2	B	601	ATP	C5-C6-N6	2.39	123.99	120.35
4	A	604	NAD	O7N-C7N-N7N	-2.39	119.19	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	ATP	PB-O3B-PG	-2.39	124.64	132.83
2	B	601	ATP	N6-C6-N1	-2.37	113.65	118.57
2	E	602	ATP	O2G-PG-O3B	2.36	112.54	104.64
4	F	604	NAD	C6N-N1N-C2N	-2.35	119.83	121.97
2	F	601	ATP	C5-C6-N6	2.35	123.92	120.35
3	C	603	IMP	O4'-C4'-C3'	-2.35	100.47	105.11
2	G	601	ATP	C3'-C2'-C1'	2.35	104.51	100.98
2	C	602	ATP	O2G-PG-O3B	2.32	112.43	104.64
2	B	602	ATP	O2G-PG-O3B	2.32	112.42	104.64
2	A	601	ATP	N6-C6-N1	-2.30	113.81	118.57
2	D	601	ATP	C5-C6-N6	2.29	123.83	120.35
4	E	604	NAD	C6N-N1N-C2N	-2.28	119.90	121.97
2	F	601	ATP	O2G-PG-O3B	2.27	112.25	104.64
2	G	602	ATP	O3G-PG-O3B	2.27	112.24	104.64
2	F	601	ATP	N6-C6-N1	-2.27	113.87	118.57
2	C	601	ATP	O2G-PG-O3B	2.26	112.21	104.64
2	D	601	ATP	O2G-PG-O3B	2.25	112.19	104.64
2	B	601	ATP	O3G-PG-O3B	2.23	112.11	104.64
2	A	602	ATP	O3G-PG-O3B	2.22	112.09	104.64
3	F	603	IMP	O4'-C4'-C3'	-2.22	100.72	105.11
4	D	604	NAD	O7N-C7N-N7N	-2.22	119.43	122.58
2	D	601	ATP	N6-C6-N1	-2.20	114.01	118.57
2	B	602	ATP	C3'-C2'-C1'	2.18	104.27	100.98
3	H	603	IMP	O4'-C4'-C3'	-2.17	100.82	105.11
3	B	603	IMP	O4'-C4'-C3'	-2.15	100.87	105.11
2	F	602	ATP	C3'-C2'-C1'	2.14	104.20	100.98
2	A	602	ATP	C3'-C2'-C1'	2.14	104.20	100.98
2	G	601	ATP	PB-O3B-PG	-2.14	125.50	132.83
2	H	602	ATP	C3'-C2'-C1'	2.12	104.17	100.98
2	E	602	ATP	C5-C6-N6	2.11	123.56	120.35
3	B	603	IMP	O6-C6-C5	2.10	128.48	124.37
3	H	603	IMP	O6-C6-C5	2.07	128.42	124.37
2	C	602	ATP	C5-C6-N6	2.07	123.50	120.35
2	G	602	ATP	C3'-C2'-C1'	2.06	104.08	100.98
3	G	603	IMP	O4'-C4'-C3'	-2.06	101.05	105.11
2	E	602	ATP	N6-C6-N1	-2.05	114.33	118.57
2	C	602	ATP	N6-C6-N1	-2.04	114.35	118.57
2	H	602	ATP	C5-C6-N6	2.03	123.43	120.35
2	D	602	ATP	N6-C6-N1	-2.01	114.40	118.57

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	602	ATP	C5'-O5'-PA-O1A
2	E	602	ATP	C5'-O5'-PA-O3A
4	A	604	NAD	C5D-O5D-PN-O3
4	A	604	NAD	O4D-C1D-N1N-C2N
4	B	604	NAD	C5D-O5D-PN-O3
4	B	604	NAD	C2N-C3N-C7N-O7N
4	B	604	NAD	C2N-C3N-C7N-N7N
4	C	604	NAD	C5D-O5D-PN-O3
4	C	604	NAD	O4D-C1D-N1N-C2N
4	C	604	NAD	C2N-C3N-C7N-O7N
4	C	604	NAD	C2N-C3N-C7N-N7N
4	D	604	NAD	PA-O3-PN-O5D
4	D	604	NAD	C5D-O5D-PN-O3
4	D	604	NAD	O4D-C1D-N1N-C2N
4	E	604	NAD	O4B-C4B-C5B-O5B
4	E	604	NAD	C3B-C4B-C5B-O5B
4	F	604	NAD	C2N-C3N-C7N-O7N
4	F	604	NAD	C2N-C3N-C7N-N7N
4	H	604	NAD	C5D-O5D-PN-O3
4	H	604	NAD	O4D-C1D-N1N-C2N
4	H	604	NAD	C2N-C3N-C7N-O7N
4	H	604	NAD	C2N-C3N-C7N-N7N
4	C	604	NAD	C4N-C3N-C7N-O7N
4	C	604	NAD	C4N-C3N-C7N-N7N
4	B	604	NAD	C4N-C3N-C7N-O7N
4	B	604	NAD	C4N-C3N-C7N-N7N
4	F	604	NAD	C4N-C3N-C7N-O7N
4	F	604	NAD	C4N-C3N-C7N-N7N
4	H	604	NAD	C4N-C3N-C7N-O7N
4	H	604	NAD	C4N-C3N-C7N-N7N
2	D	601	ATP	PB-O3A-PA-O5'
2	F	601	ATP	PB-O3A-PA-O5'
2	G	601	ATP	PB-O3A-PA-O5'
4	A	604	NAD	PA-O3-PN-O5D
4	E	604	NAD	PN-O3-PA-O5B
4	H	604	NAD	PA-O3-PN-O5D
2	E	602	ATP	O4'-C4'-C5'-O5'
2	D	602	ATP	PB-O3A-PA-O2A
4	A	604	NAD	PN-O3-PA-O2A
4	B	604	NAD	PN-O3-PA-O2A
4	C	604	NAD	PN-O3-PA-O1A
4	D	604	NAD	PN-O3-PA-O2A
4	H	604	NAD	PN-O3-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	G	604	NAD	C4D-C5D-O5D-PN
2	D	601	ATP	C5'-O5'-PA-O2A
4	A	604	NAD	C5D-O5D-PN-O1N
4	B	604	NAD	C5D-O5D-PN-O1N
4	C	604	NAD	C5D-O5D-PN-O1N
4	D	604	NAD	C5D-O5D-PN-O1N
4	H	604	NAD	C5D-O5D-PN-O1N
2	A	602	ATP	PB-O3A-PA-O2A
2	B	601	ATP	PA-O3A-PB-O2B
2	B	602	ATP	PA-O3A-PB-O2B
4	B	604	NAD	PN-O3-PA-O1A
4	C	604	NAD	PN-O3-PA-O2A
2	E	602	ATP	C4'-C5'-O5'-PA
2	A	602	ATP	PG-O3B-PB-O1B
2	C	601	ATP	PG-O3B-PB-O1B
2	C	602	ATP	PG-O3B-PB-O1B
2	H	602	ATP	PG-O3B-PB-O1B
2	H	602	ATP	PB-O3A-PA-O2A
4	A	604	NAD	PN-O3-PA-O1A
4	D	604	NAD	C4D-C5D-O5D-PN
4	H	604	NAD	PN-O3-PA-O1A
4	F	604	NAD	PN-O3-PA-O5B
4	E	604	NAD	C2N-C3N-C7N-N7N
2	D	601	ATP	C5'-O5'-PA-O3A
4	H	604	NAD	C4D-C5D-O5D-PN
2	B	601	ATP	PB-O3A-PA-O2A
2	B	602	ATP	PA-O3A-PB-O1B
2	D	601	ATP	PB-O3A-PA-O1A
2	D	602	ATP	PB-O3A-PA-O1A
2	E	602	ATP	PB-O3A-PA-O2A
2	G	602	ATP	PB-O3A-PA-O2A
2	H	602	ATP	PB-O3A-PA-O1A
4	D	604	NAD	PN-O3-PA-O1A

There are no ring outliers.

11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	603	IMP	1	0
3	D	603	IMP	1	0
3	C	603	IMP	2	0
3	H	603	IMP	4	0

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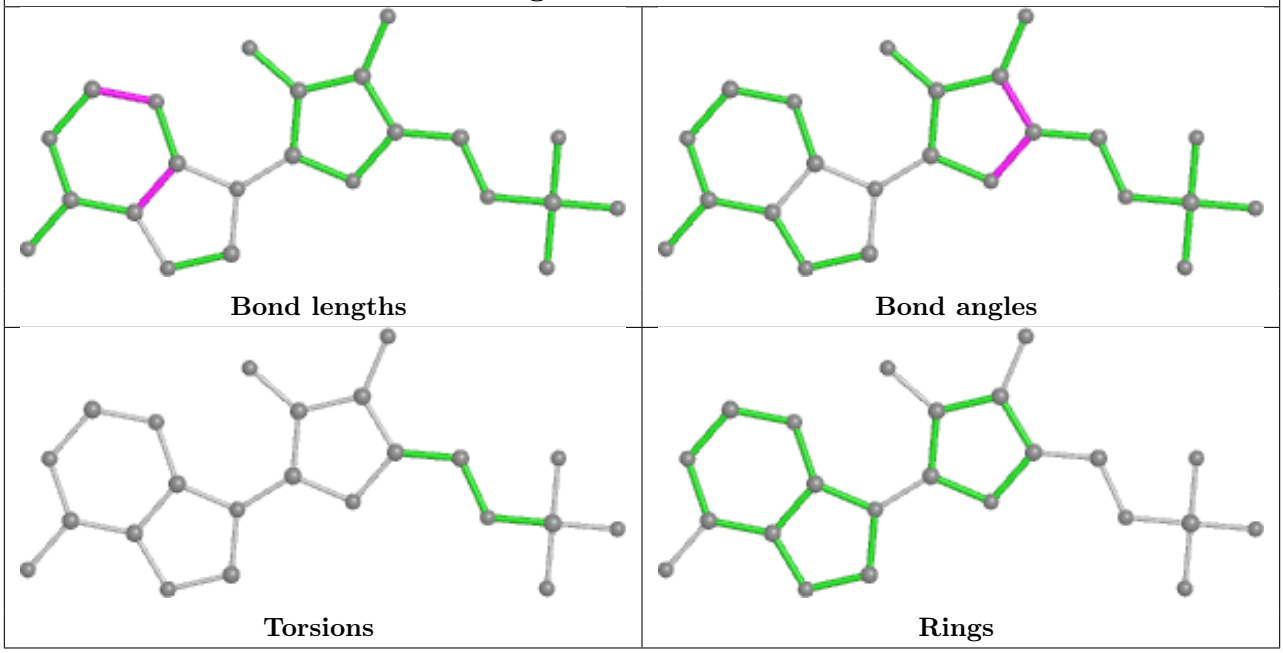
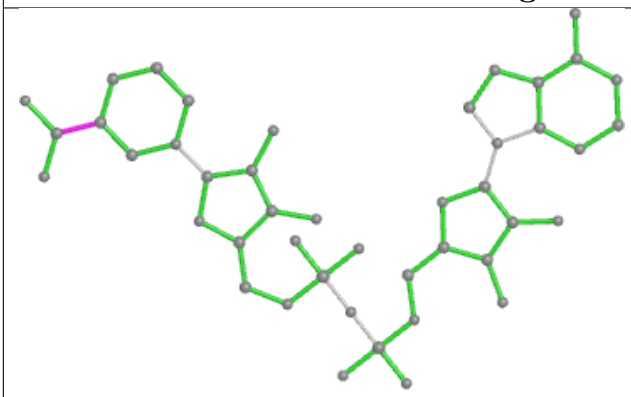
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	603	IMP	1	0
4	F	604	NAD	1	0
4	B	604	NAD	3	0
3	B	603	IMP	4	0
4	H	604	NAD	2	0
3	A	603	IMP	2	0
3	G	603	IMP	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

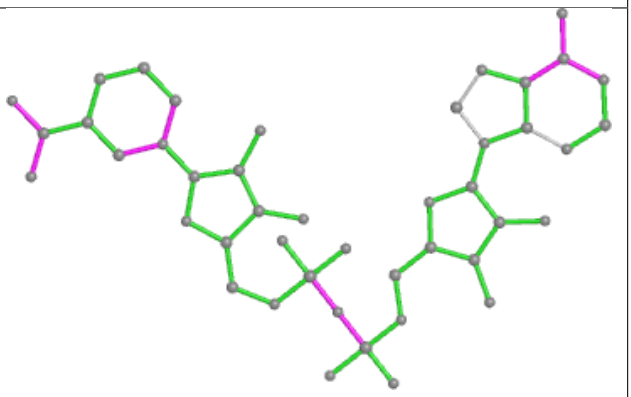
Ligand IMP F 603



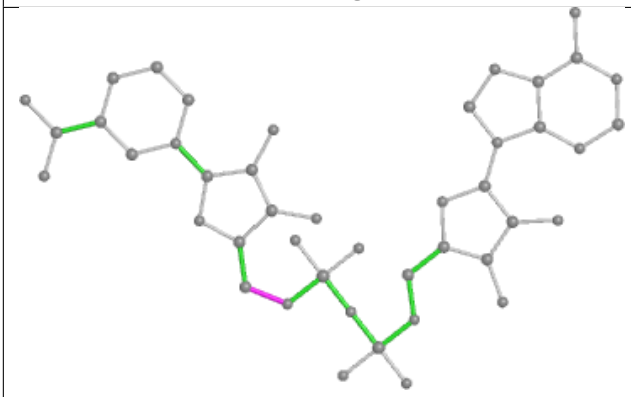
Ligand NAD G 604



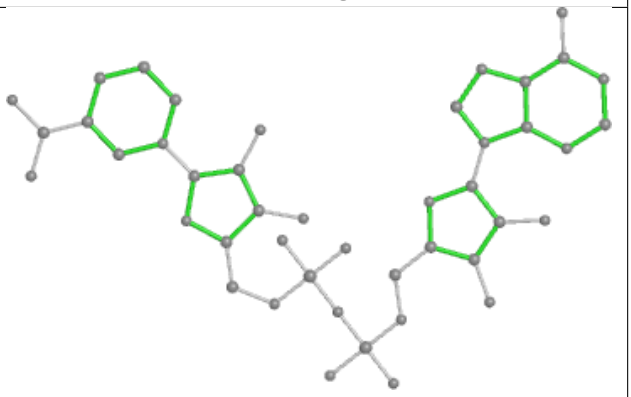
Bond lengths



Bond angles

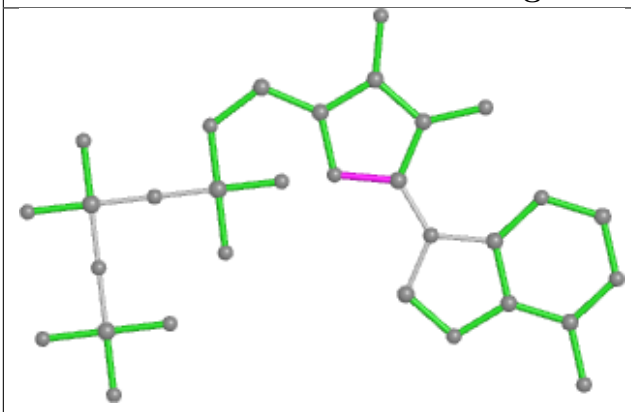


Torsions

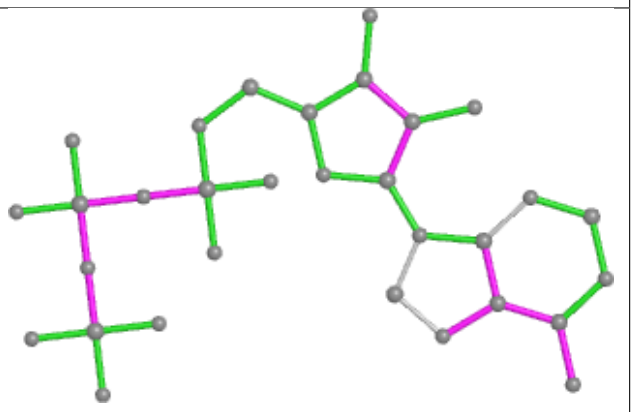


Rings

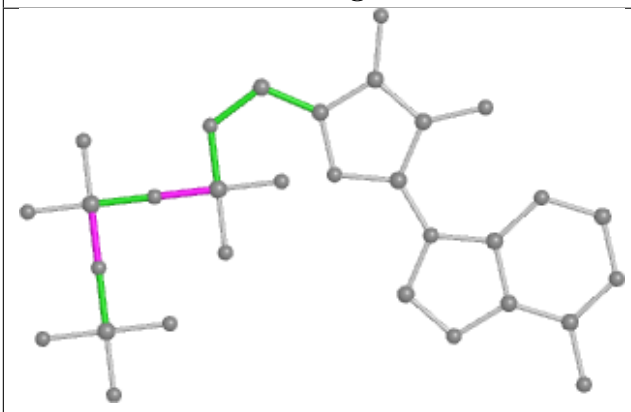
Ligand ATP H 602



Bond lengths



Bond angles



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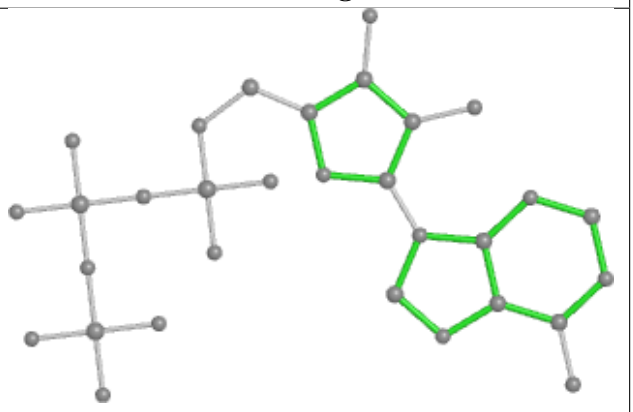
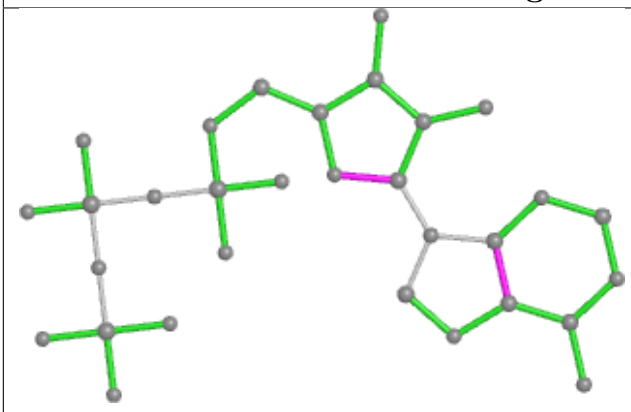
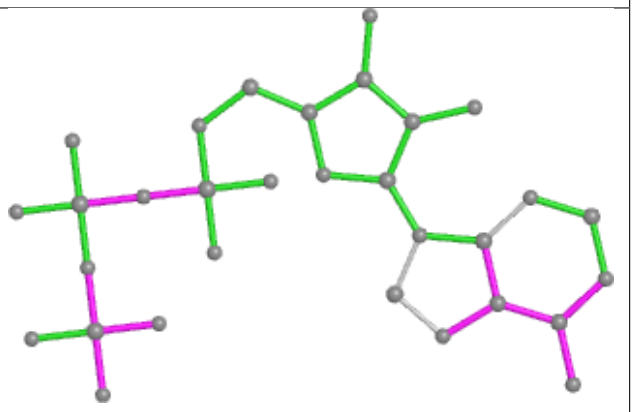


Rings

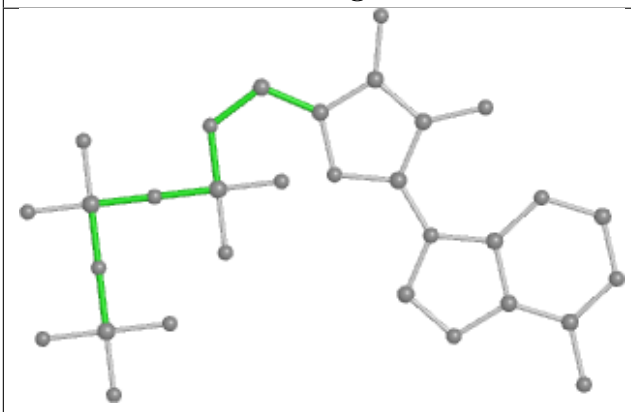
Ligand ATP E 601



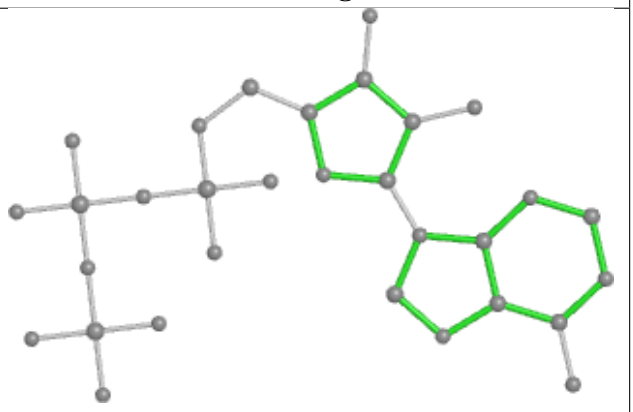
Bond lengths



Bond angles

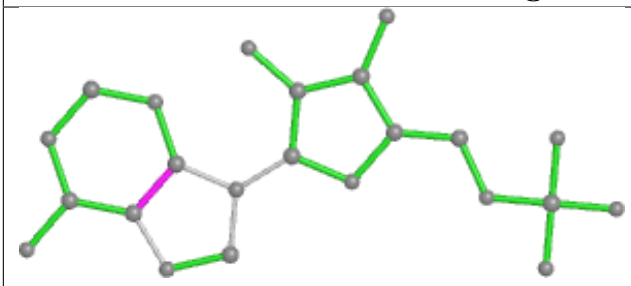


Torsions

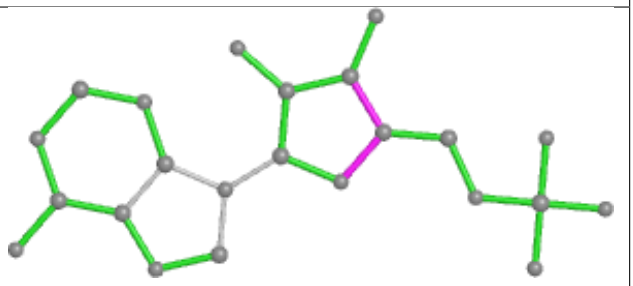


Rings

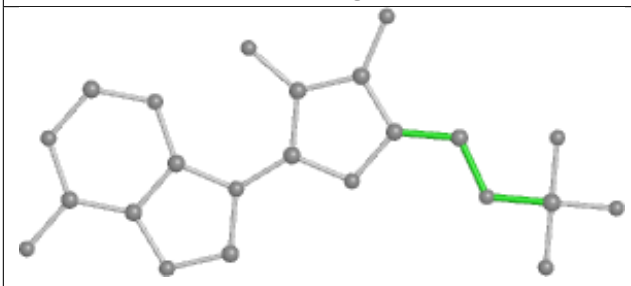
Ligand IMP D 603



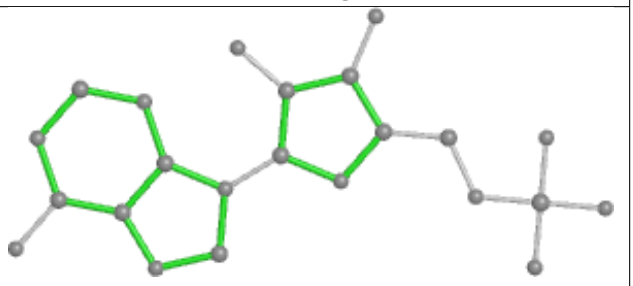
Bond lengths



Bond angles

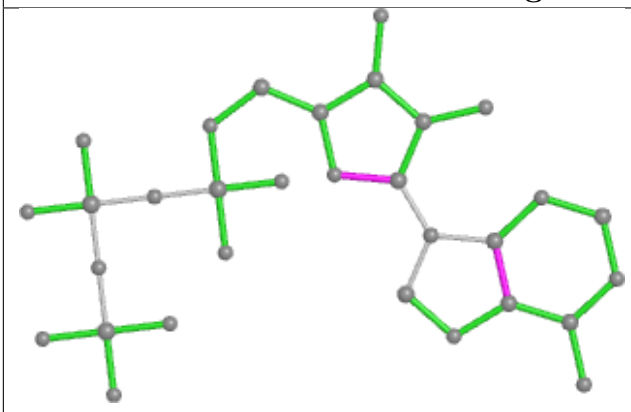


Torsions

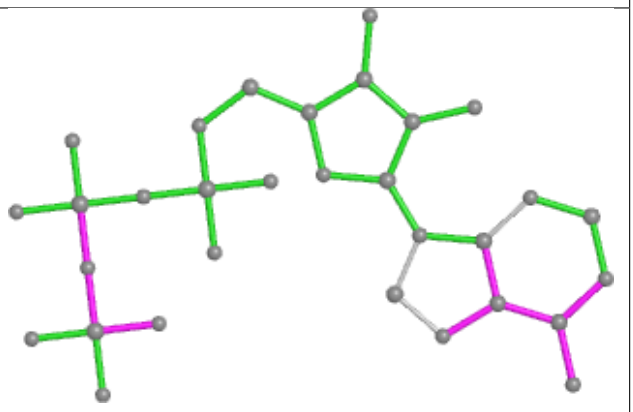


Rings

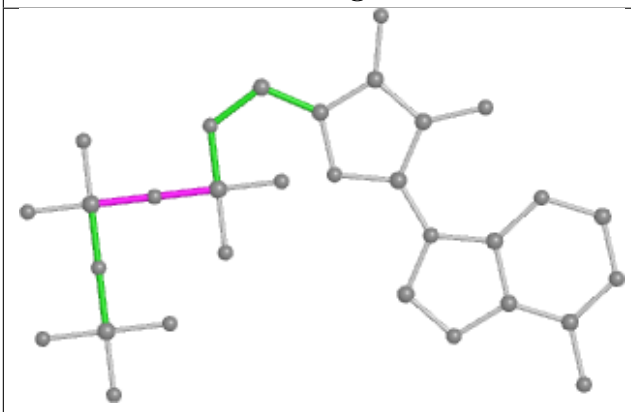
Ligand ATP B 601



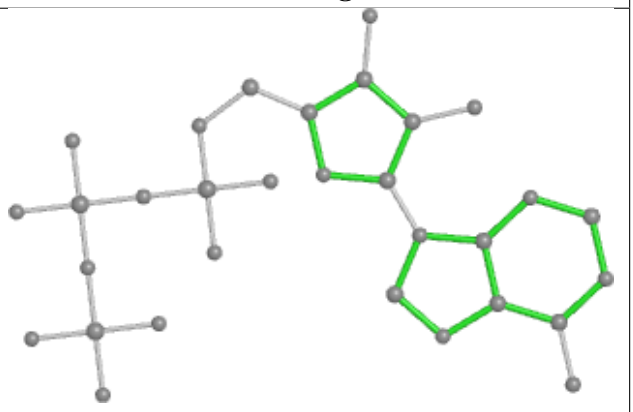
Bond lengths



Bond angles

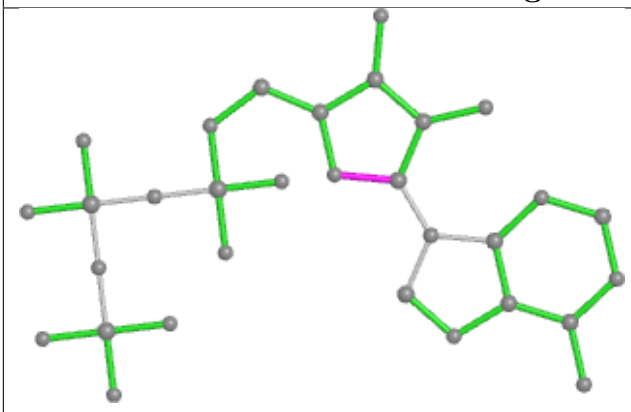


Torsions



Rings

Ligand ATP A 602



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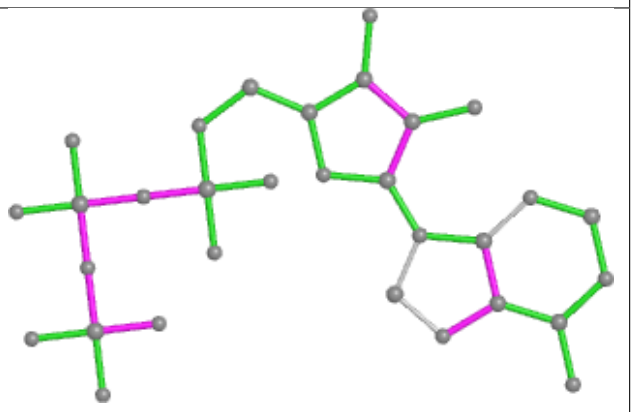
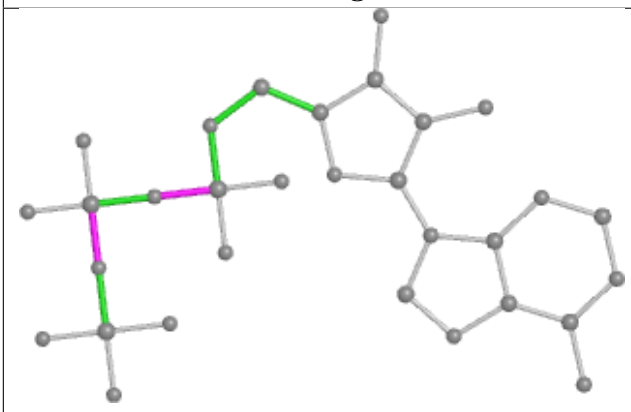


Bond angles



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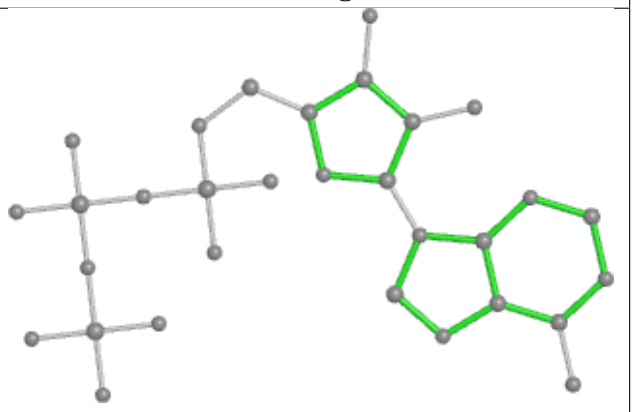
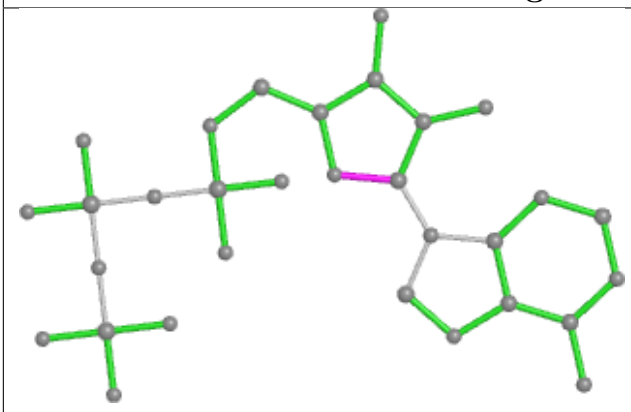


Rings

Ligand ATP E 602



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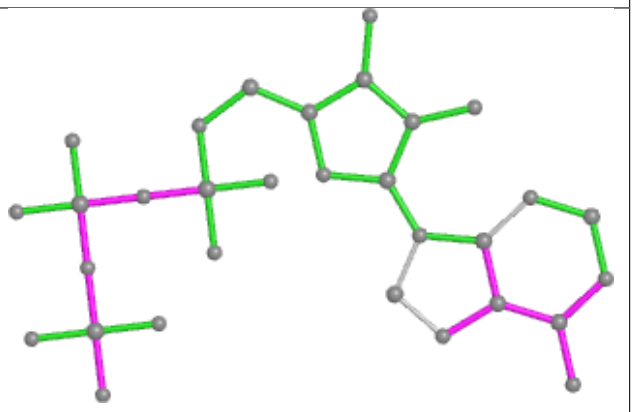
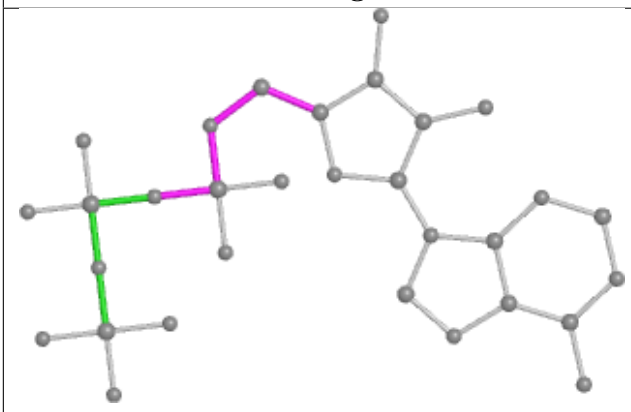
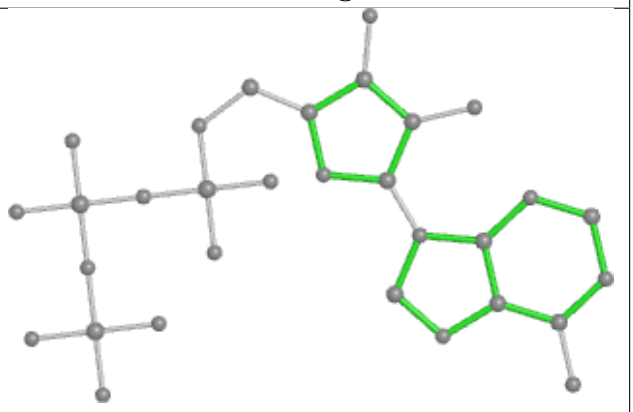


Bond angles

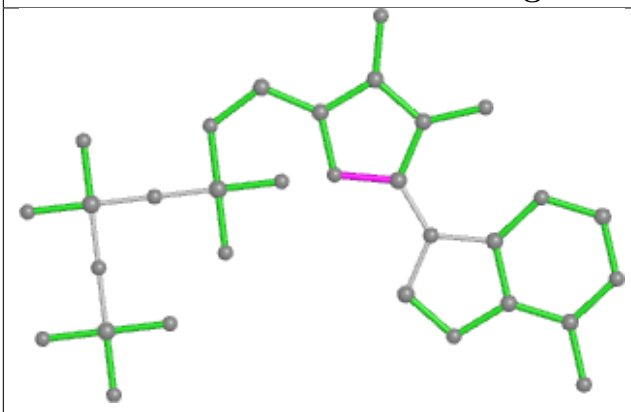


Torsions



Rings

Ligand ATP G 602



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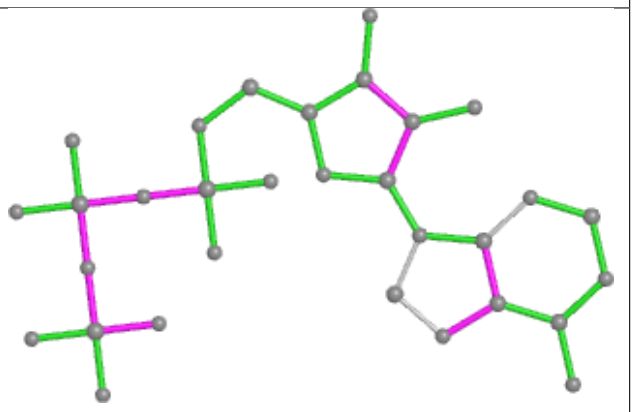
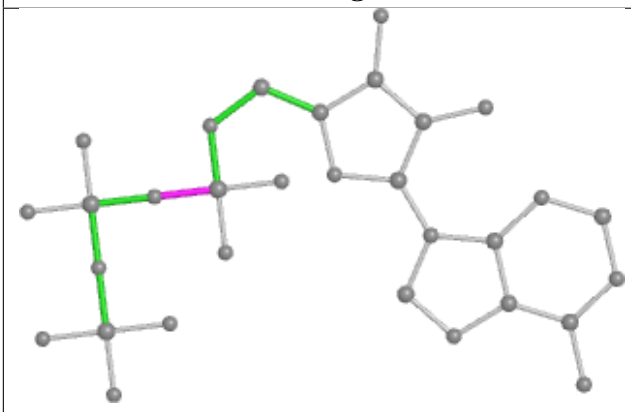
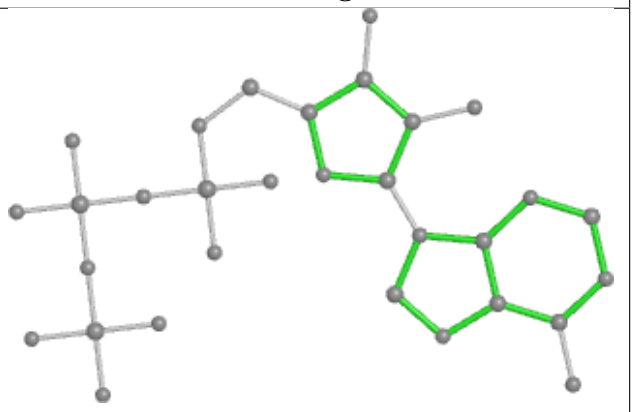


Bond angles

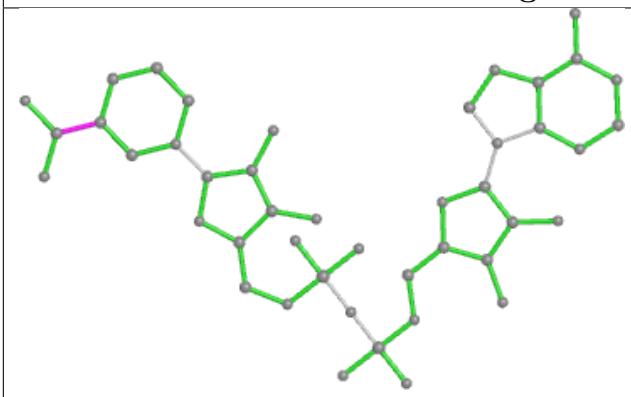


Torsions



Rings

Ligand NAD D 604



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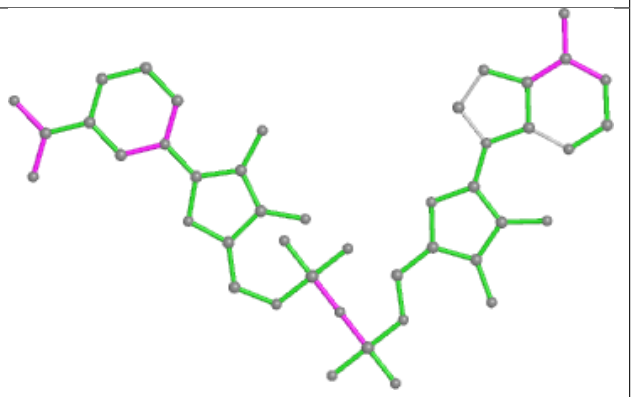
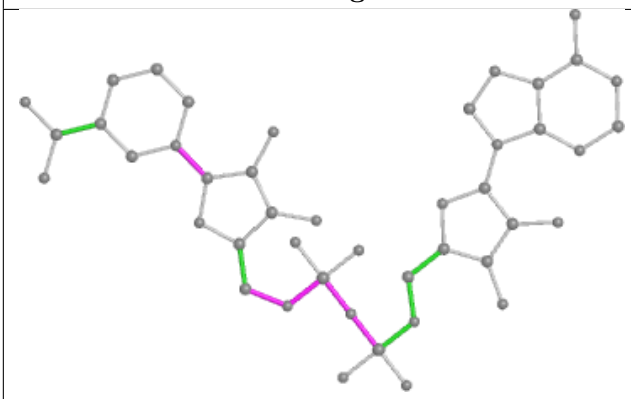


Bond angles



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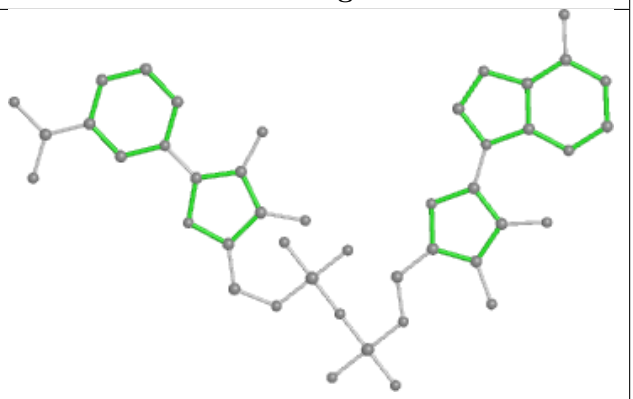
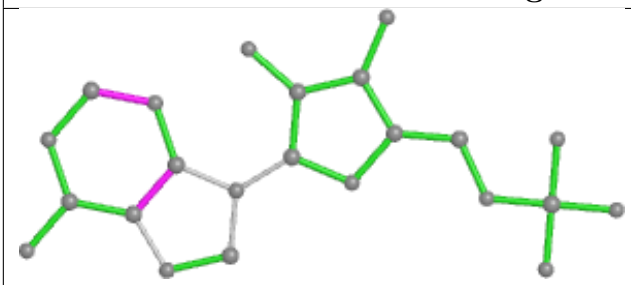


Rings

Ligand IMP C 603



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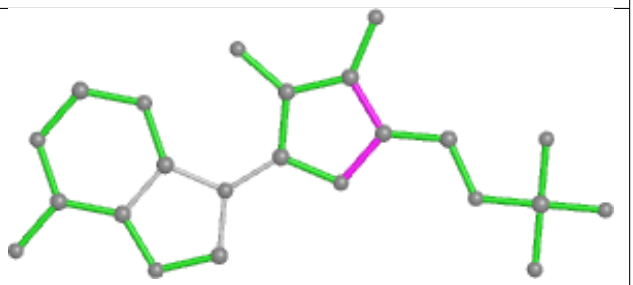
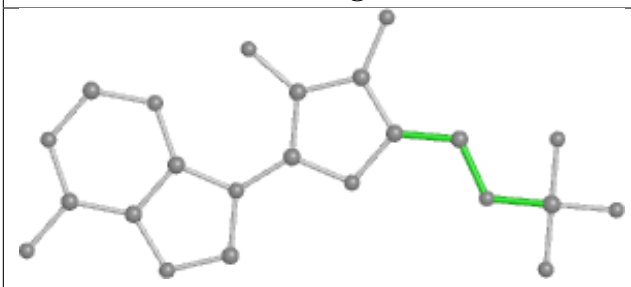


Bond angles



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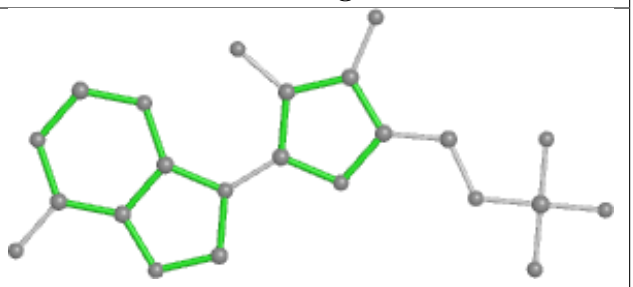
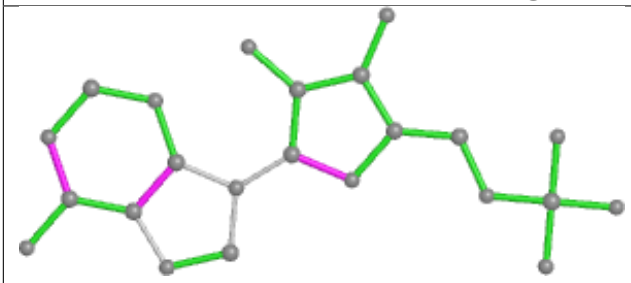


Rings

Ligand IMP H 603



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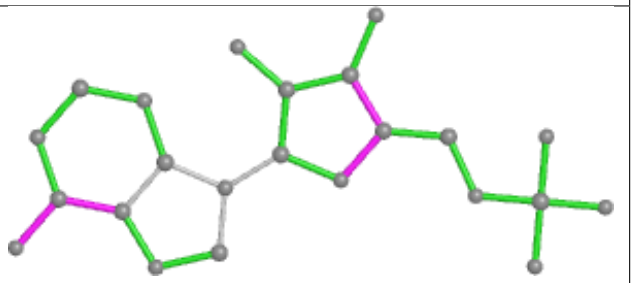
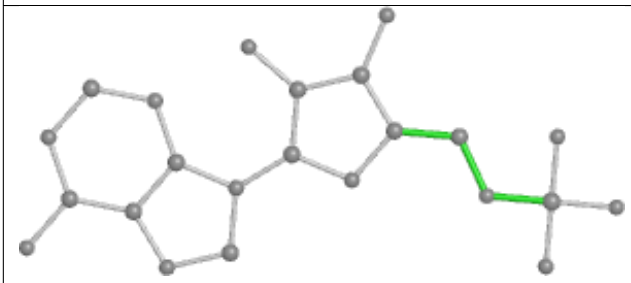


Bond angles



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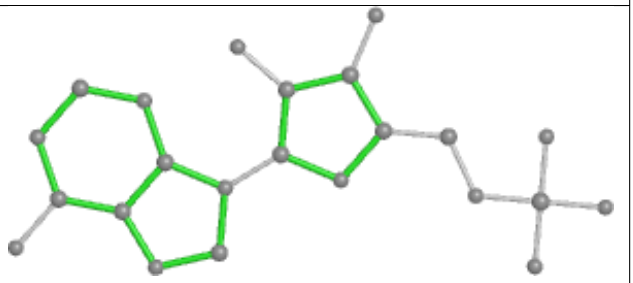
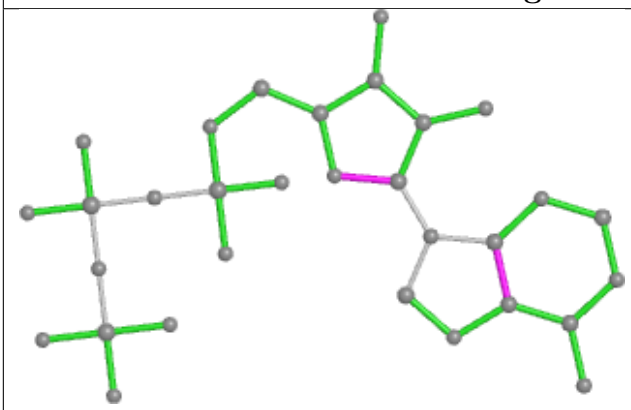


Rings

Ligand ATP A 601



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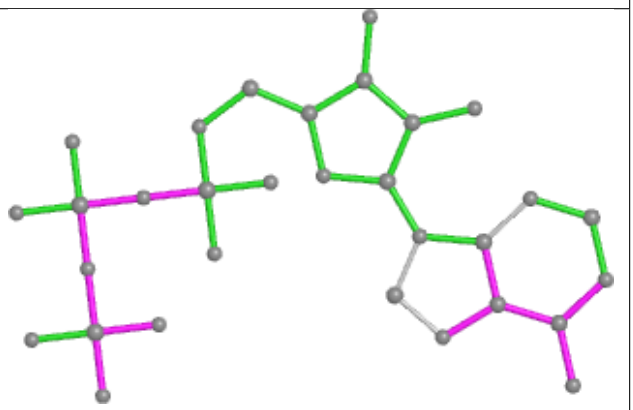

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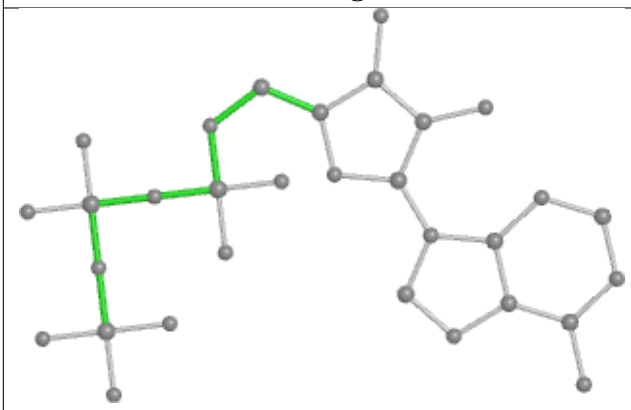

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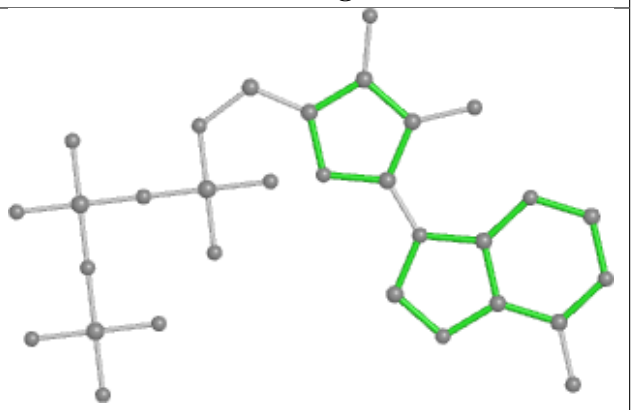
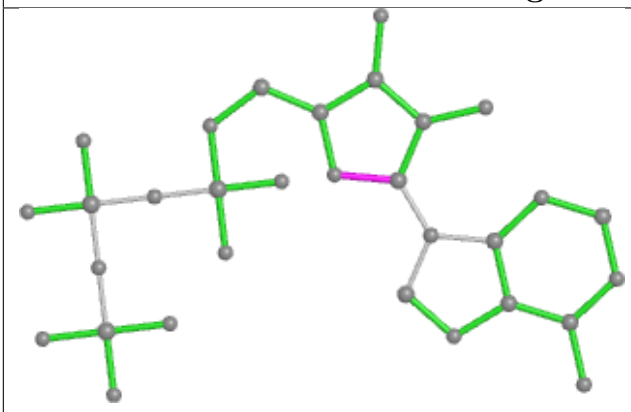


Rings

Ligand ATP F 602



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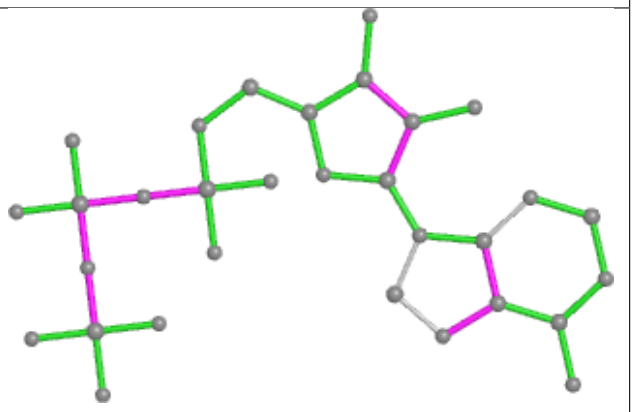
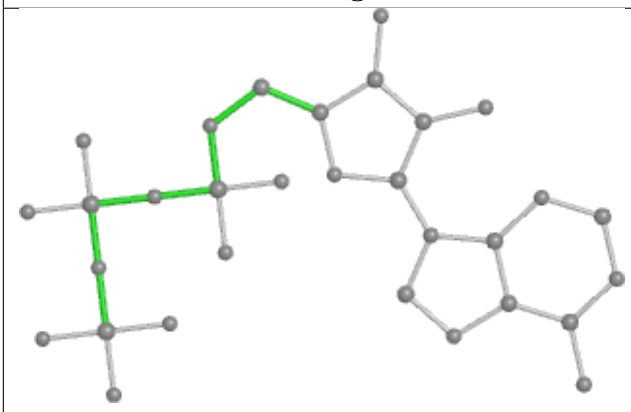


Bond angles



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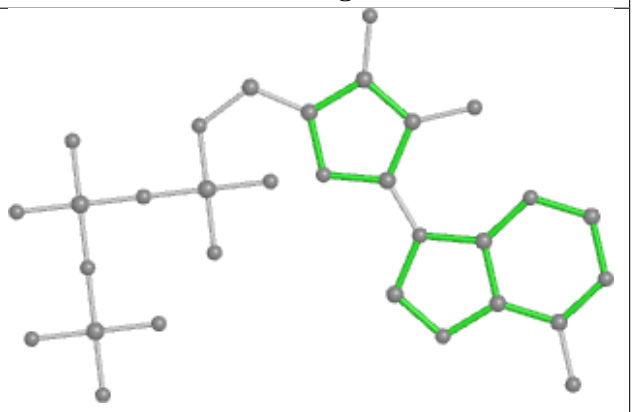
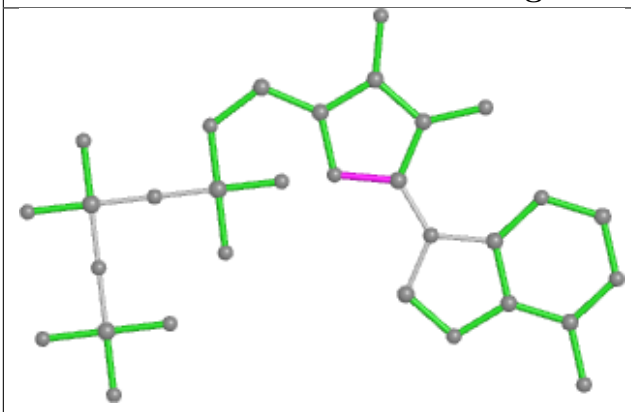


Rings

Ligand ATP B 602



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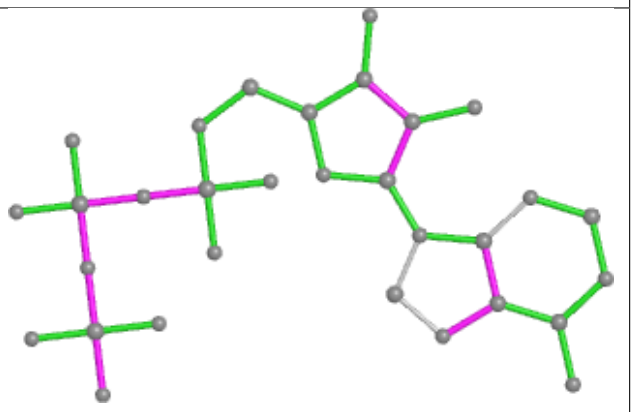
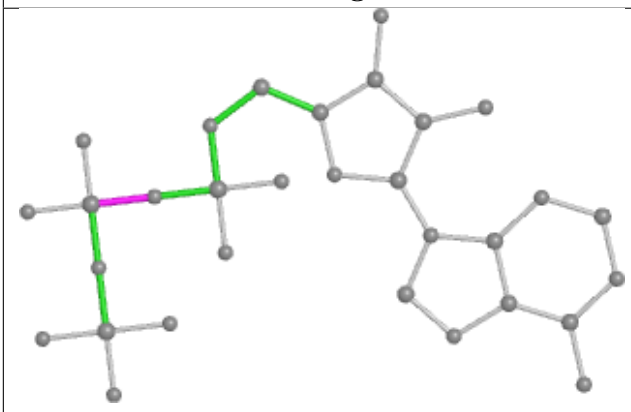


Bond angles



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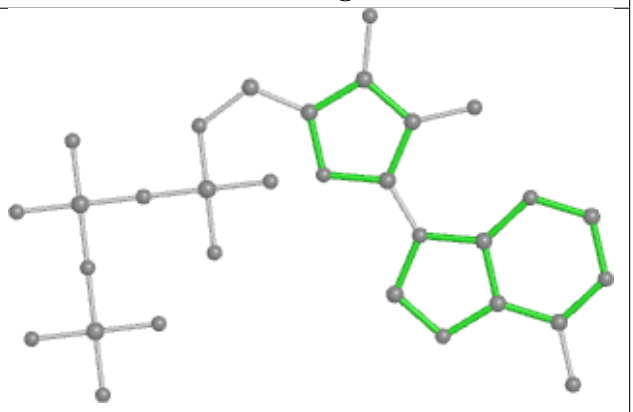
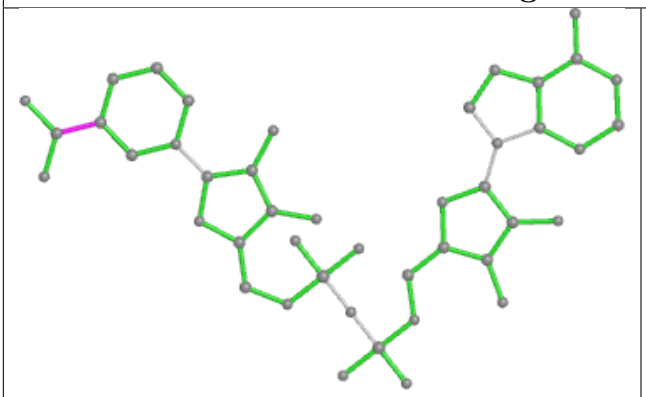


Rings

Ligand NAD A 604



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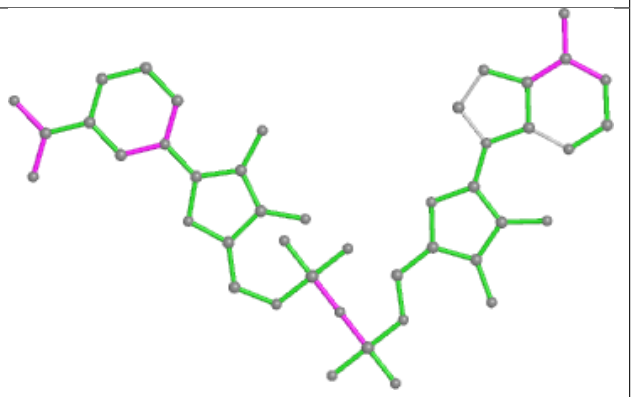
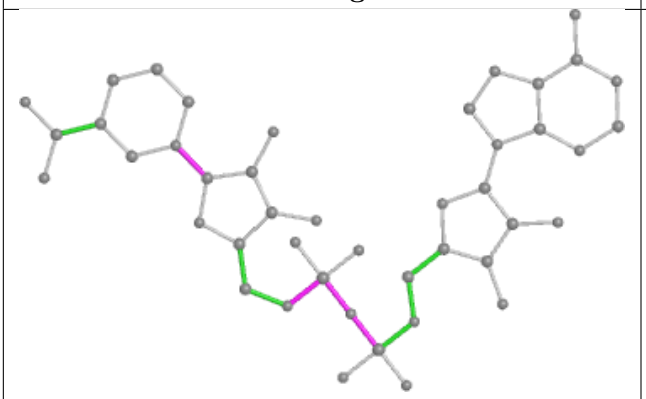


Bond angles



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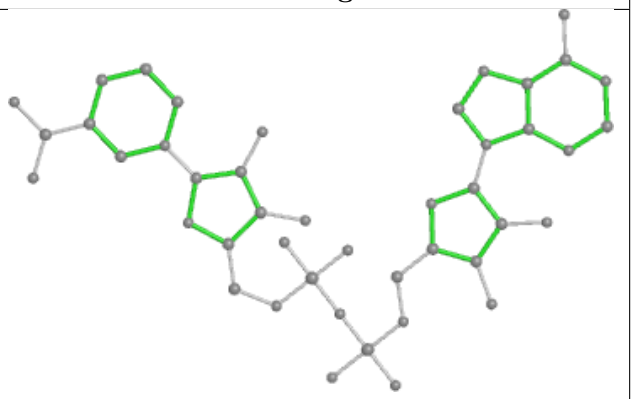
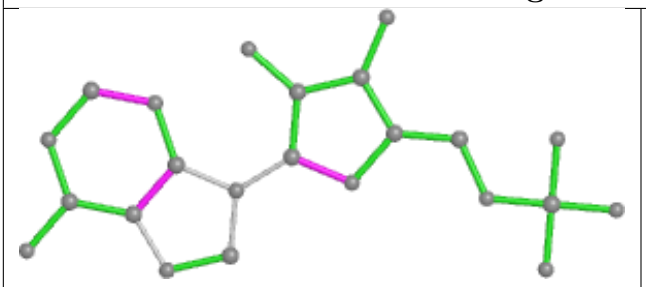


Rings

Ligand IMP E 603



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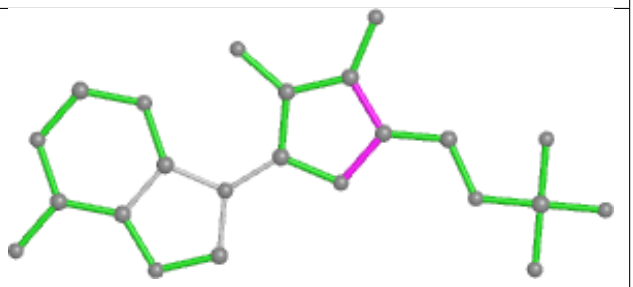

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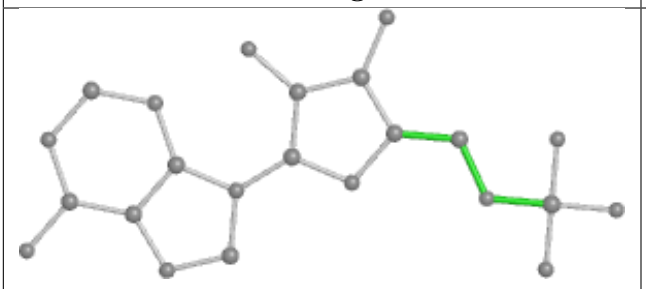

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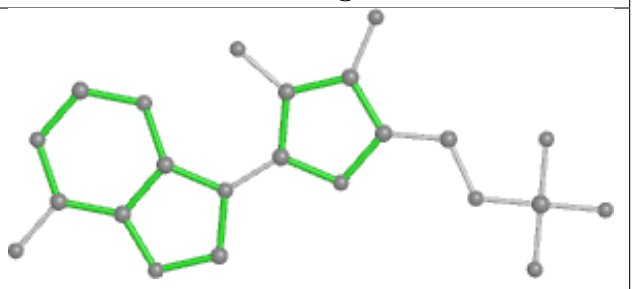
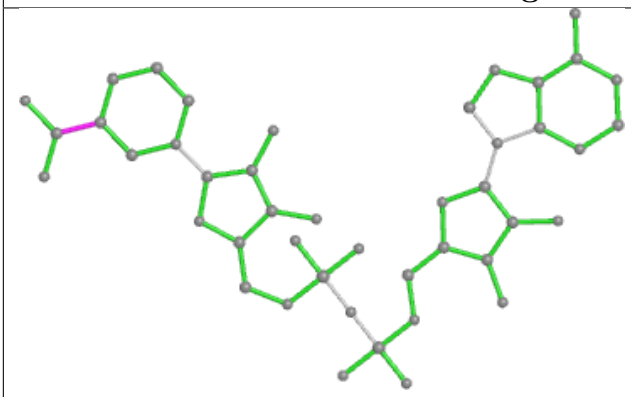


Rings

Ligand NAD E 604



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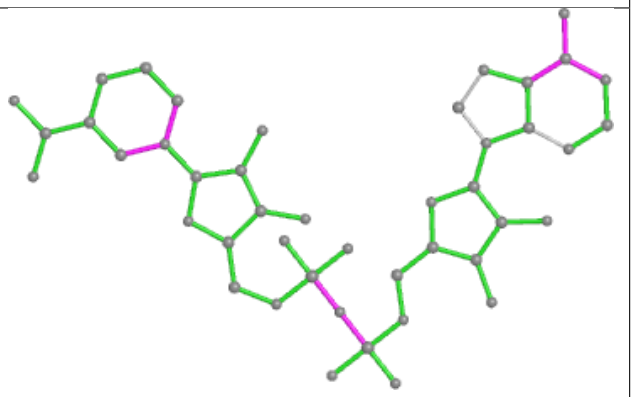
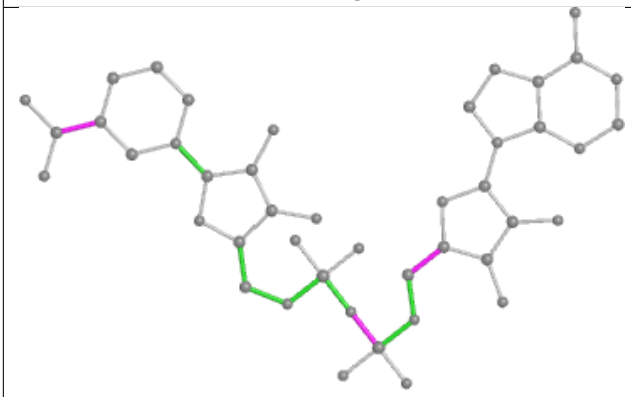


Bond angles



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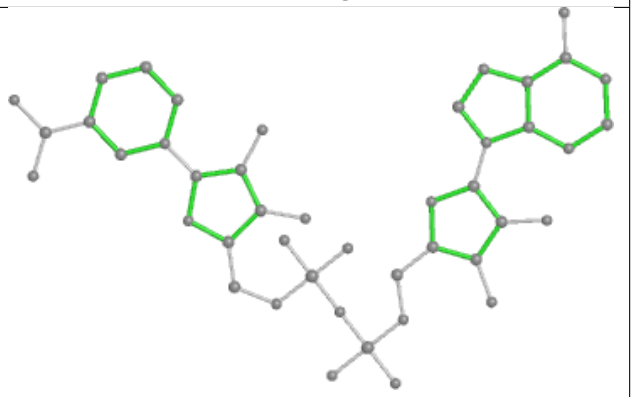
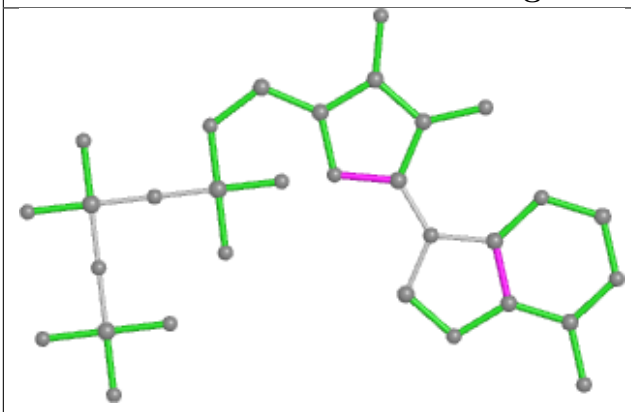
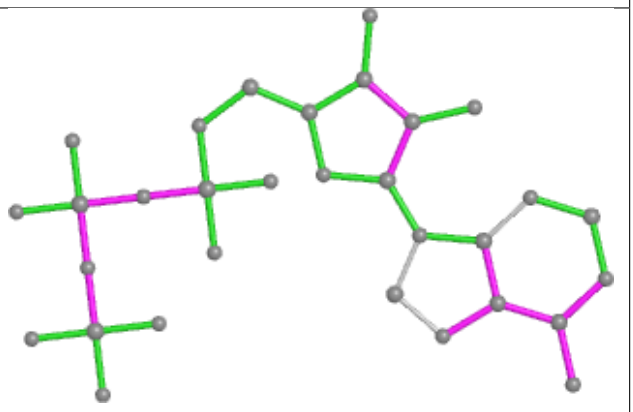


Rings

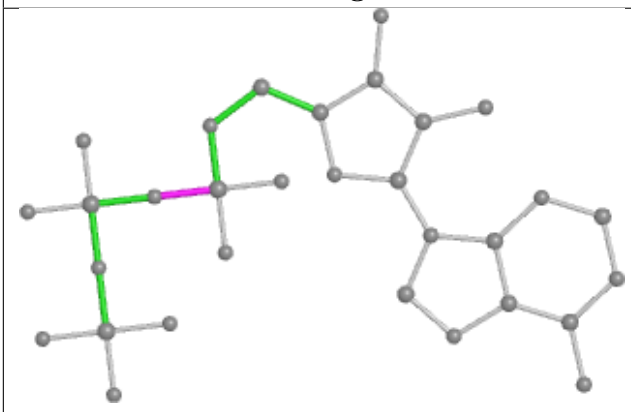
Ligand ATP G 601



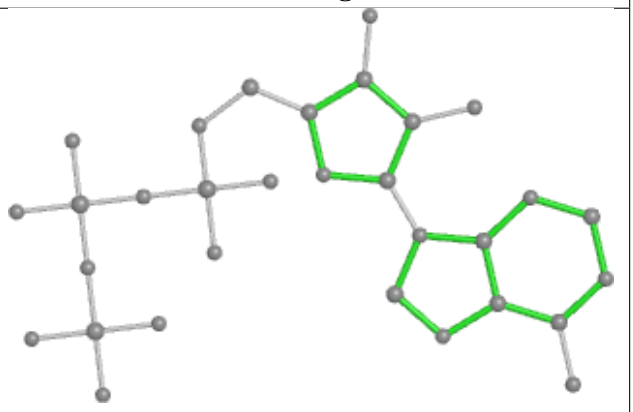
Bond lengths



Bond angles

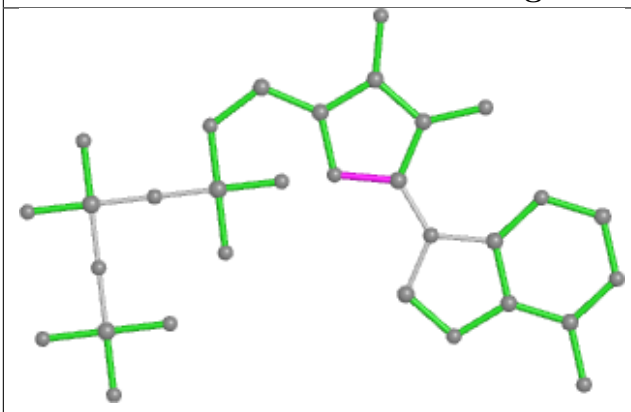


Torsions

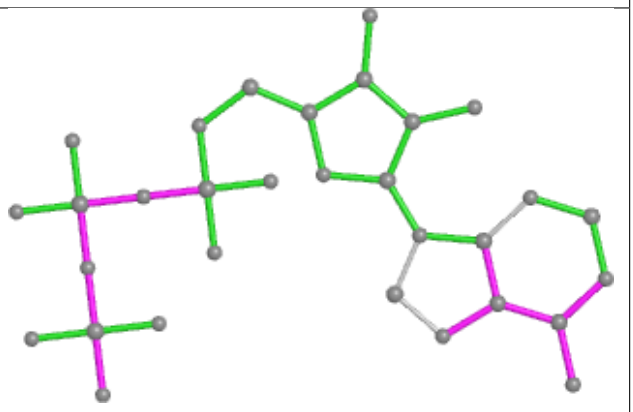


Rings

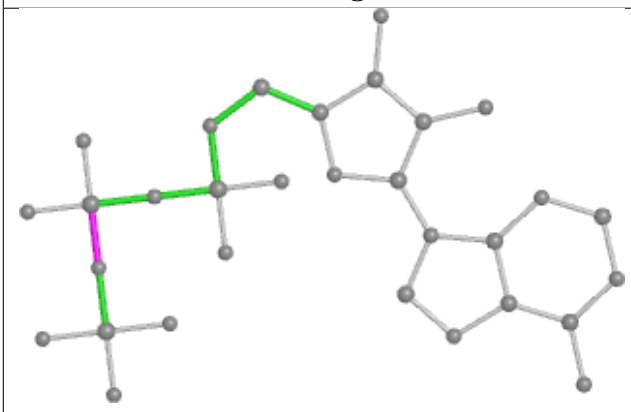
Ligand ATP C 602



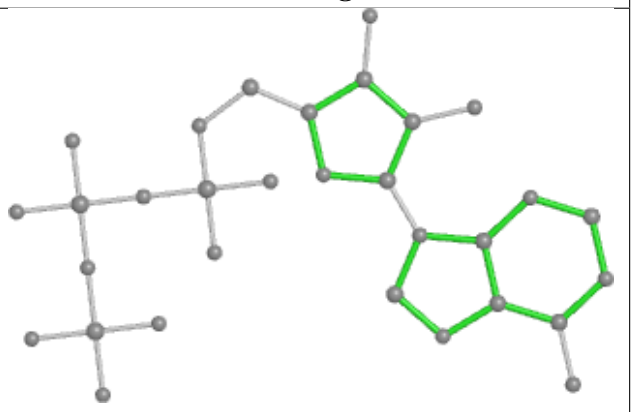
Bond lengths



Bond angles

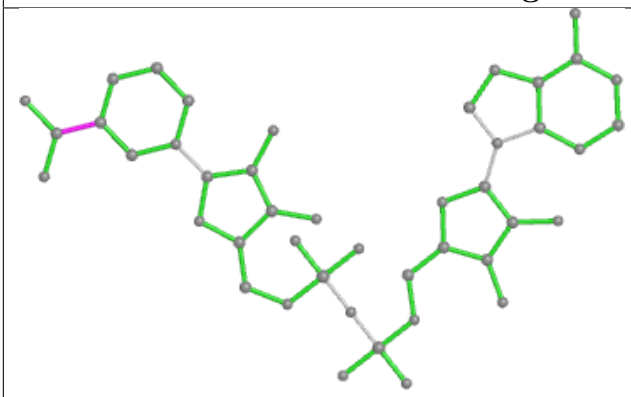


Torsions

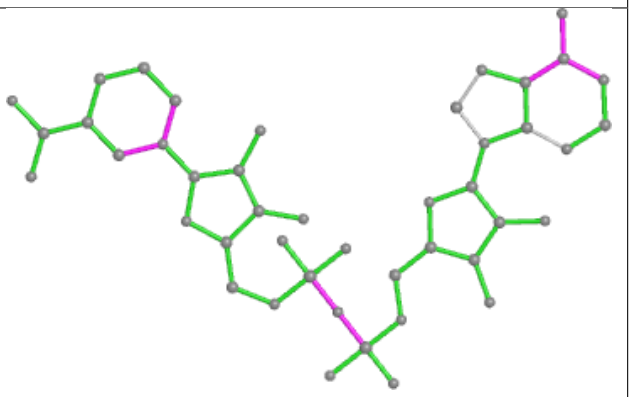


Rings

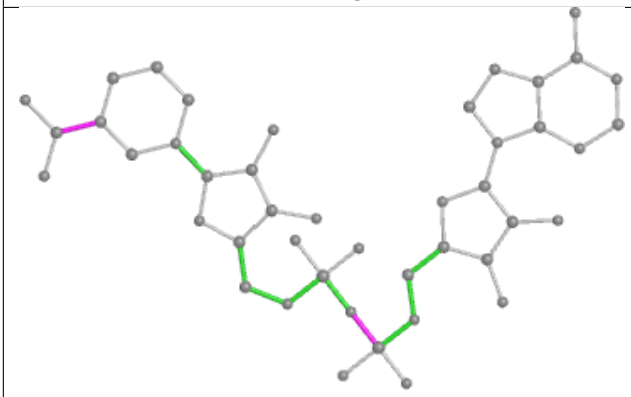
Ligand NAD F 604



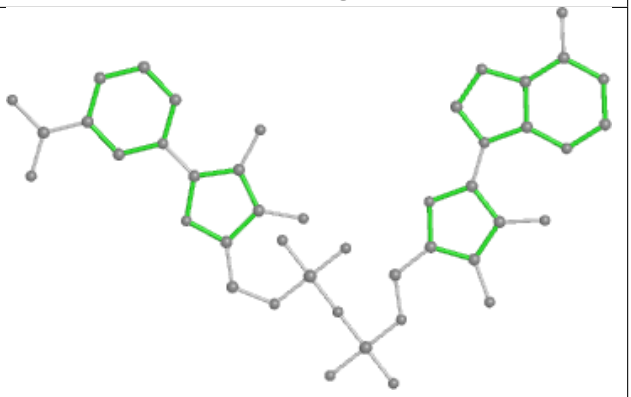
Bond lengths



Bond angles

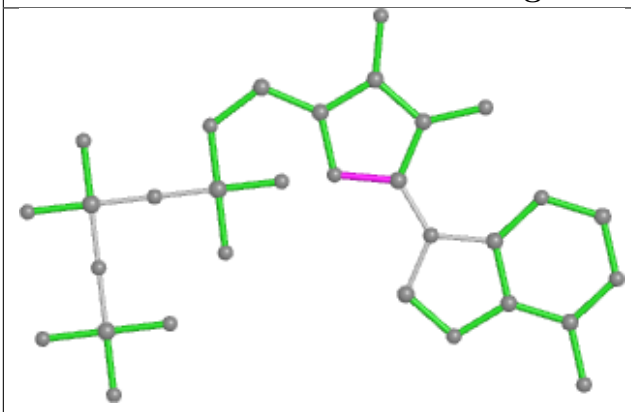


Torsions

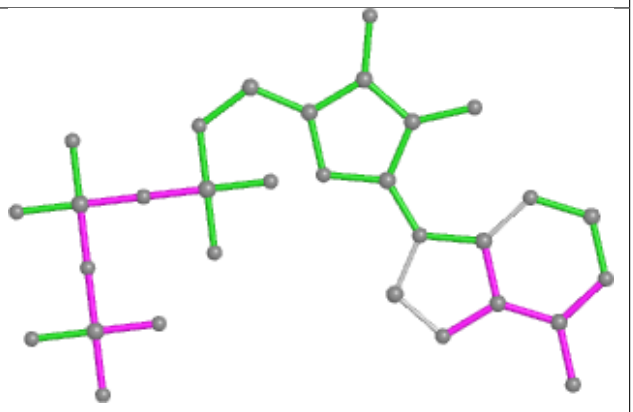


Rings

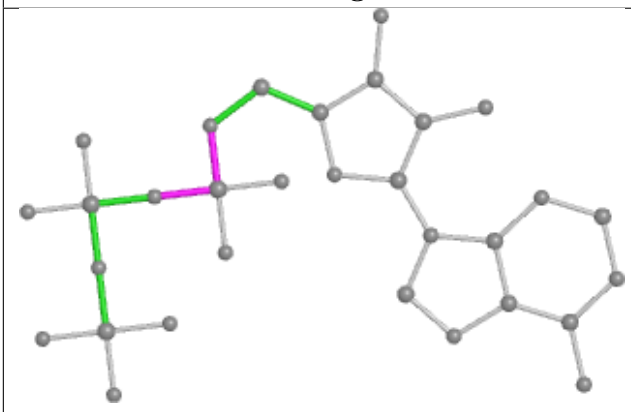
Ligand ATP D 601



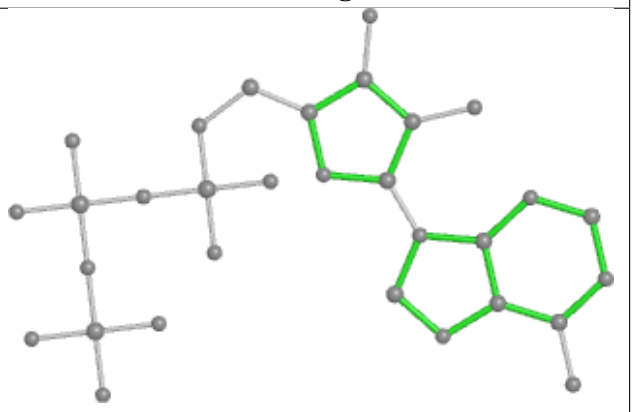
Bond lengths



Bond angles

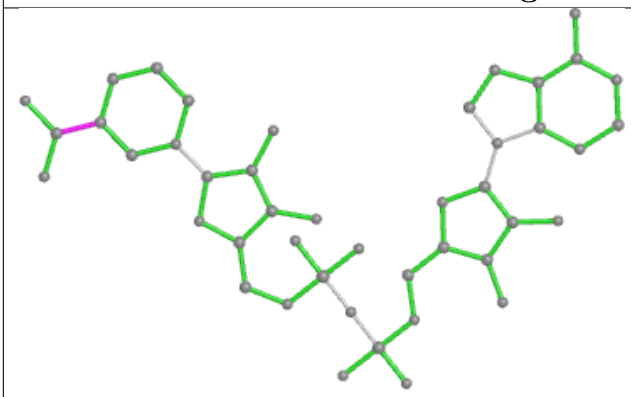


Torsions

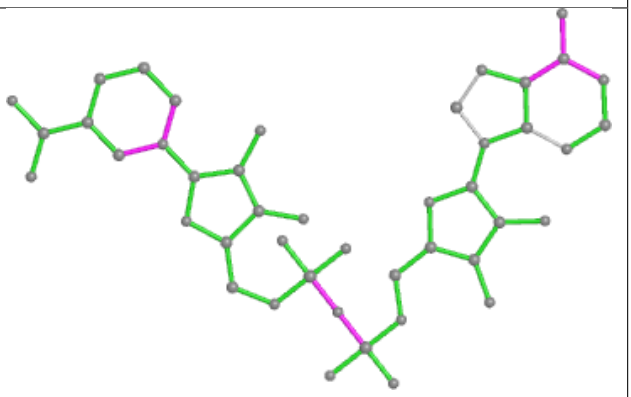


Rings

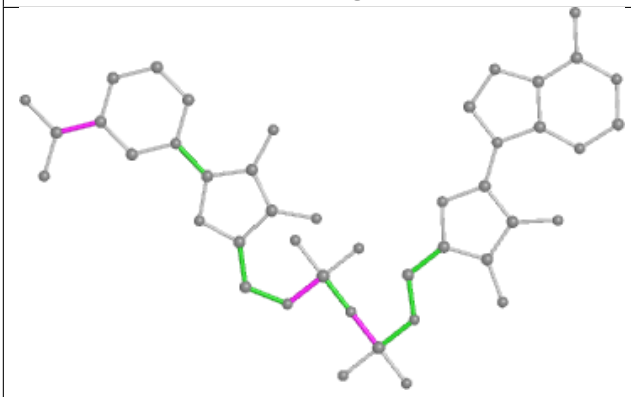
Ligand NAD B 604



Bond lengths



Bond angles



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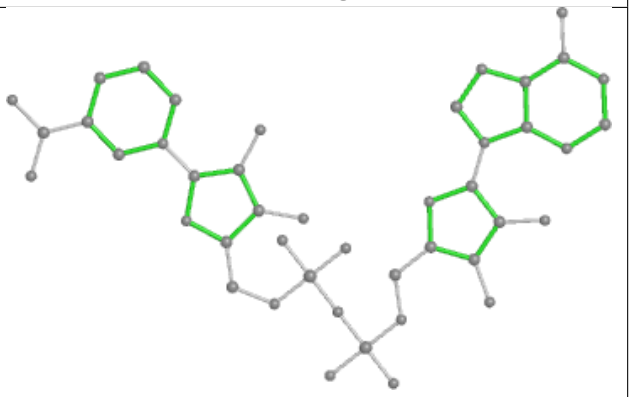
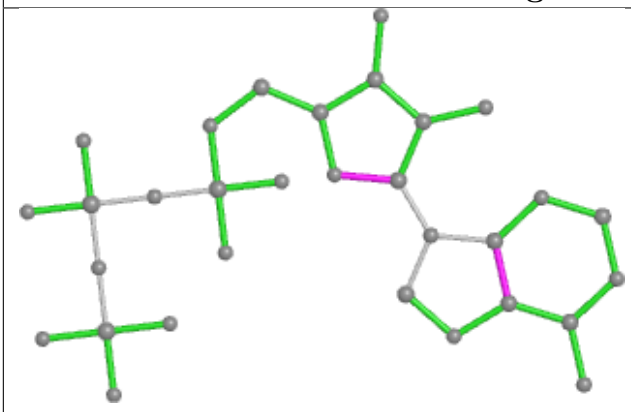
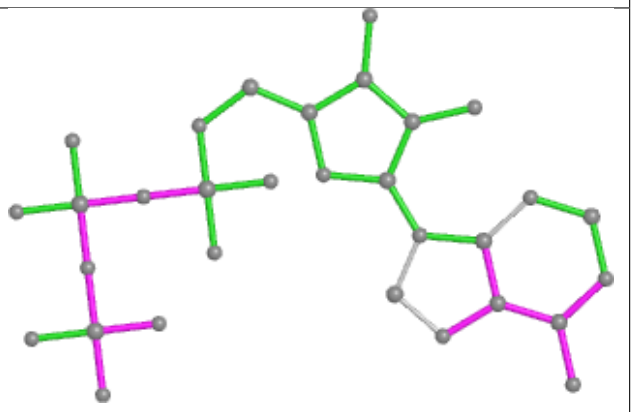


Rings

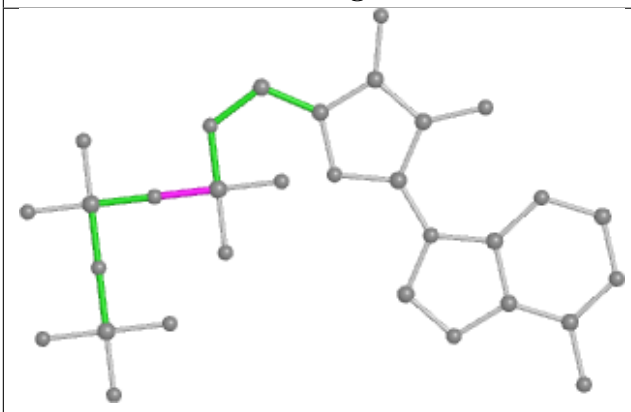
Ligand ATP F 601



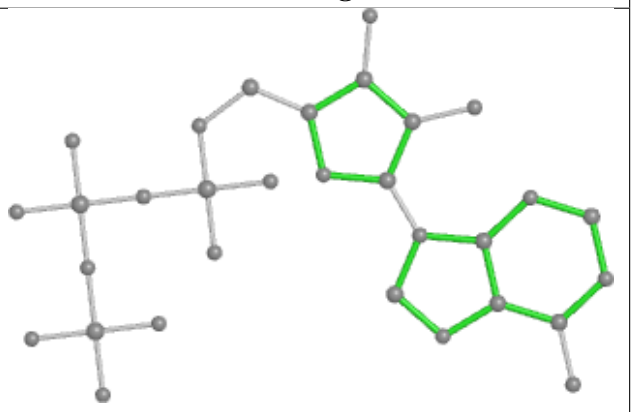
Bond lengths



Bond angles

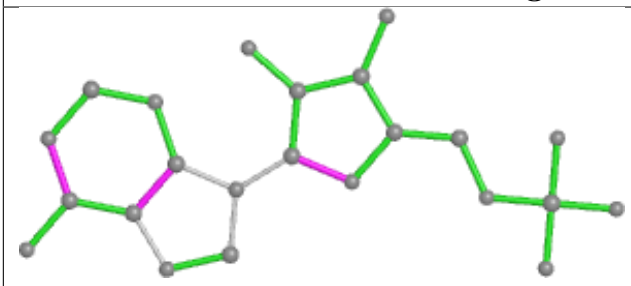


Torsions

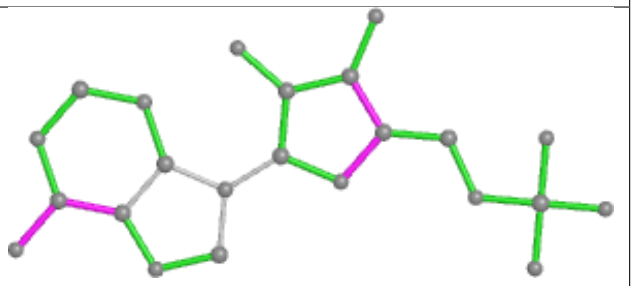


Rings

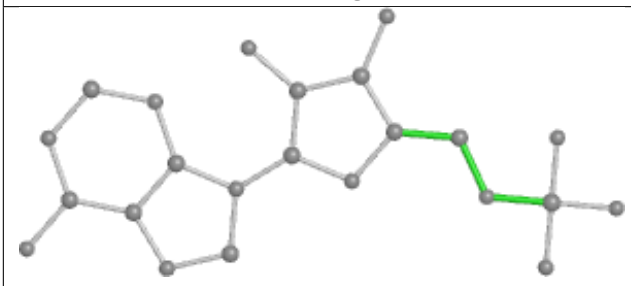
Ligand IMP B 603



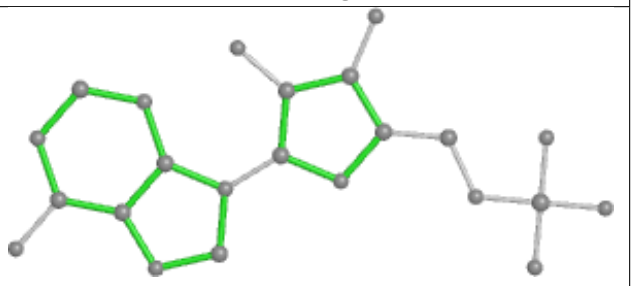
Bond lengths



Bond angles

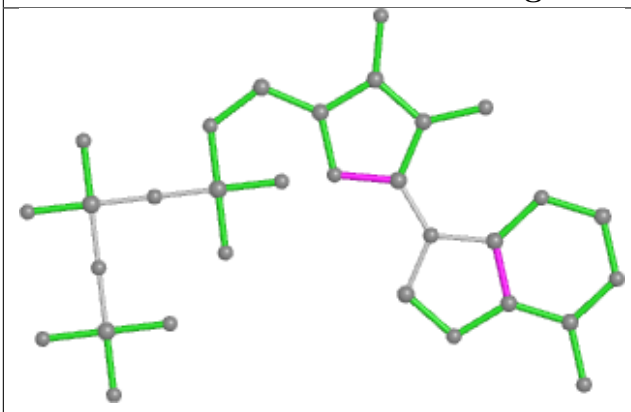


Torsions

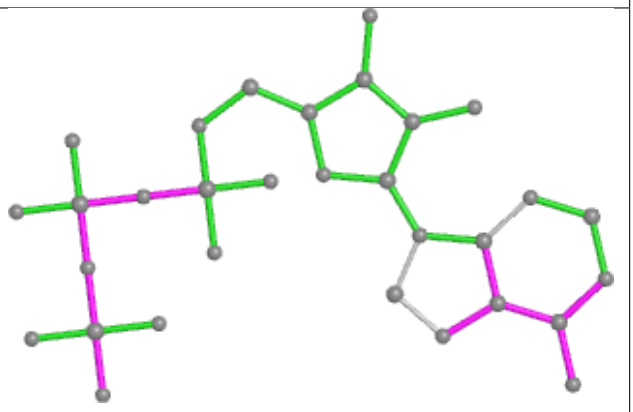


Rings

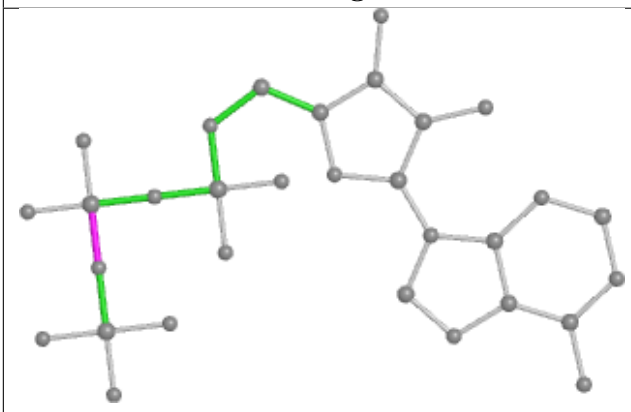
Ligand ATP C 601



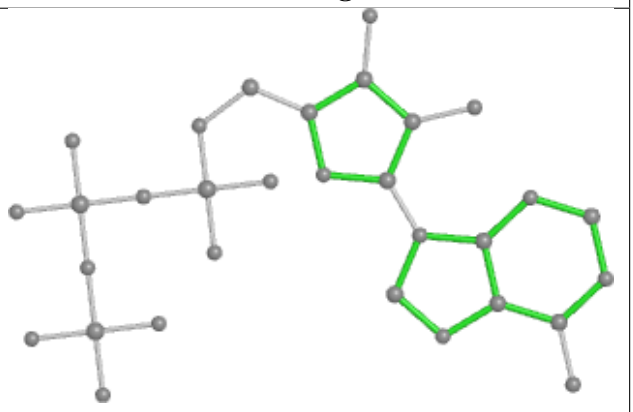
Bond lengths



Bond angles

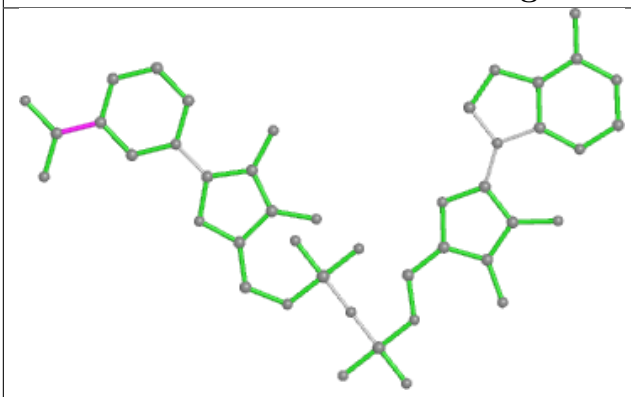


Torsions



Rings

Ligand NAD C 604



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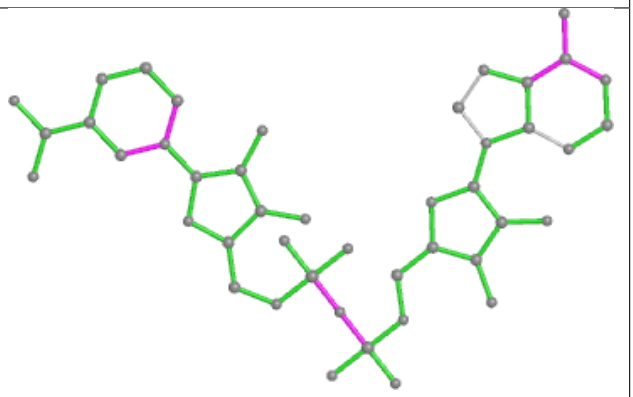
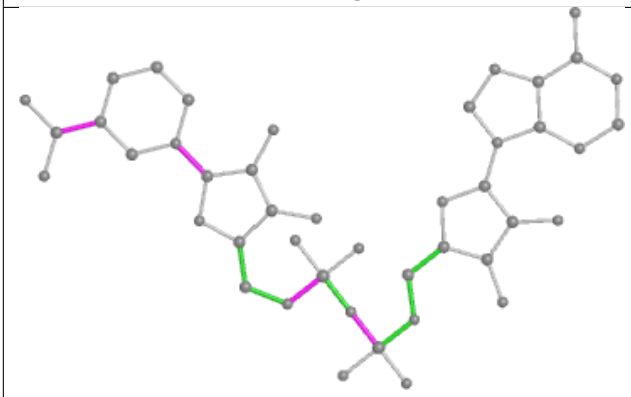
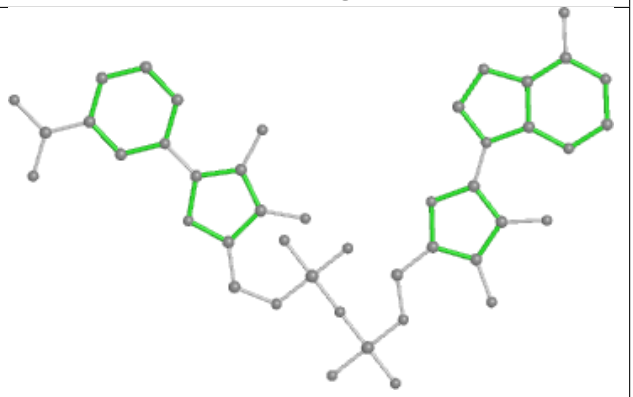


Bond angles

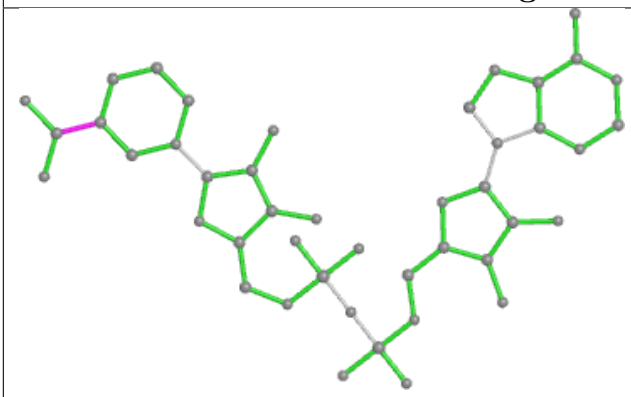


Torsions

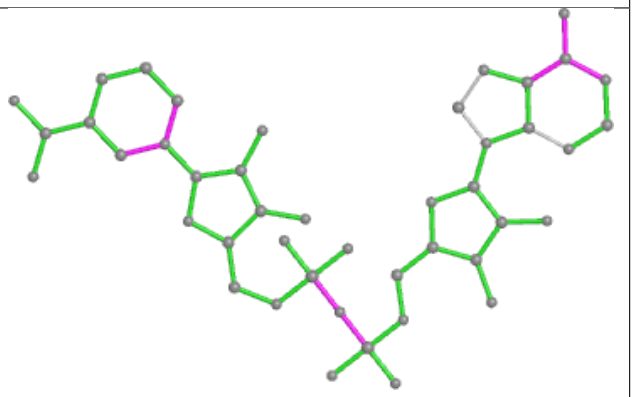


Rings

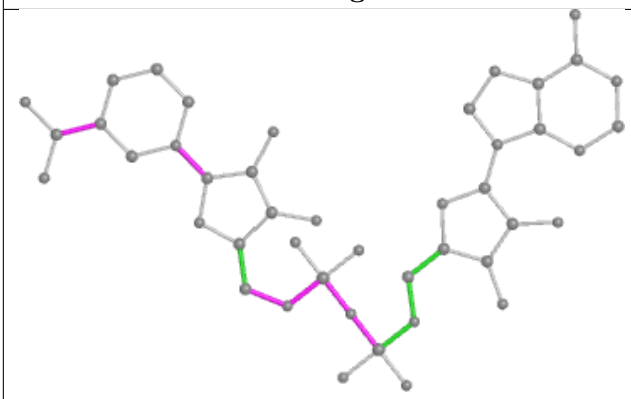
Ligand NAD H 604



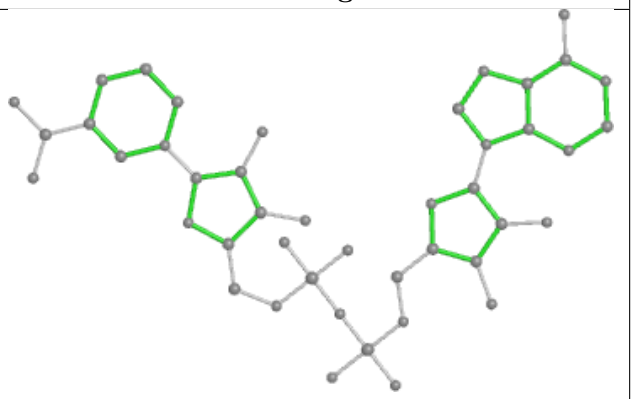
Bond lengths



Bond angles

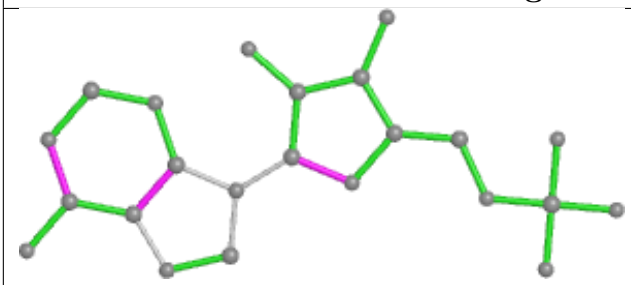


Torsions

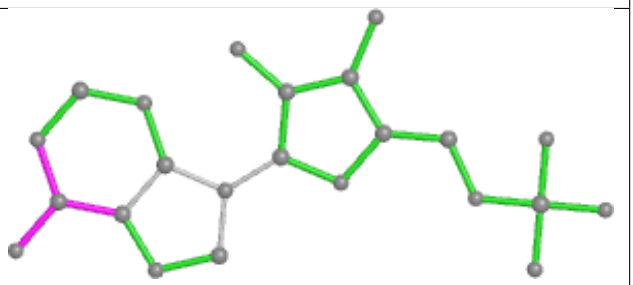


Rings

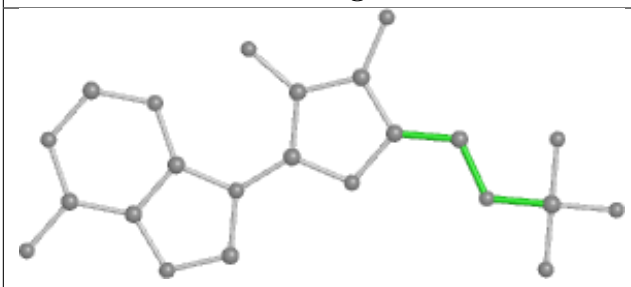
Ligand IMP A 603



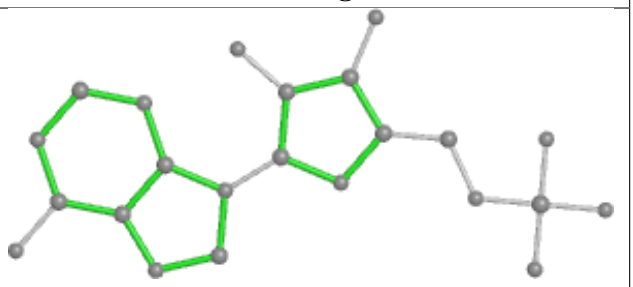
Bond lengths



Bond angles

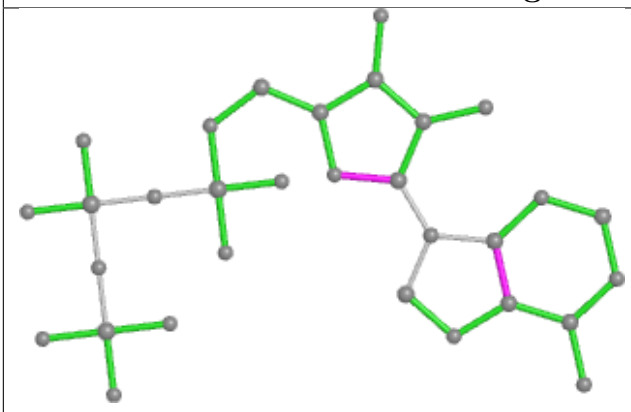


Torsions

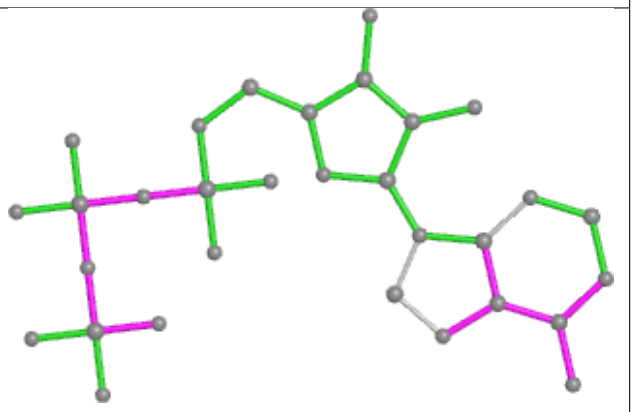


Rings

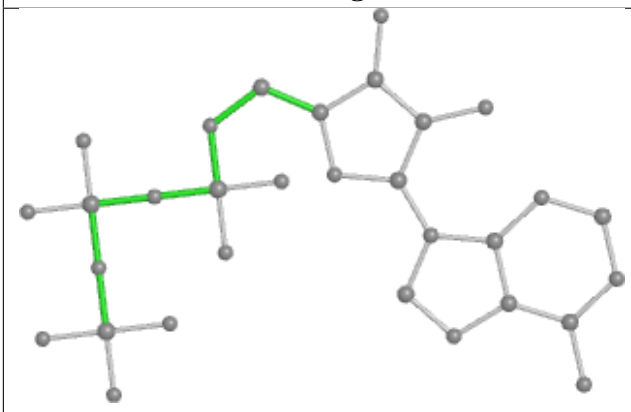
Ligand ATP H 601



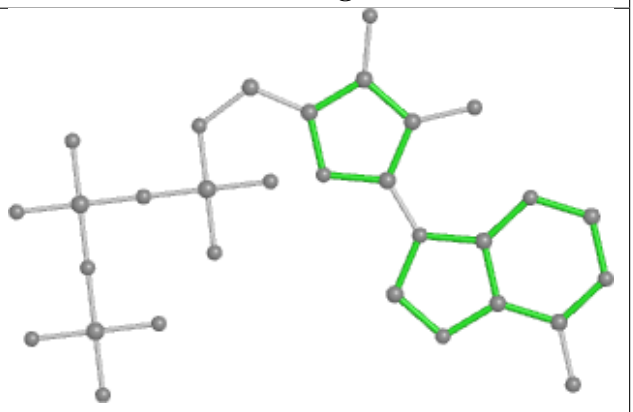
Bond lengths



Bond angles

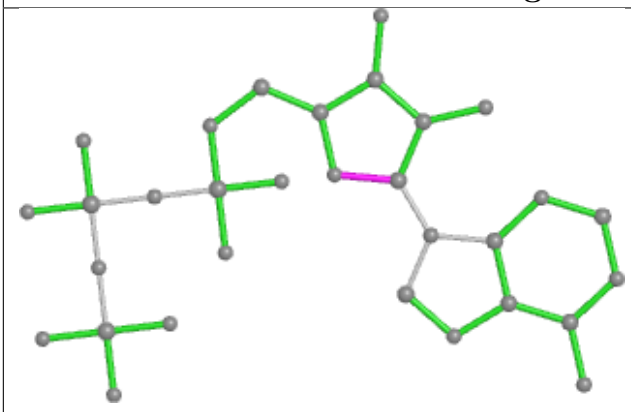


Torsions

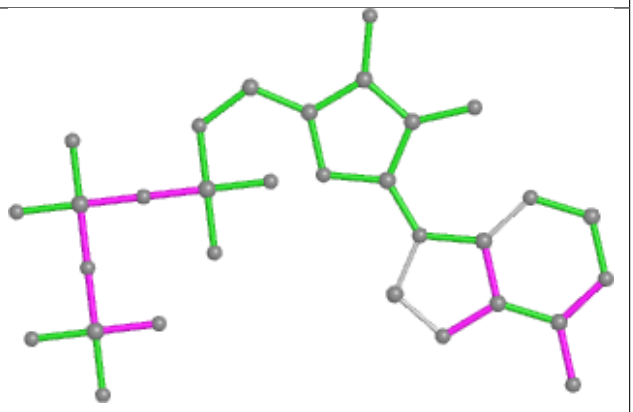


Rings

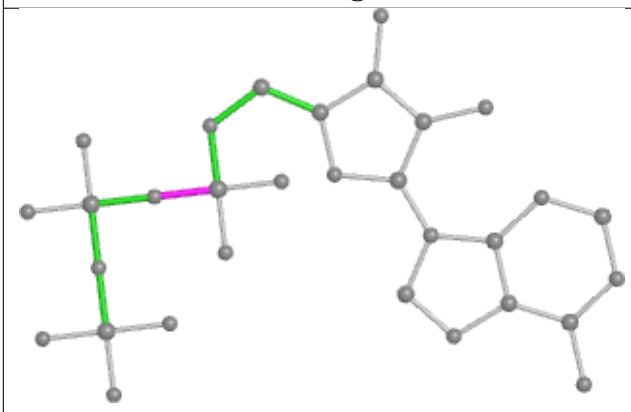
Ligand ATP D 602



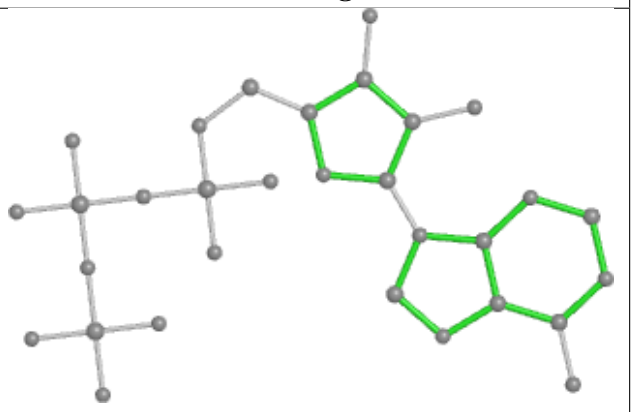
Bond lengths



Bond angles

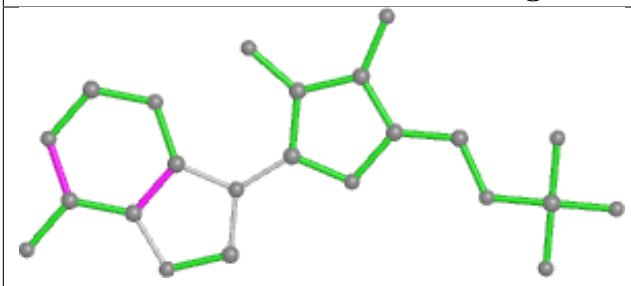


Torsions

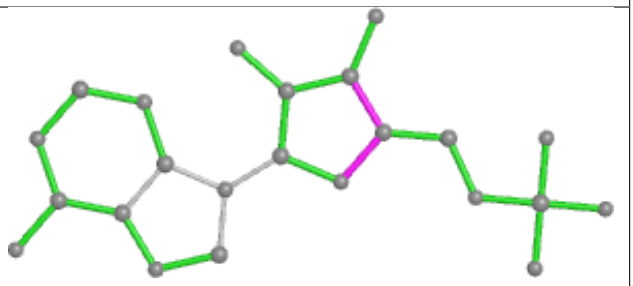


Rings

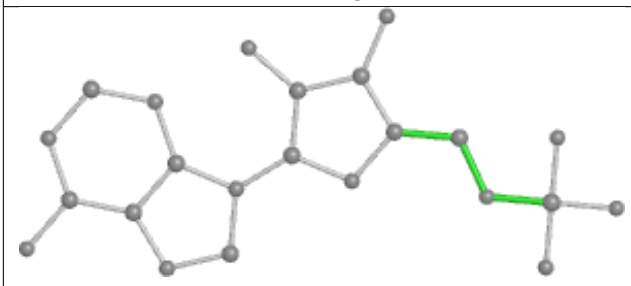
Ligand IMP G 603



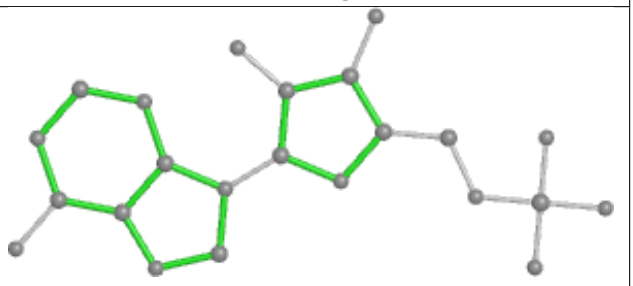
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

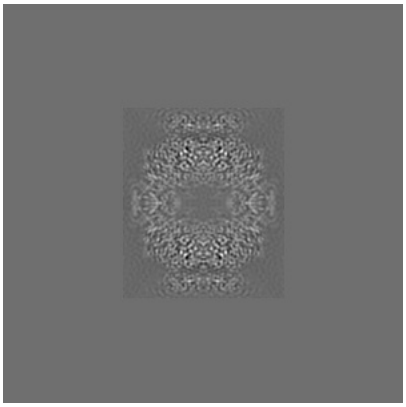
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24452. These allow visual inspection of the internal detail of the map and identification of artifacts.

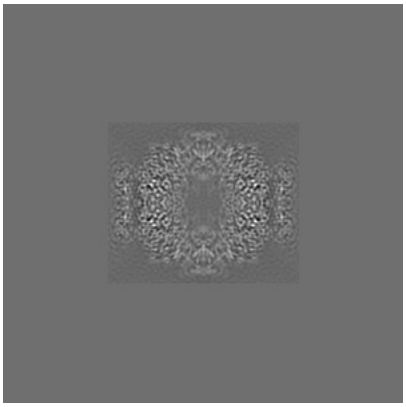
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

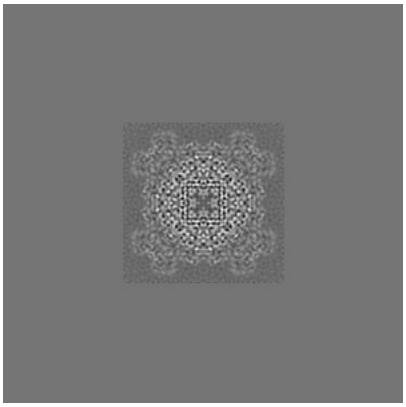
6.1.1 Primary map



X



Y

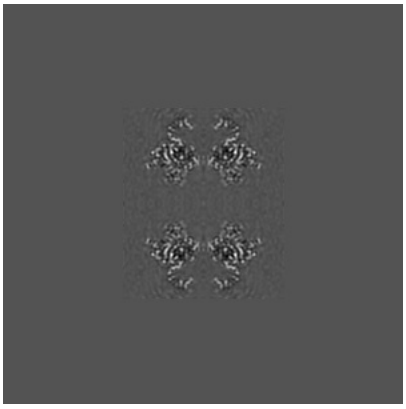


Z

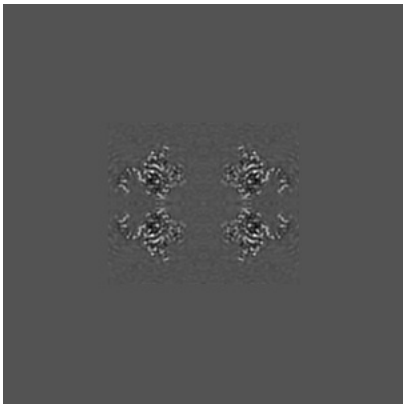
The images above show the map projected in three orthogonal directions.

6.2 Central slices

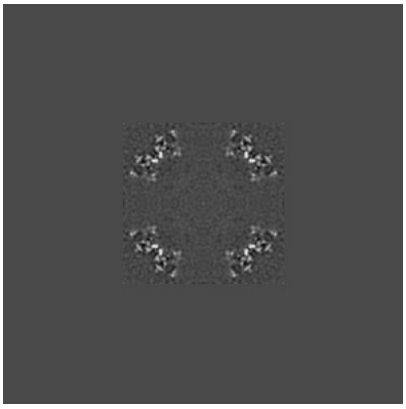
6.2.1 Primary map



X Index: 200



Y Index: 200

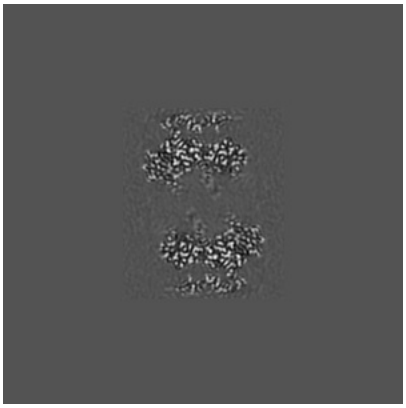


Z Index: 200

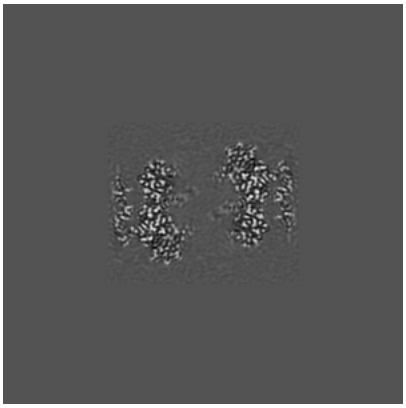
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

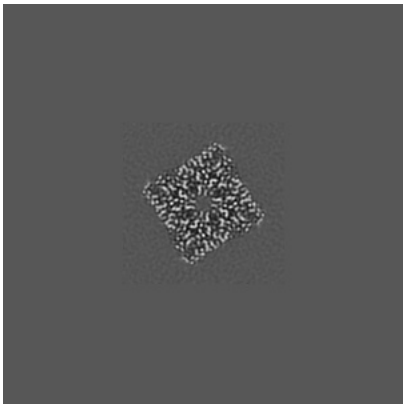
6.3.1 Primary map



X Index: 219



Y Index: 219

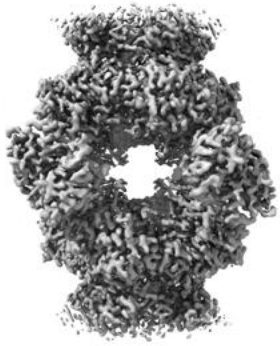


Z Index: 149

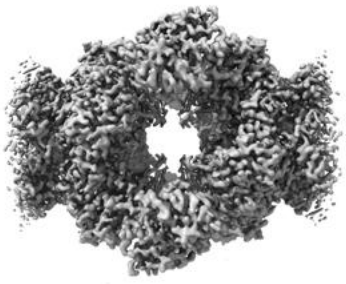
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

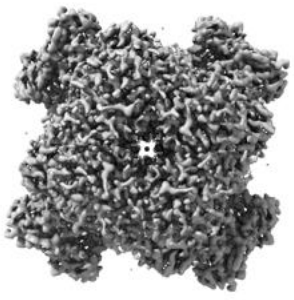
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

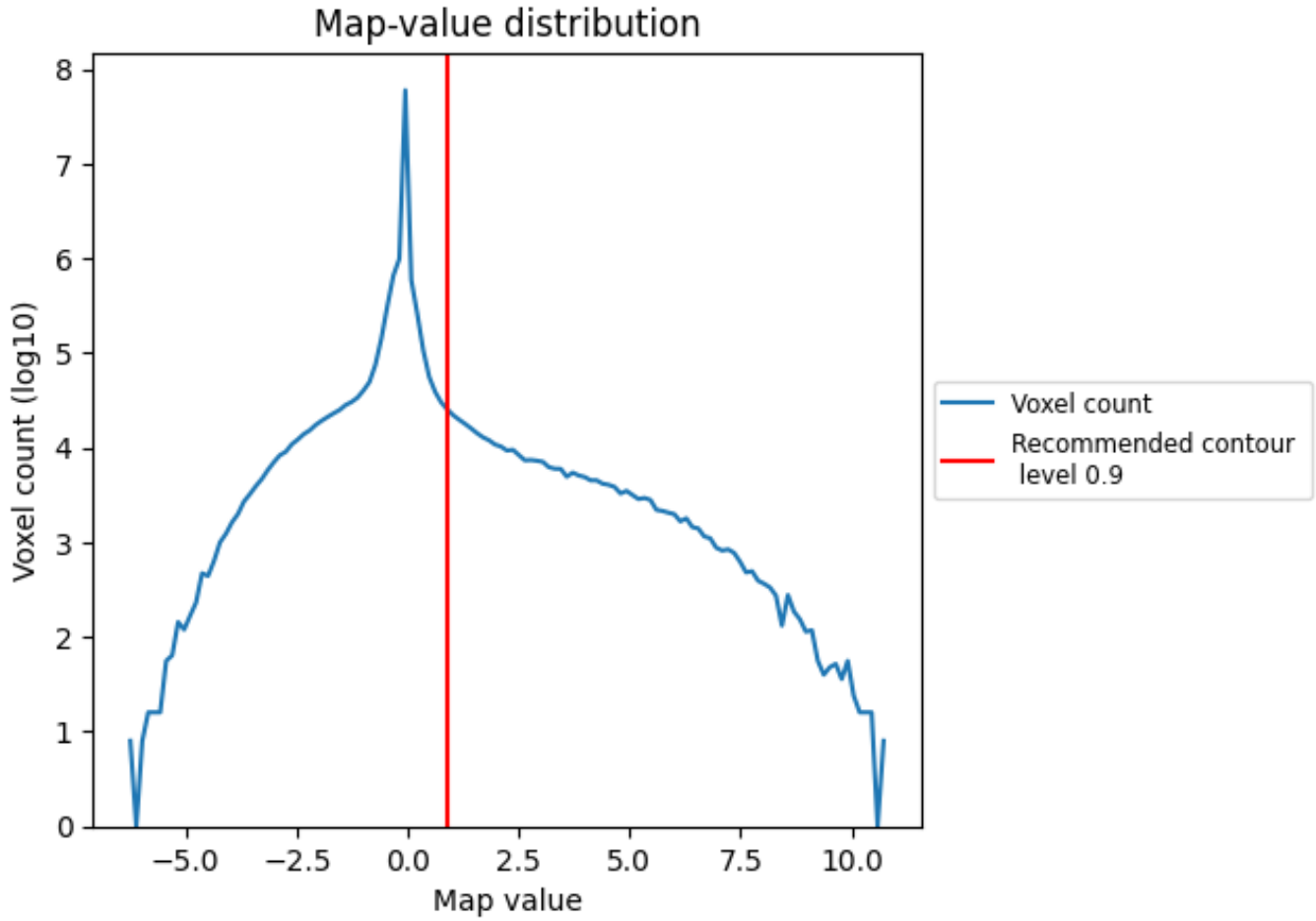
6.5 Mask visualisation (i)

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

7 Map analysis

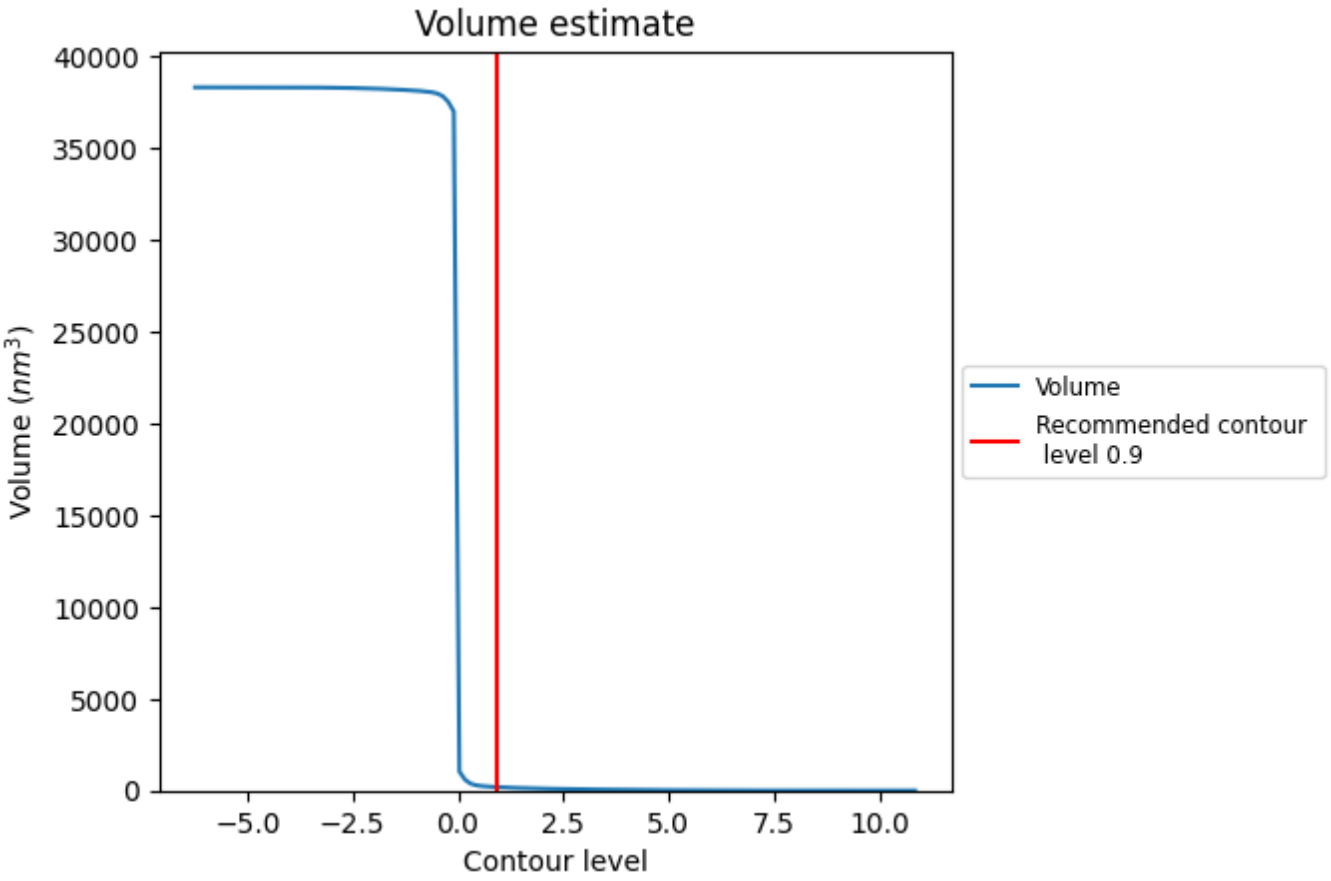
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

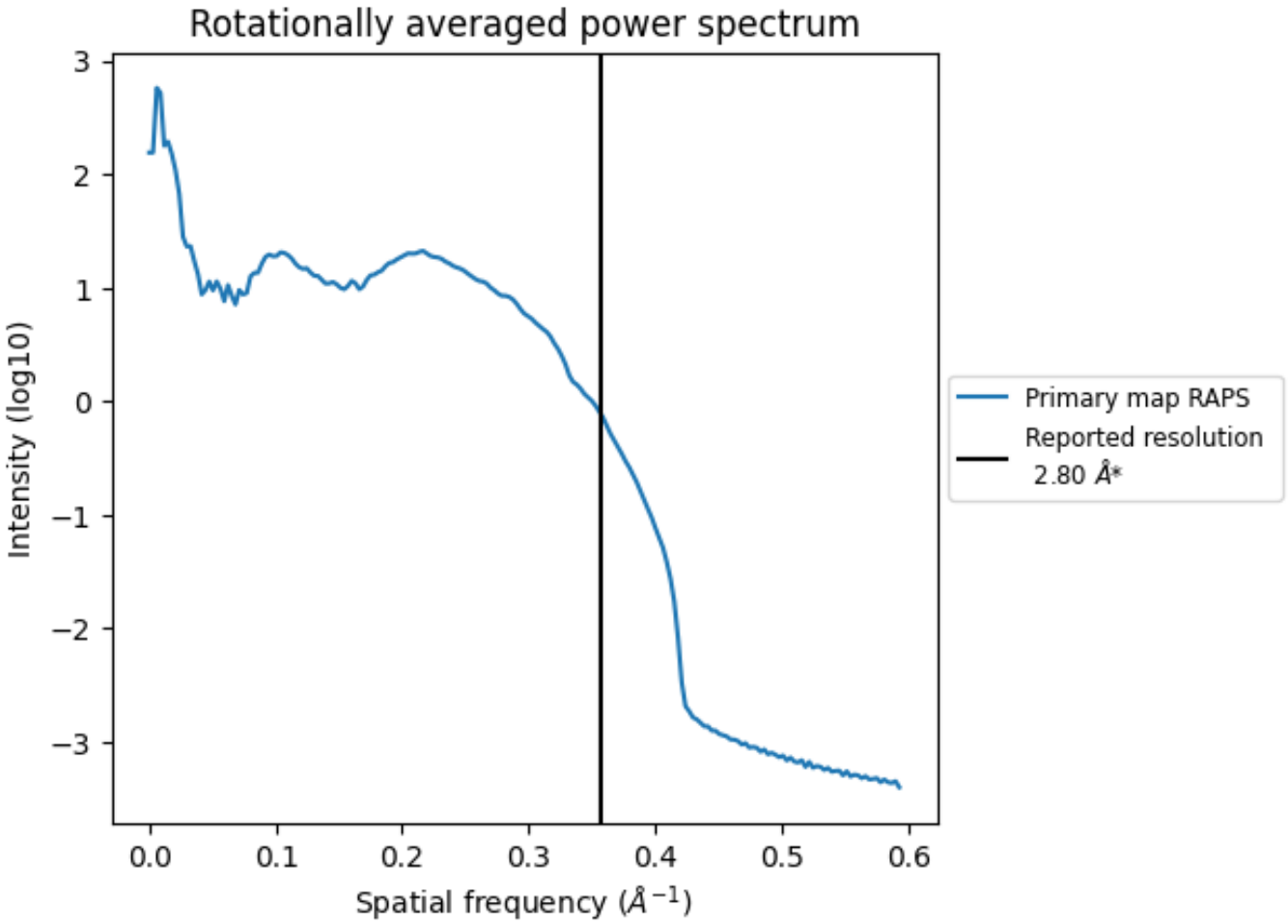
7.2 Volume estimate



The volume at the recommended contour level is 191 nm^3; this corresponds to an approximate mass of 173 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

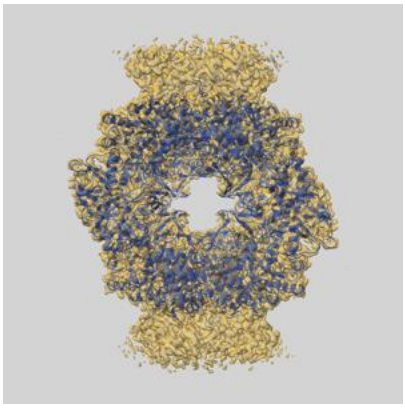
8 Fourier-Shell correlation (i)

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

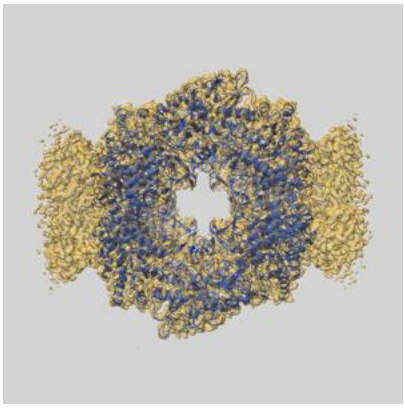
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24452 and PDB model 7RGM. Per-residue inclusion information can be found in section 3 on page 14.

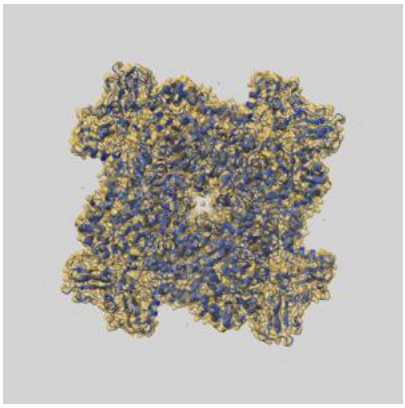
9.1 Map-model overlay



X



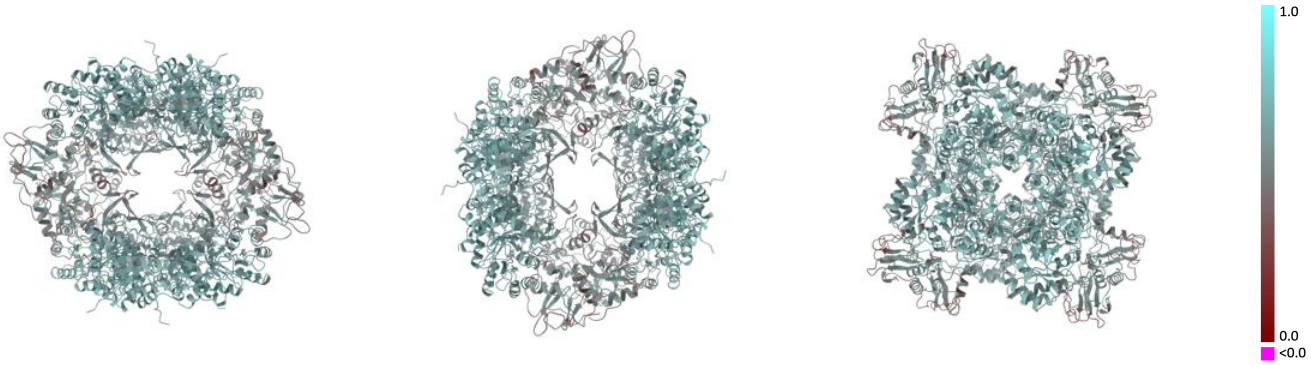
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

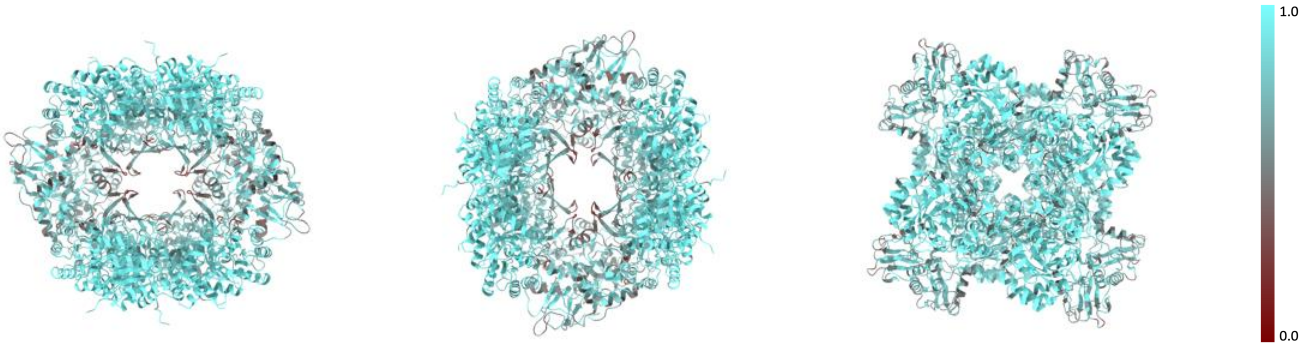
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

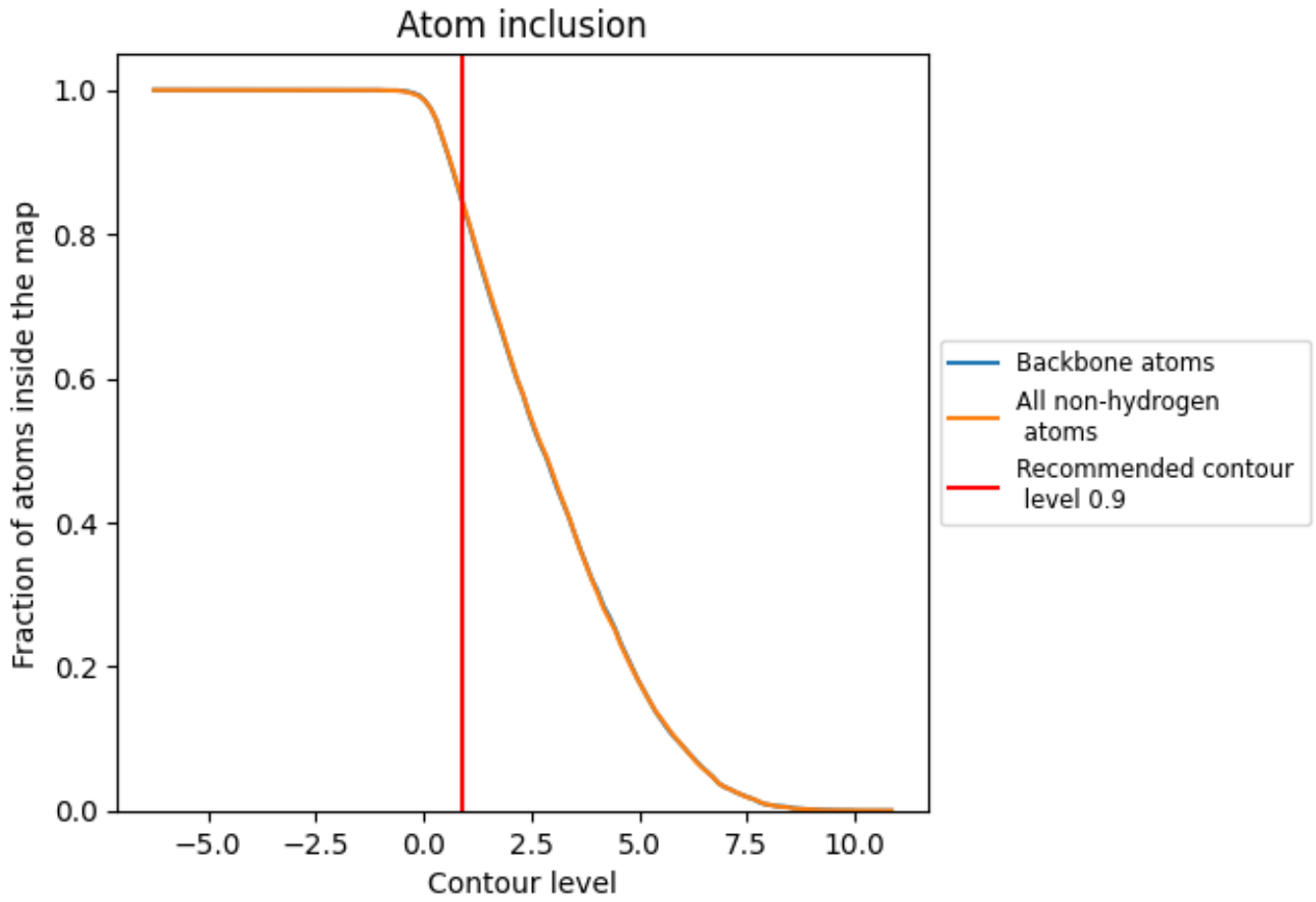
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8461	0.5870
A	0.8479	0.5860
B	0.8479	0.5870
C	0.8466	0.5860
D	0.8479	0.5880
E	0.8469	0.5860
F	0.8528	0.5900
G	0.8514	0.5870
H	0.8477	0.5880