wwPDB X-ray Structure Validation Summary Report (i)

Apr 20, 2022 – 10:16 am BST

PDB ID	:	7R50
Title	:	Crystal structure of GMP reductase from mycobacterium smegmatis in complex with GMP.
Authors	:	Dolezal, M.; Klima, M.; Pichova, I.
Deposited on	:	2022-02-09
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

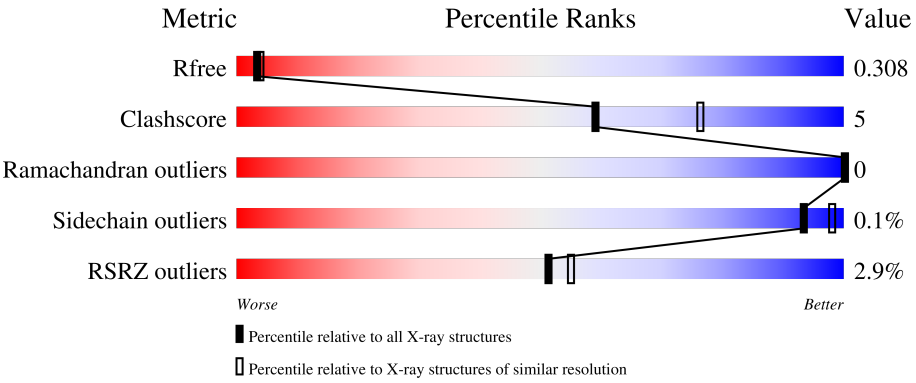
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	2% 88% 7% 5%
1	B	496	2% 80% 9% 10%
1	C	496	2% 81% 9% 10%
1	D	496	86% 8% 6%
1	E	496	2% 84% 10% 6%

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Mol	Chain	Length	Quality of chain
1	F	496	4% 74% 14% 11%
1	G	496	7% 74% 11% 15%
1	H	496	2% 82% 12% 6%
1	I	496	3% 83% 11% 6%
1	J	496	3% 76% 12% 11%
1	K	496	4% 79% 12% 9%
1	L	496	% 83% 11% 6%
1	M	496	3% 85% 9% 5%
1	N	496	4% 85% 8% 7%
1	O	496	2% 81% 11% 8%
1	P	496	% 81% 12% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 53060 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 guaB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3403	2125	603	661	14			
1	B	447	Total	C	N	O	S	0	0	0
			3230	2017	572	628	13			
1	C	446	Total	C	N	O	S	0	0	0
			3235	2024	574	624	13			
1	D	468	Total	C	N	O	S	0	0	0
			3389	2118	601	656	14			
1	E	468	Total	C	N	O	S	0	0	0
			3390	2119	601	656	14			
1	F	440	Total	C	N	O	S	0	0	0
			3168	1986	561	608	13			
1	G	424	Total	C	N	O	S	0	0	0
			3017	1896	521	587	13			
1	H	468	Total	C	N	O	S	0	0	0
			3378	2107	601	656	14			
1	I	466	Total	C	N	O	S	0	0	0
			3375	2110	599	652	14			
1	J	440	Total	C	N	O	S	0	0	0
			3154	1976	551	614	13			
1	K	450	Total	C	N	O	S	0	0	0
			3216	2021	566	617	12			
1	L	465	Total	C	N	O	S	0	0	0
			3346	2089	594	649	14			
1	M	471	Total	C	N	O	S	0	0	0
			3376	2114	592	656	14			
1	N	461	Total	C	N	O	S	0	0	0
			3350	2093	597	646	14			
1	O	455	Total	C	N	O	S	0	0	0
			3280	2049	582	636	13			
1	P	465	Total	C	N	O	S	0	0	0
			3369	2108	601	646	14			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	insertion	UNP I7GA39
A	480	THR	-	expression tag	UNP I7GA39
A	481	ALA	-	expression tag	UNP I7GA39
A	482	ALA	-	expression tag	UNP I7GA39
A	483	ALA	-	expression tag	UNP I7GA39
A	484	LYS	-	expression tag	UNP I7GA39
A	485	GLU	-	expression tag	UNP I7GA39
A	486	ASP	-	expression tag	UNP I7GA39
A	487	LEU	-	expression tag	UNP I7GA39
A	488	GLU	-	expression tag	UNP I7GA39
A	489	HIS	-	expression tag	UNP I7GA39
A	490	HIS	-	expression tag	UNP I7GA39
A	491	HIS	-	expression tag	UNP I7GA39
A	492	HIS	-	expression tag	UNP I7GA39
A	493	HIS	-	expression tag	UNP I7GA39
A	494	HIS	-	expression tag	UNP I7GA39
A	495	HIS	-	expression tag	UNP I7GA39
A	496	HIS	-	expression tag	UNP I7GA39
B	2	VAL	-	insertion	UNP I7GA39
B	480	THR	-	expression tag	UNP I7GA39
B	481	ALA	-	expression tag	UNP I7GA39
B	482	ALA	-	expression tag	UNP I7GA39
B	483	ALA	-	expression tag	UNP I7GA39
B	484	LYS	-	expression tag	UNP I7GA39
B	485	GLU	-	expression tag	UNP I7GA39
B	486	ASP	-	expression tag	UNP I7GA39
B	487	LEU	-	expression tag	UNP I7GA39
B	488	GLU	-	expression tag	UNP I7GA39
B	489	HIS	-	expression tag	UNP I7GA39
B	490	HIS	-	expression tag	UNP I7GA39
B	491	HIS	-	expression tag	UNP I7GA39
B	492	HIS	-	expression tag	UNP I7GA39
B	493	HIS	-	expression tag	UNP I7GA39
B	494	HIS	-	expression tag	UNP I7GA39
B	495	HIS	-	expression tag	UNP I7GA39
B	496	HIS	-	expression tag	UNP I7GA39
C	2	VAL	-	insertion	UNP I7GA39
C	480	THR	-	expression tag	UNP I7GA39
C	481	ALA	-	expression tag	UNP I7GA39
C	482	ALA	-	expression tag	UNP I7GA39
C	483	ALA	-	expression tag	UNP I7GA39
C	484	LYS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	485	GLU	-	expression tag	UNP I7GA39
C	486	ASP	-	expression tag	UNP I7GA39
C	487	LEU	-	expression tag	UNP I7GA39
C	488	GLU	-	expression tag	UNP I7GA39
C	489	HIS	-	expression tag	UNP I7GA39
C	490	HIS	-	expression tag	UNP I7GA39
C	491	HIS	-	expression tag	UNP I7GA39
C	492	HIS	-	expression tag	UNP I7GA39
C	493	HIS	-	expression tag	UNP I7GA39
C	494	HIS	-	expression tag	UNP I7GA39
C	495	HIS	-	expression tag	UNP I7GA39
C	496	HIS	-	expression tag	UNP I7GA39
D	2	VAL	-	insertion	UNP I7GA39
D	480	THR	-	expression tag	UNP I7GA39
D	481	ALA	-	expression tag	UNP I7GA39
D	482	ALA	-	expression tag	UNP I7GA39
D	483	ALA	-	expression tag	UNP I7GA39
D	484	LYS	-	expression tag	UNP I7GA39
D	485	GLU	-	expression tag	UNP I7GA39
D	486	ASP	-	expression tag	UNP I7GA39
D	487	LEU	-	expression tag	UNP I7GA39
D	488	GLU	-	expression tag	UNP I7GA39
D	489	HIS	-	expression tag	UNP I7GA39
D	490	HIS	-	expression tag	UNP I7GA39
D	491	HIS	-	expression tag	UNP I7GA39
D	492	HIS	-	expression tag	UNP I7GA39
D	493	HIS	-	expression tag	UNP I7GA39
D	494	HIS	-	expression tag	UNP I7GA39
D	495	HIS	-	expression tag	UNP I7GA39
D	496	HIS	-	expression tag	UNP I7GA39
E	2	VAL	-	insertion	UNP I7GA39
E	480	THR	-	expression tag	UNP I7GA39
E	481	ALA	-	expression tag	UNP I7GA39
E	482	ALA	-	expression tag	UNP I7GA39
E	483	ALA	-	expression tag	UNP I7GA39
E	484	LYS	-	expression tag	UNP I7GA39
E	485	GLU	-	expression tag	UNP I7GA39
E	486	ASP	-	expression tag	UNP I7GA39
E	487	LEU	-	expression tag	UNP I7GA39
E	488	GLU	-	expression tag	UNP I7GA39
E	489	HIS	-	expression tag	UNP I7GA39
E	490	HIS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
E	491	HIS	-	expression tag	UNP I7GA39
E	492	HIS	-	expression tag	UNP I7GA39
E	493	HIS	-	expression tag	UNP I7GA39
E	494	HIS	-	expression tag	UNP I7GA39
E	495	HIS	-	expression tag	UNP I7GA39
E	496	HIS	-	expression tag	UNP I7GA39
F	2	VAL	-	insertion	UNP I7GA39
F	480	THR	-	expression tag	UNP I7GA39
F	481	ALA	-	expression tag	UNP I7GA39
F	482	ALA	-	expression tag	UNP I7GA39
F	483	ALA	-	expression tag	UNP I7GA39
F	484	LYS	-	expression tag	UNP I7GA39
F	485	GLU	-	expression tag	UNP I7GA39
F	486	ASP	-	expression tag	UNP I7GA39
F	487	LEU	-	expression tag	UNP I7GA39
F	488	GLU	-	expression tag	UNP I7GA39
F	489	HIS	-	expression tag	UNP I7GA39
F	490	HIS	-	expression tag	UNP I7GA39
F	491	HIS	-	expression tag	UNP I7GA39
F	492	HIS	-	expression tag	UNP I7GA39
F	493	HIS	-	expression tag	UNP I7GA39
F	494	HIS	-	expression tag	UNP I7GA39
F	495	HIS	-	expression tag	UNP I7GA39
F	496	HIS	-	expression tag	UNP I7GA39
G	2	VAL	-	insertion	UNP I7GA39
G	480	THR	-	expression tag	UNP I7GA39
G	481	ALA	-	expression tag	UNP I7GA39
G	482	ALA	-	expression tag	UNP I7GA39
G	483	ALA	-	expression tag	UNP I7GA39
G	484	LYS	-	expression tag	UNP I7GA39
G	485	GLU	-	expression tag	UNP I7GA39
G	486	ASP	-	expression tag	UNP I7GA39
G	487	LEU	-	expression tag	UNP I7GA39
G	488	GLU	-	expression tag	UNP I7GA39
G	489	HIS	-	expression tag	UNP I7GA39
G	490	HIS	-	expression tag	UNP I7GA39
G	491	HIS	-	expression tag	UNP I7GA39
G	492	HIS	-	expression tag	UNP I7GA39
G	493	HIS	-	expression tag	UNP I7GA39
G	494	HIS	-	expression tag	UNP I7GA39
G	495	HIS	-	expression tag	UNP I7GA39
G	496	HIS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
H	2	VAL	-	insertion	UNP I7GA39
H	480	THR	-	expression tag	UNP I7GA39
H	481	ALA	-	expression tag	UNP I7GA39
H	482	ALA	-	expression tag	UNP I7GA39
H	483	ALA	-	expression tag	UNP I7GA39
H	484	LYS	-	expression tag	UNP I7GA39
H	485	GLU	-	expression tag	UNP I7GA39
H	486	ASP	-	expression tag	UNP I7GA39
H	487	LEU	-	expression tag	UNP I7GA39
H	488	GLU	-	expression tag	UNP I7GA39
H	489	HIS	-	expression tag	UNP I7GA39
H	490	HIS	-	expression tag	UNP I7GA39
H	491	HIS	-	expression tag	UNP I7GA39
H	492	HIS	-	expression tag	UNP I7GA39
H	493	HIS	-	expression tag	UNP I7GA39
H	494	HIS	-	expression tag	UNP I7GA39
H	495	HIS	-	expression tag	UNP I7GA39
H	496	HIS	-	expression tag	UNP I7GA39
I	2	VAL	-	insertion	UNP I7GA39
I	480	THR	-	expression tag	UNP I7GA39
I	481	ALA	-	expression tag	UNP I7GA39
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I	483	ALA	-	expression tag	UNP I7GA39
I	484	LYS	-	expression tag	UNP I7GA39
I	485	GLU	-	expression tag	UNP I7GA39
I	486	ASP	-	expression tag	UNP I7GA39
I	487	LEU	-	expression tag	UNP I7GA39
I	488	GLU	-	expression tag	UNP I7GA39
I	489	HIS	-	expression tag	UNP I7GA39
I	490	HIS	-	expression tag	UNP I7GA39
I	491	HIS	-	expression tag	UNP I7GA39
I	492	HIS	-	expression tag	UNP I7GA39
I	493	HIS	-	expression tag	UNP I7GA39
I	494	HIS	-	expression tag	UNP I7GA39
I	495	HIS	-	expression tag	UNP I7GA39
I	496	HIS	-	expression tag	UNP I7GA39
J	2	VAL	-	insertion	UNP I7GA39
J	480	THR	-	expression tag	UNP I7GA39
J	481	ALA	-	expression tag	UNP I7GA39
J	482	ALA	-	expression tag	UNP I7GA39
J	483	ALA	-	expression tag	UNP I7GA39
J	484	LYS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
J	485	GLU	-	expression tag	UNP I7GA39
J	486	ASP	-	expression tag	UNP I7GA39
J	487	LEU	-	expression tag	UNP I7GA39
J	488	GLU	-	expression tag	UNP I7GA39
J	489	HIS	-	expression tag	UNP I7GA39
J	490	HIS	-	expression tag	UNP I7GA39
J	491	HIS	-	expression tag	UNP I7GA39
J	492	HIS	-	expression tag	UNP I7GA39
J	493	HIS	-	expression tag	UNP I7GA39
J	494	HIS	-	expression tag	UNP I7GA39
J	495	HIS	-	expression tag	UNP I7GA39
J	496	HIS	-	expression tag	UNP I7GA39
K	2	VAL	-	insertion	UNP I7GA39
K	480	THR	-	expression tag	UNP I7GA39
K	481	ALA	-	expression tag	UNP I7GA39
K	482	ALA	-	expression tag	UNP I7GA39
K	483	ALA	-	expression tag	UNP I7GA39
K	484	LYS	-	expression tag	UNP I7GA39
K	485	GLU	-	expression tag	UNP I7GA39
K	486	ASP	-	expression tag	UNP I7GA39
K	487	LEU	-	expression tag	UNP I7GA39
K	488	GLU	-	expression tag	UNP I7GA39
K	489	HIS	-	expression tag	UNP I7GA39
K	490	HIS	-	expression tag	UNP I7GA39
K	491	HIS	-	expression tag	UNP I7GA39
K	492	HIS	-	expression tag	UNP I7GA39
K	493	HIS	-	expression tag	UNP I7GA39
K	494	HIS	-	expression tag	UNP I7GA39
K	495	HIS	-	expression tag	UNP I7GA39
K	496	HIS	-	expression tag	UNP I7GA39
L	2	VAL	-	insertion	UNP I7GA39
L	480	THR	-	expression tag	UNP I7GA39
L	481	ALA	-	expression tag	UNP I7GA39
L	482	ALA	-	expression tag	UNP I7GA39
L	483	ALA	-	expression tag	UNP I7GA39
L	484	LYS	-	expression tag	UNP I7GA39
L	485	GLU	-	expression tag	UNP I7GA39
L	486	ASP	-	expression tag	UNP I7GA39
L	487	LEU	-	expression tag	UNP I7GA39
L	488	GLU	-	expression tag	UNP I7GA39
L	489	HIS	-	expression tag	UNP I7GA39
L	490	HIS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
L	491	HIS	-	expression tag	UNP I7GA39
L	492	HIS	-	expression tag	UNP I7GA39
L	493	HIS	-	expression tag	UNP I7GA39
L	494	HIS	-	expression tag	UNP I7GA39
L	495	HIS	-	expression tag	UNP I7GA39
L	496	HIS	-	expression tag	UNP I7GA39
M	2	VAL	-	insertion	UNP I7GA39
M	480	THR	-	expression tag	UNP I7GA39
M	481	ALA	-	expression tag	UNP I7GA39
M	482	ALA	-	expression tag	UNP I7GA39
M	483	ALA	-	expression tag	UNP I7GA39
M	484	LYS	-	expression tag	UNP I7GA39
M	485	GLU	-	expression tag	UNP I7GA39
M	486	ASP	-	expression tag	UNP I7GA39
M	487	LEU	-	expression tag	UNP I7GA39
M	488	GLU	-	expression tag	UNP I7GA39
M	489	HIS	-	expression tag	UNP I7GA39
M	490	HIS	-	expression tag	UNP I7GA39
M	491	HIS	-	expression tag	UNP I7GA39
M	492	HIS	-	expression tag	UNP I7GA39
M	493	HIS	-	expression tag	UNP I7GA39
M	494	HIS	-	expression tag	UNP I7GA39
M	495	HIS	-	expression tag	UNP I7GA39
M	496	HIS	-	expression tag	UNP I7GA39
N	2	VAL	-	insertion	UNP I7GA39
N	480	THR	-	expression tag	UNP I7GA39
N	481	ALA	-	expression tag	UNP I7GA39
N	482	ALA	-	expression tag	UNP I7GA39
N	483	ALA	-	expression tag	UNP I7GA39
N	484	LYS	-	expression tag	UNP I7GA39
N	485	GLU	-	expression tag	UNP I7GA39
N	486	ASP	-	expression tag	UNP I7GA39
N	487	LEU	-	expression tag	UNP I7GA39
N	488	GLU	-	expression tag	UNP I7GA39
N	489	HIS	-	expression tag	UNP I7GA39
N	490	HIS	-	expression tag	UNP I7GA39
N	491	HIS	-	expression tag	UNP I7GA39
N	492	HIS	-	expression tag	UNP I7GA39
N	493	HIS	-	expression tag	UNP I7GA39
N	494	HIS	-	expression tag	UNP I7GA39
N	495	HIS	-	expression tag	UNP I7GA39
N	496	HIS	-	expression tag	UNP I7GA39

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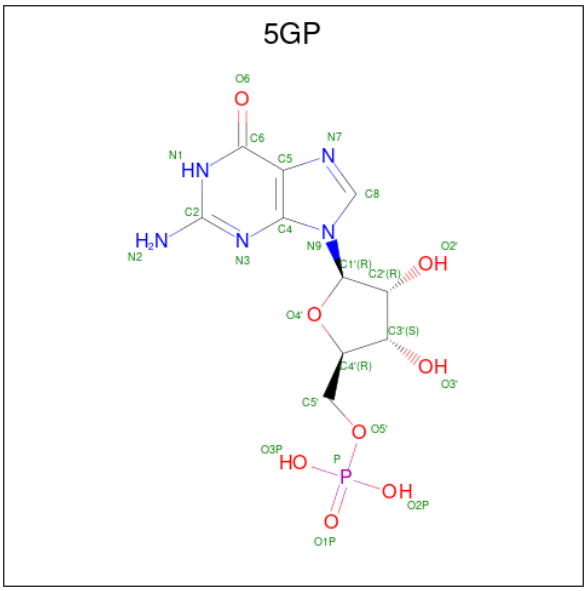
Chain	Residue	Modelled	Actual	Comment	Reference
O	2	VAL	-	insertion	UNP I7GA39
O	480	THR	-	expression tag	UNP I7GA39
O	481	ALA	-	expression tag	UNP I7GA39
O	482	ALA	-	expression tag	UNP I7GA39
O	483	ALA	-	expression tag	UNP I7GA39
O	484	LYS	-	expression tag	UNP I7GA39
O	485	GLU	-	expression tag	UNP I7GA39
O	486	ASP	-	expression tag	UNP I7GA39
O	487	LEU	-	expression tag	UNP I7GA39
O	488	GLU	-	expression tag	UNP I7GA39
O	489	HIS	-	expression tag	UNP I7GA39
O	490	HIS	-	expression tag	UNP I7GA39
O	491	HIS	-	expression tag	UNP I7GA39
O	492	HIS	-	expression tag	UNP I7GA39
O	493	HIS	-	expression tag	UNP I7GA39
O	494	HIS	-	expression tag	UNP I7GA39
O	495	HIS	-	expression tag	UNP I7GA39
O	496	HIS	-	expression tag	UNP I7GA39
P	2	VAL	-	insertion	UNP I7GA39
P	480	THR	-	expression tag	UNP I7GA39
P	481	ALA	-	expression tag	UNP I7GA39
P	482	ALA	-	expression tag	UNP I7GA39
P	483	ALA	-	expression tag	UNP I7GA39
P	484	LYS	-	expression tag	UNP I7GA39
P	485	GLU	-	expression tag	UNP I7GA39
P	486	ASP	-	expression tag	UNP I7GA39
P	487	LEU	-	expression tag	UNP I7GA39
P	488	GLU	-	expression tag	UNP I7GA39
P	489	HIS	-	expression tag	UNP I7GA39
P	490	HIS	-	expression tag	UNP I7GA39
P	491	HIS	-	expression tag	UNP I7GA39
P	492	HIS	-	expression tag	UNP I7GA39
P	493	HIS	-	expression tag	UNP I7GA39
P	494	HIS	-	expression tag	UNP I7GA39
P	495	HIS	-	expression tag	UNP I7GA39
P	496	HIS	-	expression tag	UNP I7GA39

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	F	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	G	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	H	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	I	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	J	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	K	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	L	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	M	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	N	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

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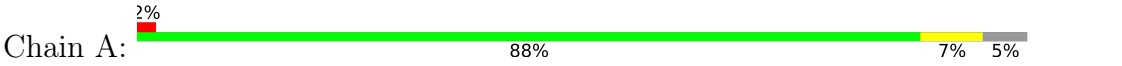
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	P	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

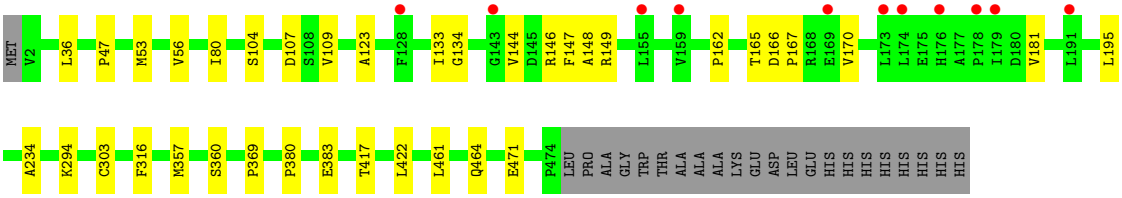
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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 guaB1

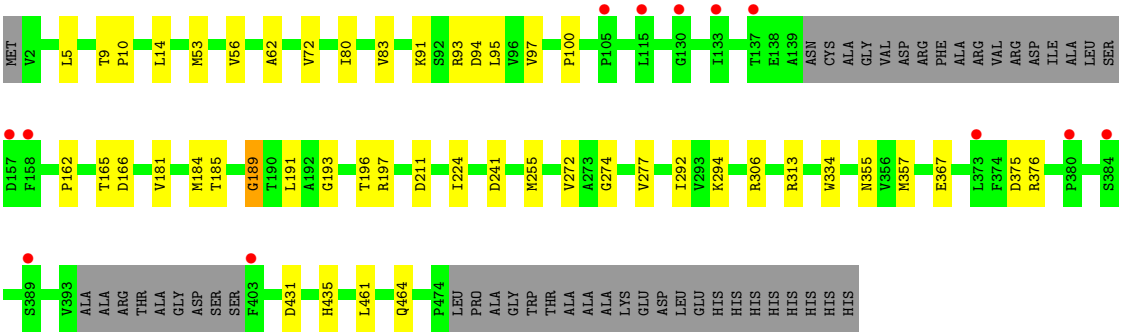
Chain A:





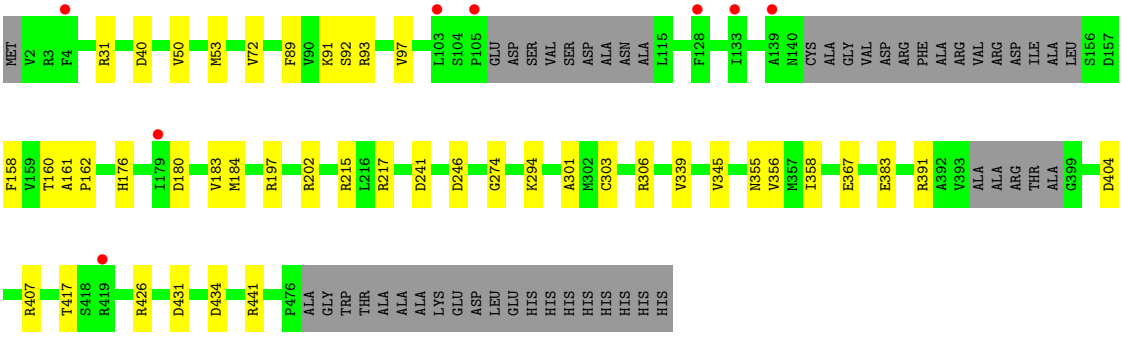
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain B:



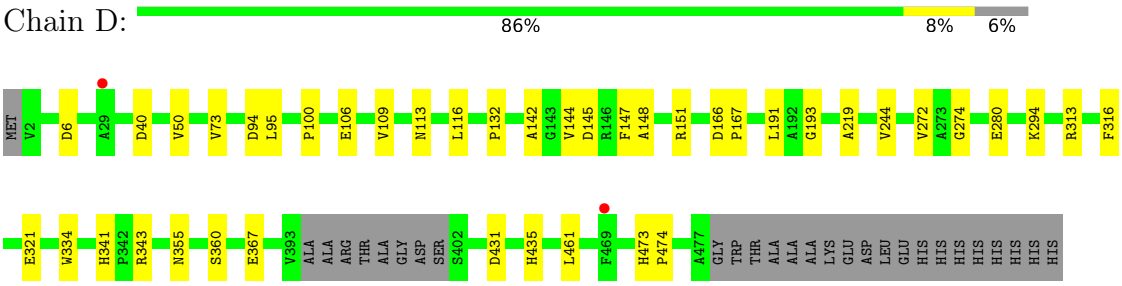
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain C:



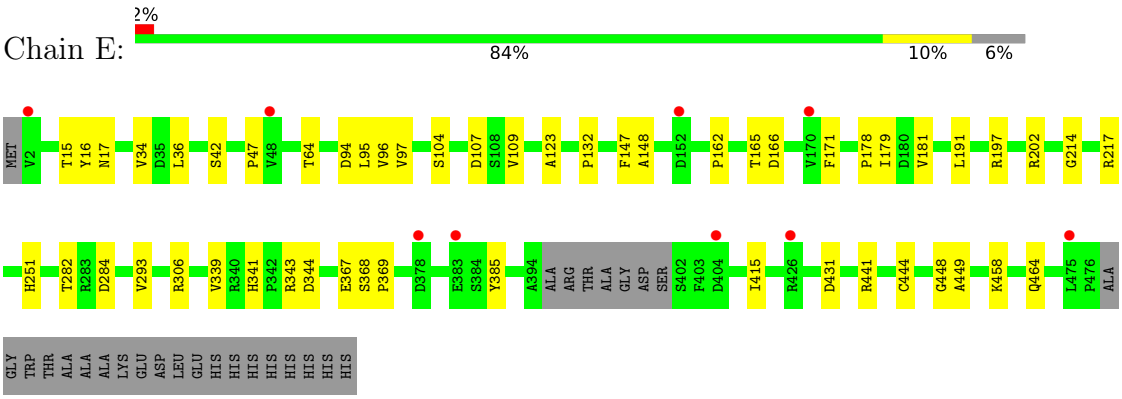
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain D:



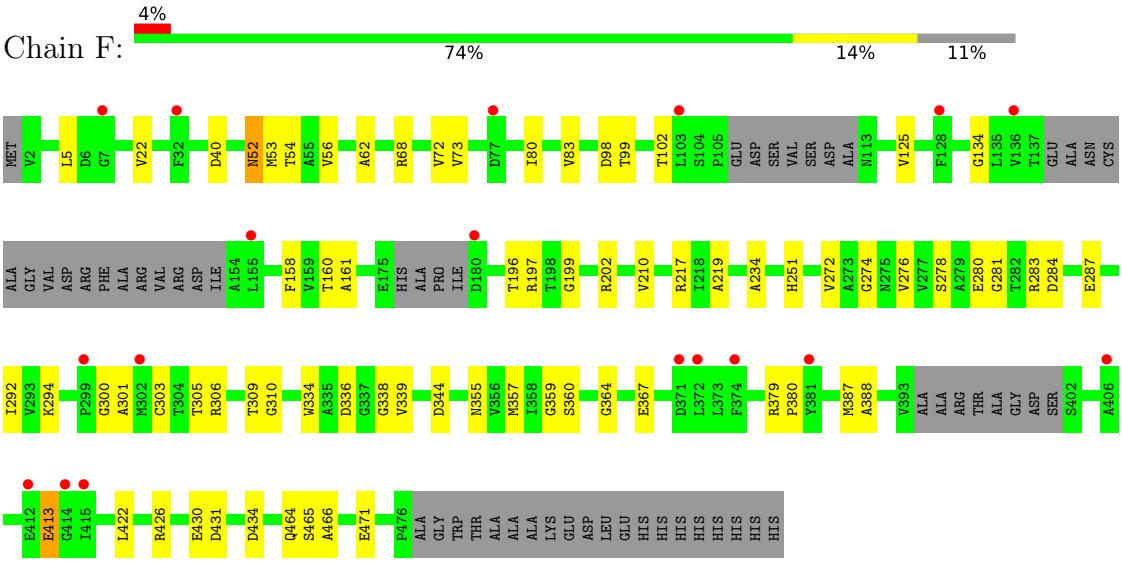
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain E:



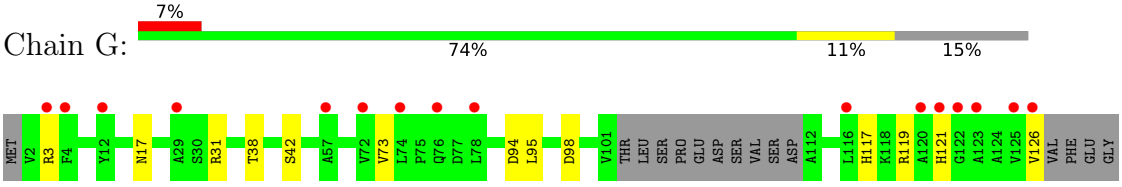
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

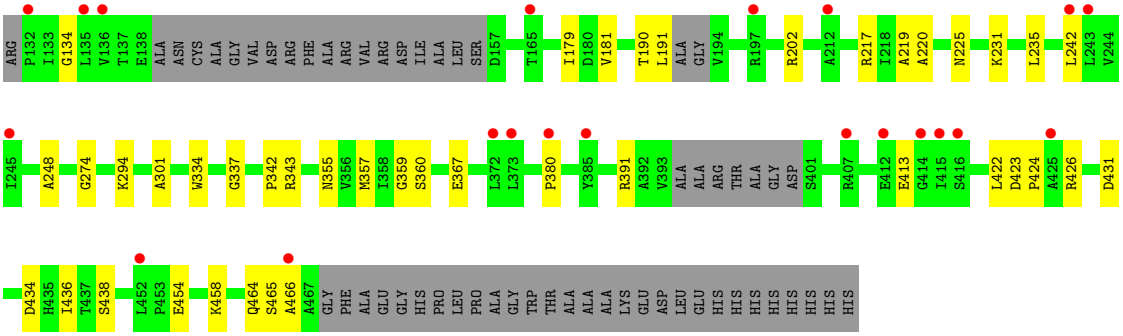
Chain F:



• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

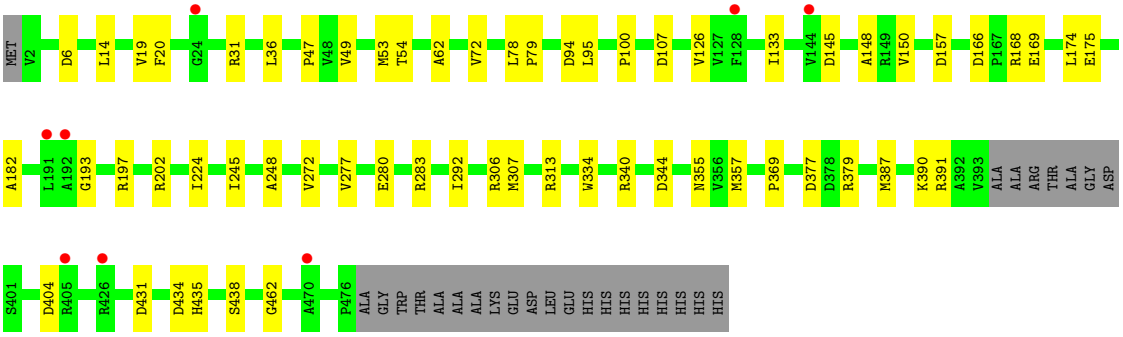
Chain G:





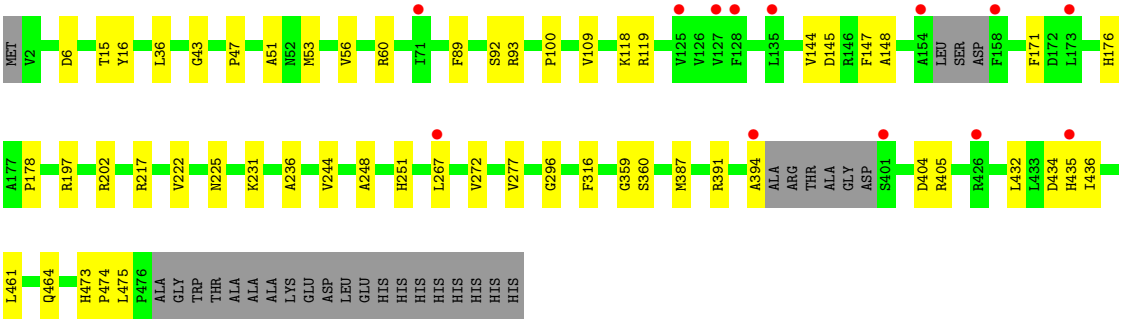
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain H:



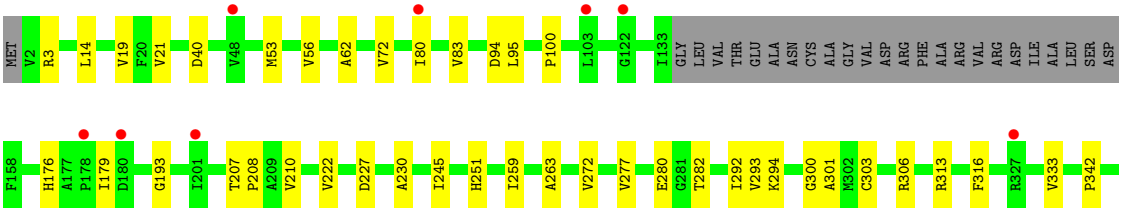
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

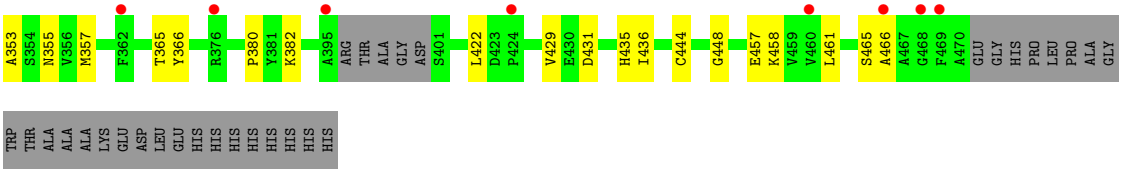
Chain I:



• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

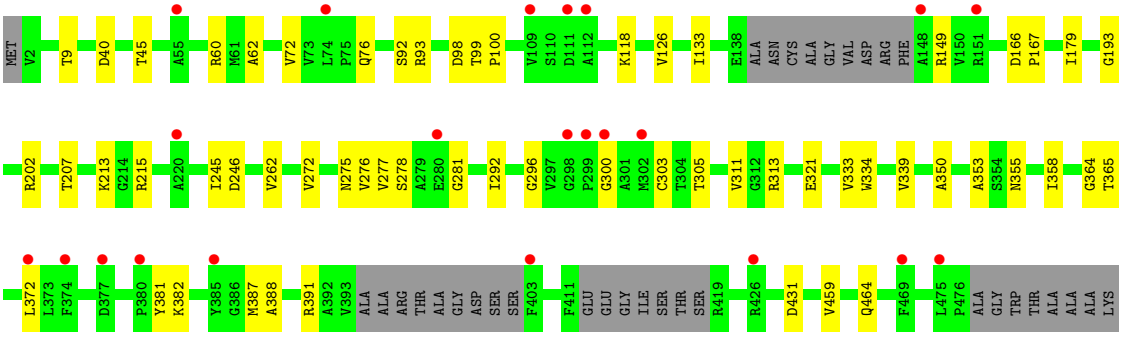
Chain J:





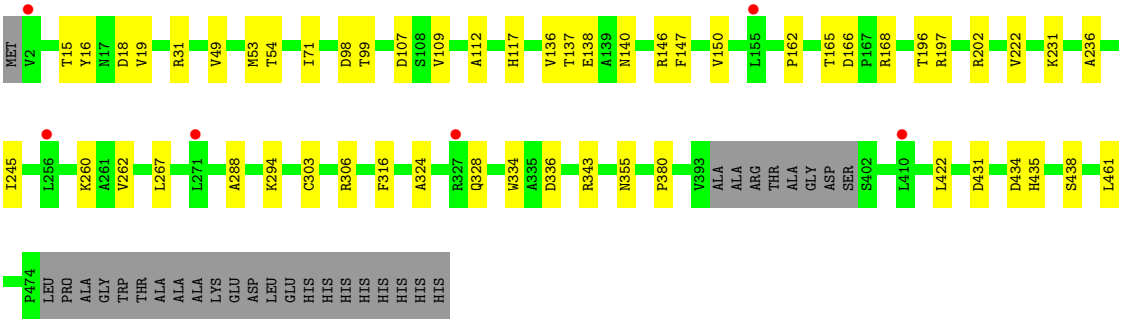
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain K:



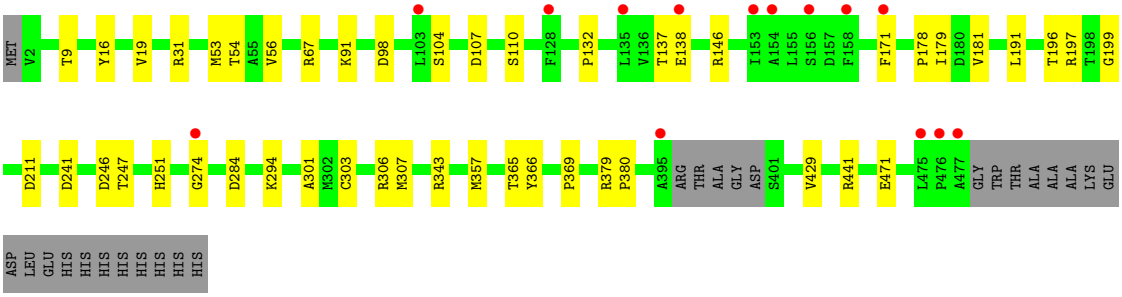
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain L:



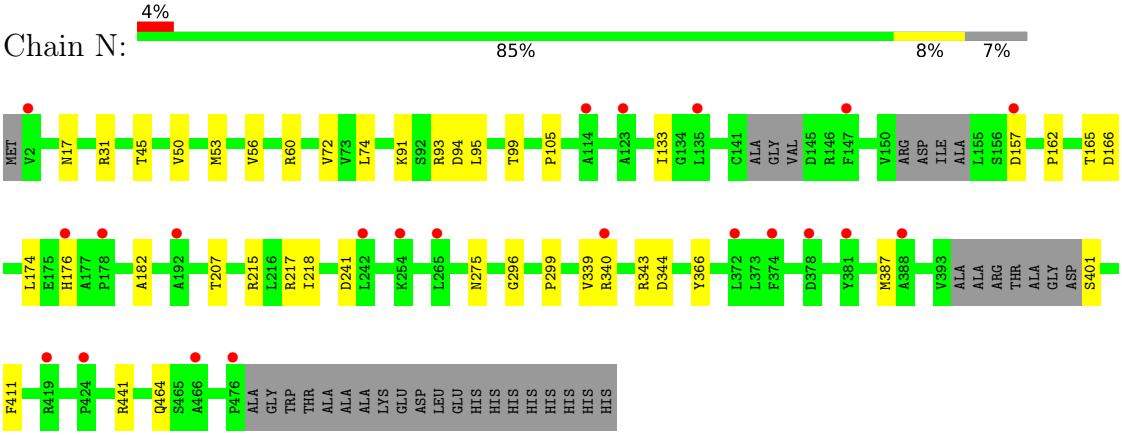
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain M:



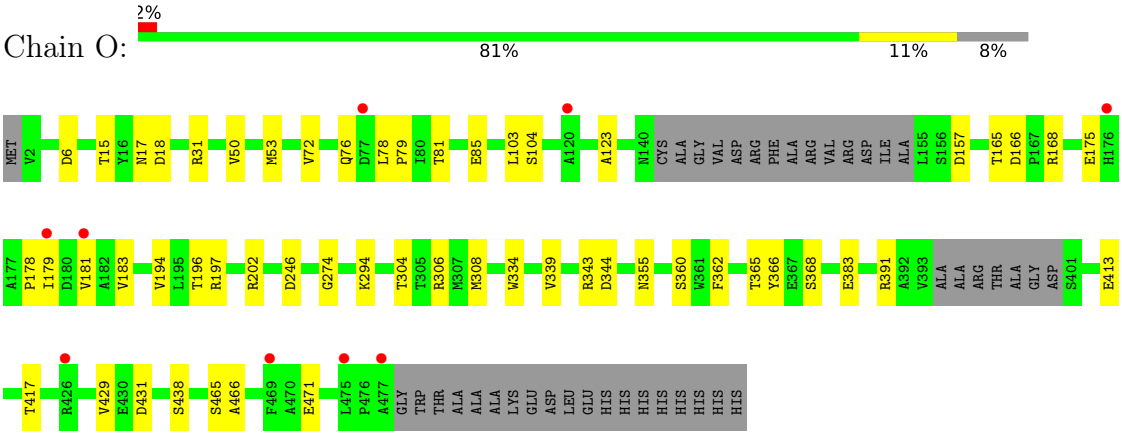
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain N:



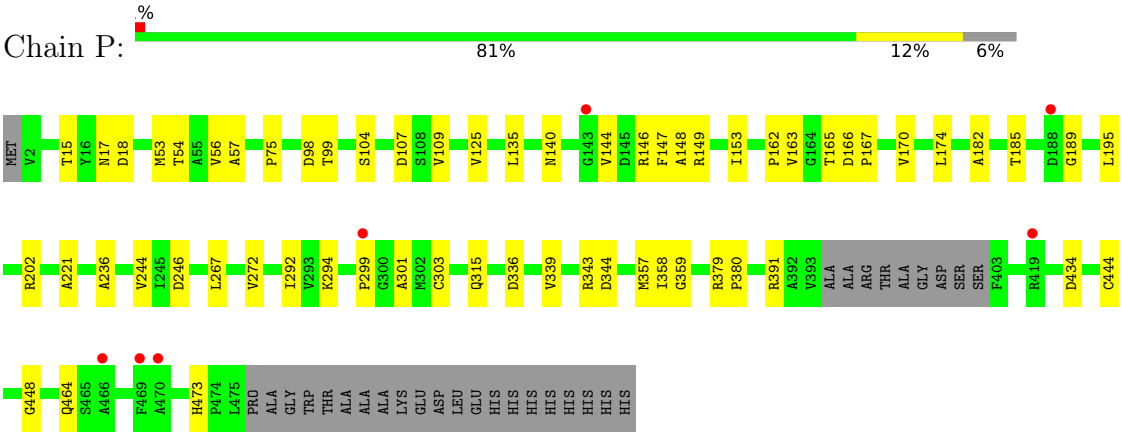
• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain O:



• Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	104.79Å 105.10Å 170.47Å 76.92° 81.86° 69.01°	Depositor
Resolution (Å)	47.69 – 2.50 47.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (47.69-2.50) 91.0 (47.69-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.263 , 0.306 0.266 , 0.308	Depositor DCC
R_{free} test set	10296 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	53060	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP

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	0.21	0/3460	0.41	0/4717
1	B	0.23	0/3283	0.46	0/4474
1	C	0.21	0/3289	0.42	0/4478
1	D	0.22	0/3446	0.44	1/4696 (0.0%)
1	E	0.21	0/3447	0.41	0/4697
1	F	0.22	0/3218	0.43	0/4381
1	G	0.21	0/3063	0.43	0/4176
1	H	0.21	0/3433	0.42	0/4678
1	I	0.21	0/3431	0.42	0/4673
1	J	0.24	0/3206	0.45	1/4372 (0.0%)
1	K	0.22	0/3270	0.45	0/4462
1	L	0.21	0/3401	0.42	0/4637
1	M	0.21	0/3433	0.42	0/4683
1	N	0.21	0/3405	0.42	0/4635
1	O	0.22	0/3334	0.41	0/4544
1	P	0.21	0/3425	0.43	1/4665 (0.0%)
All	All	0.22	0/53544	0.43	3/72968 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	116	LEU	CA-CB-CG	8.43	134.68	115.30
1	P	189	GLY	N-CA-C	5.47	126.79	113.10
1	J	210	VAL	N-CA-C	5.10	124.76	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	189	GLY	Peptide
1	G	117	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3371	21	0
1	B	3230	0	3204	28	1
1	C	3235	0	3222	27	0
1	D	3389	0	3370	26	1
1	E	3390	0	3372	32	0
1	F	3168	0	3163	44	0
1	G	3017	0	2977	36	0
1	H	3378	0	3358	41	0
1	I	3375	0	3358	38	0
1	J	3154	0	3119	39	0
1	K	3216	0	3177	36	0
1	L	3346	0	3312	33	0
1	M	3376	0	3339	32	1
1	N	3350	0	3336	27	0
1	O	3280	0	3262	37	1
1	P	3369	0	3360	39	0
2	A	24	0	12	2	0
2	B	24	0	12	0	0
2	C	24	0	12	3	0
2	D	24	0	12	1	0
2	E	24	0	12	0	0
2	F	24	0	12	2	0
2	G	24	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	24	0	12	0	0
2	I	24	0	12	2	0
2	J	24	0	12	3	0
2	K	24	0	12	5	0
2	L	24	0	12	2	0
2	M	24	0	12	3	0
2	N	24	0	12	1	0
2	O	24	0	12	2	0
2	P	24	0	12	4	0
All	All	53060	0	52492	494	2

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 5.

The worst 5 of 494 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:O:175:GLU:OE2	1:O:197:ARG:NH2	2.14	0.80
1:K:372:LEU:H	1:K:382:LYS:HE3	1.47	0.79
1:B:185:THR:OG1	1:B:189:GLY:O	2.00	0.78
1:G:202:ARG:NH1	1:G:434:ASP:OD2	2.16	0.78
1:H:272:VAL:HG12	1:H:292:ILE:HB	1.66	0.77

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ASP:OD2	1:M:9:THR:OG1[1_646]	1.95	0.25
1:B:9:THR:OG1	1:O:6:ASP:OD2[1_646]	2.17	0.03

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 X-ray entries followed by that with respect to entries of similar resolution.

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	471/496 (95%)	459 (98%)	12 (2%)	0	100	100
1	B	441/496 (89%)	430 (98%)	11 (2%)	0	100	100
1	C	438/496 (88%)	425 (97%)	13 (3%)	0	100	100
1	D	464/496 (94%)	456 (98%)	8 (2%)	0	100	100
1	E	464/496 (94%)	449 (97%)	15 (3%)	0	100	100
1	F	430/496 (87%)	415 (96%)	15 (4%)	0	100	100
1	G	412/496 (83%)	395 (96%)	17 (4%)	0	100	100
1	H	464/496 (94%)	445 (96%)	19 (4%)	0	100	100
1	I	460/496 (93%)	448 (97%)	12 (3%)	0	100	100
1	J	434/496 (88%)	419 (96%)	15 (4%)	0	100	100
1	K	442/496 (89%)	423 (96%)	19 (4%)	0	100	100
1	L	461/496 (93%)	452 (98%)	9 (2%)	0	100	100
1	M	467/496 (94%)	456 (98%)	11 (2%)	0	100	100
1	N	453/496 (91%)	442 (98%)	11 (2%)	0	100	100
1	O	449/496 (90%)	434 (97%)	15 (3%)	0	100	100
1	P	461/496 (93%)	449 (97%)	12 (3%)	0	100	100
All	All	7211/7936 (91%)	6997 (97%)	214 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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	346/372 (93%)	346 (100%)	0	100	100
1	B	331/372 (89%)	330 (100%)	1 (0%)	92	97
1	C	333/372 (90%)	333 (100%)	0	100	100
1	D	348/372 (94%)	348 (100%)	0	100	100
1	E	348/372 (94%)	348 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	324/372 (87%)	322 (99%)	2 (1%)	86 95
1	G	305/372 (82%)	305 (100%)	0	100 100
1	H	347/372 (93%)	347 (100%)	0	100 100
1	I	346/372 (93%)	345 (100%)	1 (0%)	92 97
1	J	321/372 (86%)	321 (100%)	0	100 100
1	K	323/372 (87%)	322 (100%)	1 (0%)	92 97
1	L	341/372 (92%)	340 (100%)	1 (0%)	92 97
1	M	343/372 (92%)	343 (100%)	0	100 100
1	N	346/372 (93%)	346 (100%)	0	100 100
1	O	337/372 (91%)	337 (100%)	0	100 100
1	P	344/372 (92%)	344 (100%)	0	100 100
All	All	5383/5952 (90%)	5377 (100%)	6 (0%)	93 98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	251	HIS
1	K	381	TYR
1	L	146	ARG
1	F	52	ASN
1	B	93	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	5GP	M	501	-	22,26,26	0.64	0	27,40,40	0.68	0
2	5GP	G	501	-	22,26,26	0.63	0	27,40,40	0.78	0
2	5GP	J	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.75	1 (3%)
2	5GP	D	501	-	22,26,26	0.85	1 (4%)	27,40,40	0.70	0
2	5GP	L	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.73	1 (3%)
2	5GP	H	501	-	22,26,26	0.64	0	27,40,40	0.69	0
2	5GP	C	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.75	1 (3%)
2	5GP	K	501	-	22,26,26	0.90	1 (4%)	27,40,40	0.71	0
2	5GP	N	501	-	22,26,26	0.64	0	27,40,40	0.70	0
2	5GP	E	501	-	22,26,26	0.85	1 (4%)	27,40,40	0.69	0
2	5GP	A	501	-	22,26,26	0.88	1 (4%)	27,40,40	0.76	0
2	5GP	F	501	-	22,26,26	0.86	1 (4%)	27,40,40	0.75	0
2	5GP	B	501	-	22,26,26	0.86	1 (4%)	27,40,40	0.69	0
2	5GP	O	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.74	1 (3%)
2	5GP	I	501	-	22,26,26	0.88	1 (4%)	27,40,40	0.80	1 (3%)
2	5GP	P	501	-	22,26,26	0.67	0	27,40,40	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5GP	M	501	-	-	5/6/26/26	0/3/3/3
2	5GP	G	501	-	-	5/6/26/26	0/3/3/3
2	5GP	J	501	-	-	5/6/26/26	0/3/3/3
2	5GP	D	501	-	-	5/6/26/26	0/3/3/3
2	5GP	L	501	-	-	1/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5GP	H	501	-	-	0/6/26/26	0/3/3/3
2	5GP	C	501	-	-	5/6/26/26	0/3/3/3
2	5GP	K	501	-	-	5/6/26/26	0/3/3/3
2	5GP	N	501	-	-	3/6/26/26	0/3/3/3
2	5GP	E	501	-	-	3/6/26/26	0/3/3/3
2	5GP	A	501	-	-	0/6/26/26	0/3/3/3
2	5GP	F	501	-	-	0/6/26/26	0/3/3/3
2	5GP	B	501	-	-	5/6/26/26	0/3/3/3
2	5GP	O	501	-	-	1/6/26/26	0/3/3/3
2	5GP	I	501	-	-	1/6/26/26	0/3/3/3
2	5GP	P	501	-	-	5/6/26/26	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	5GP	P-O1P	2.90	1.59	1.50
2	C	501	5GP	P-O1P	2.84	1.59	1.50
2	L	501	5GP	P-O1P	2.83	1.59	1.50
2	O	501	5GP	P-O1P	2.83	1.59	1.50
2	J	501	5GP	P-O1P	2.83	1.59	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	501	5GP	O3P-P-O2P	2.39	116.76	107.64
2	O	501	5GP	O3P-P-O2P	2.28	116.35	107.64
2	C	501	5GP	O3P-P-O2P	2.24	116.19	107.64
2	J	501	5GP	O3P-P-O2P	2.18	115.95	107.64
2	L	501	5GP	O3P-P-O2P	2.01	115.31	107.64

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	5GP	C5'-O5'-P-O1P
2	B	501	5GP	C5'-O5'-P-O2P
2	B	501	5GP	C5'-O5'-P-O3P
2	B	501	5GP	C3'-C4'-C5'-O5'
2	C	501	5GP	C5'-O5'-P-O1P

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	501	5GP	3	0
2	G	501	5GP	4	0
2	J	501	5GP	3	0
2	D	501	5GP	1	0
2	L	501	5GP	2	0
2	C	501	5GP	3	0
2	K	501	5GP	5	0
2	N	501	5GP	1	0
2	A	501	5GP	2	0
2	F	501	5GP	2	0
2	O	501	5GP	2	0
2	I	501	5GP	2	0
2	P	501	5GP	4	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.

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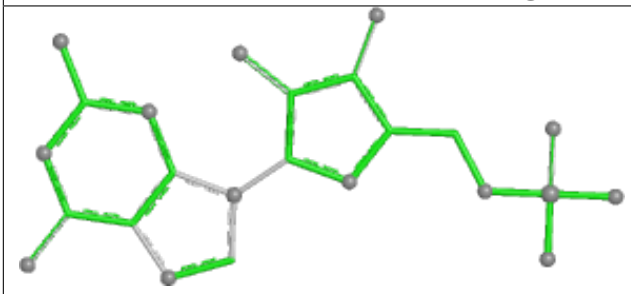	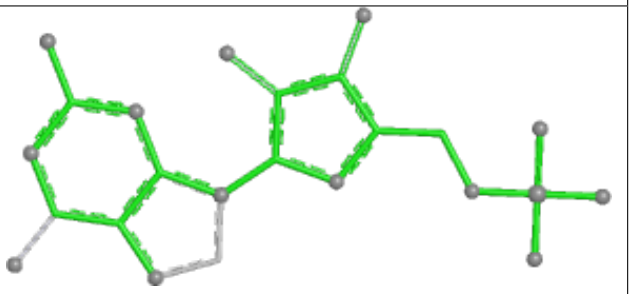
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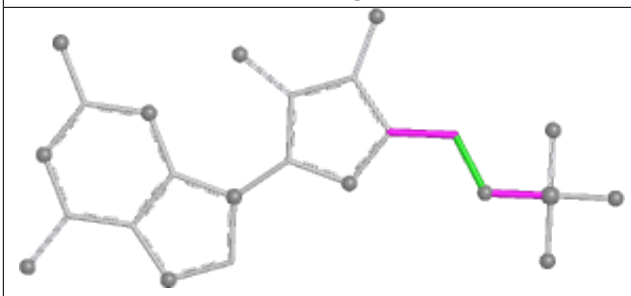	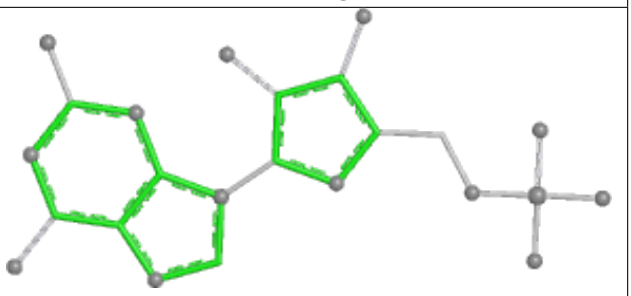
Torsions	Rings

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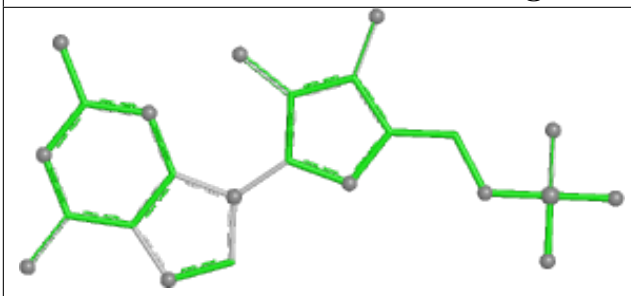	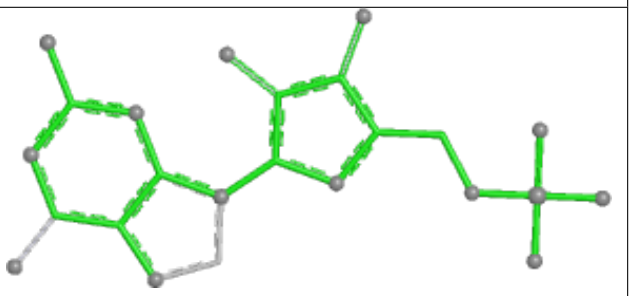
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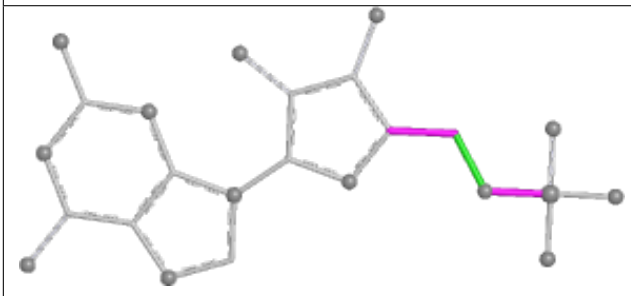	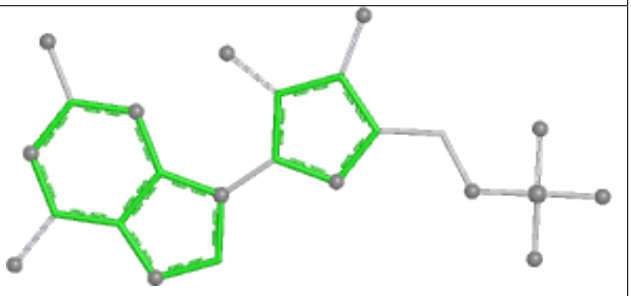
Torsions	Rings

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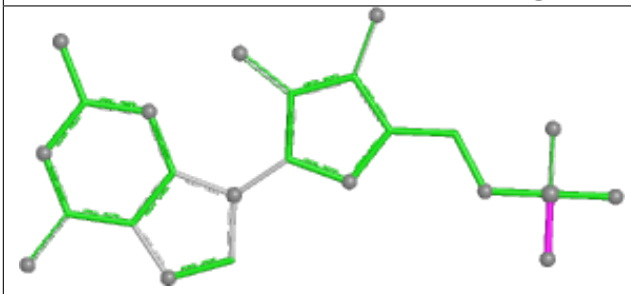	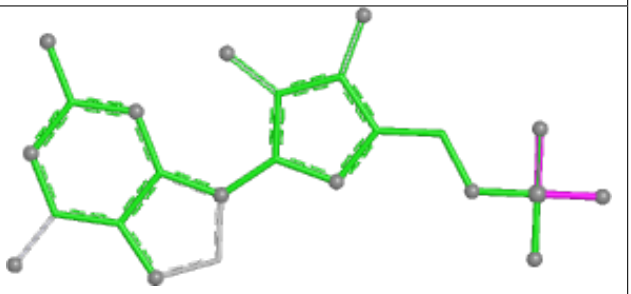
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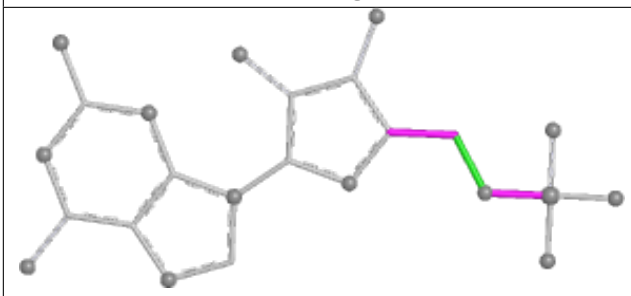	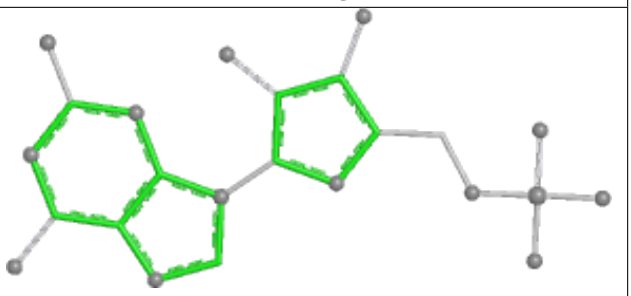
Torsions	**Rings**

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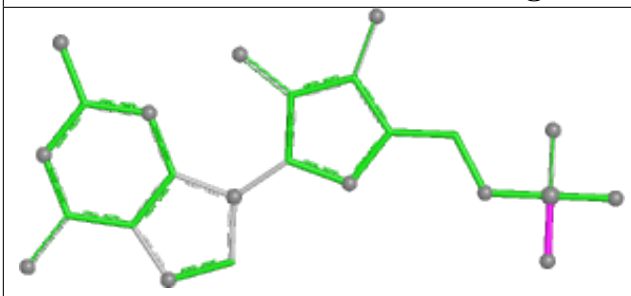	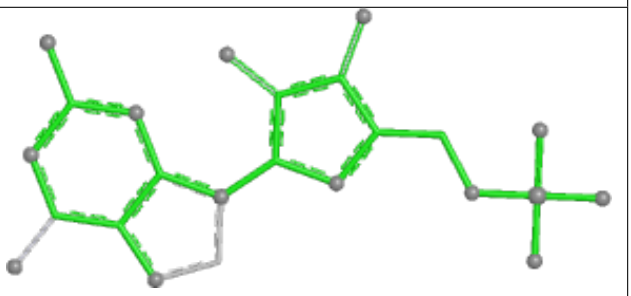
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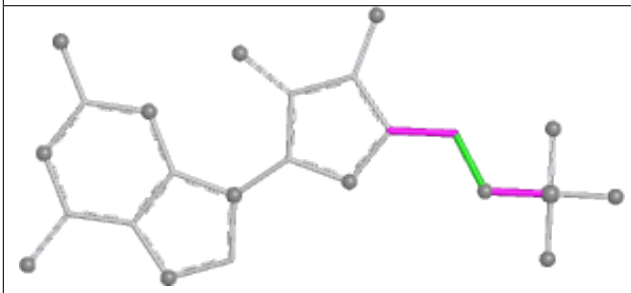	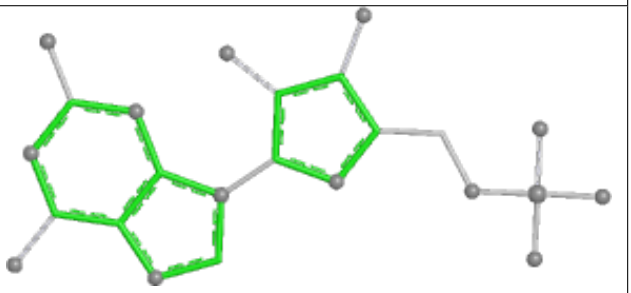
Torsions	**Rings**

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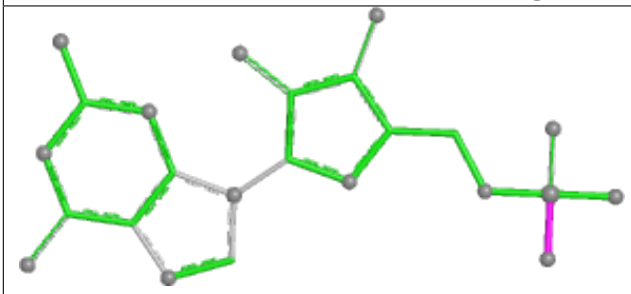
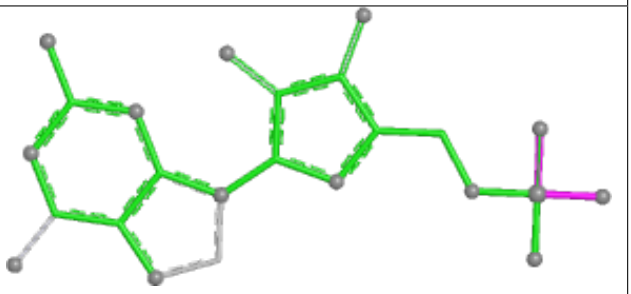
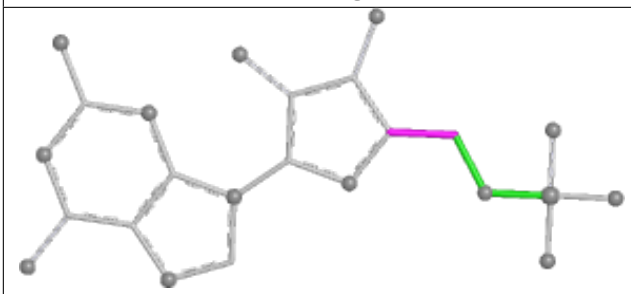
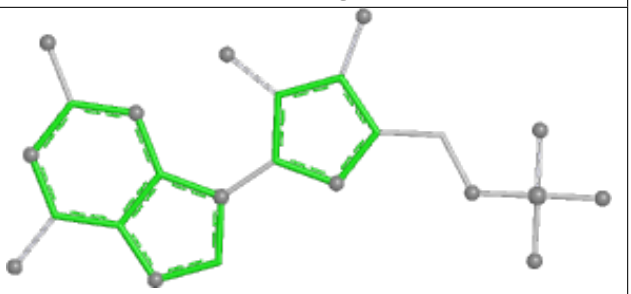
 Bond lengths	 Bond angles
 Torsions	 Rings

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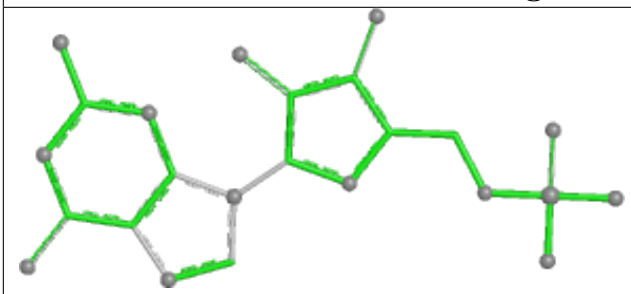
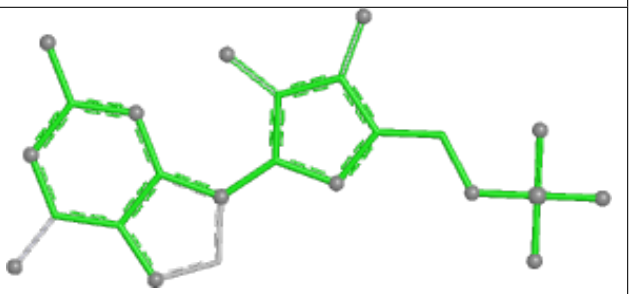
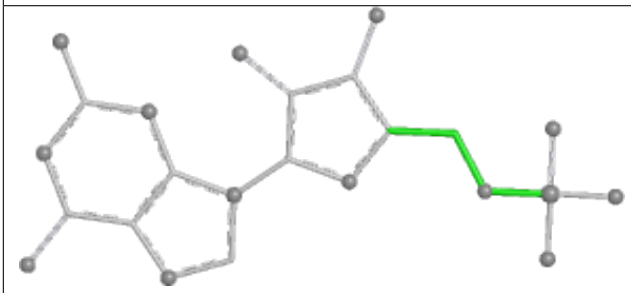
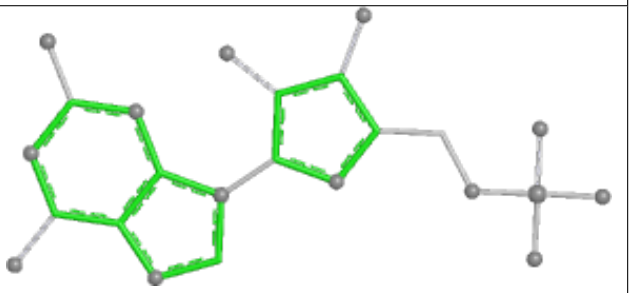
 Bond lengths	 Bond angles
 Torsions	 Rings

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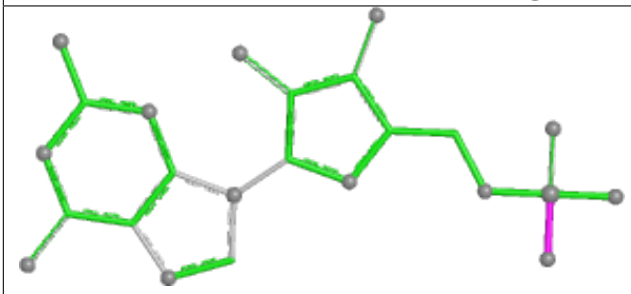

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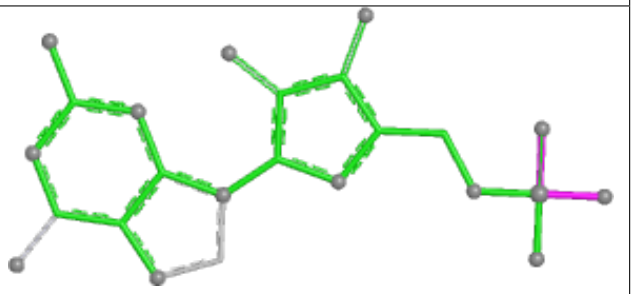

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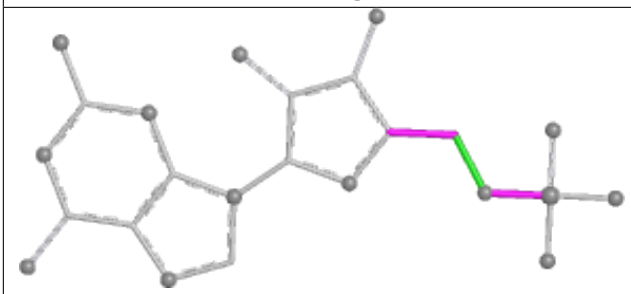

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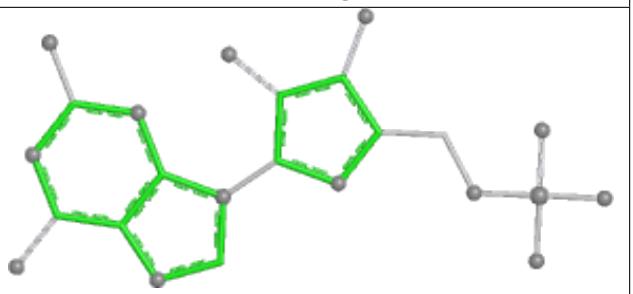

Rings

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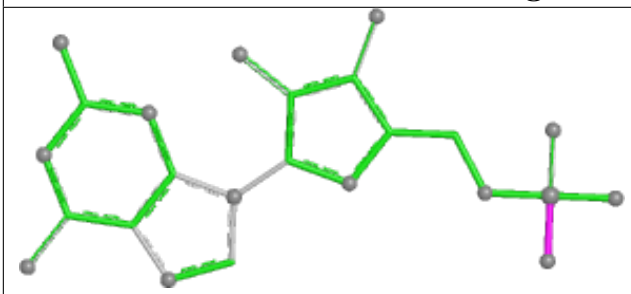

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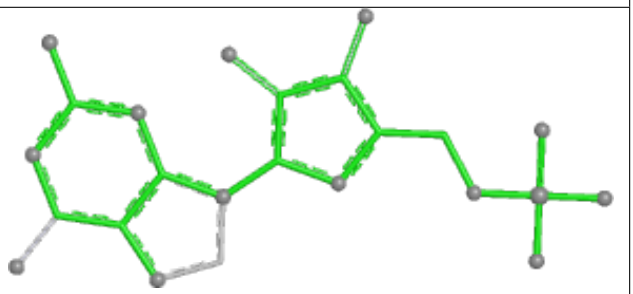

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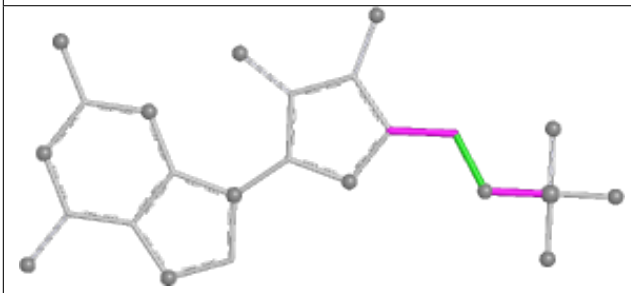

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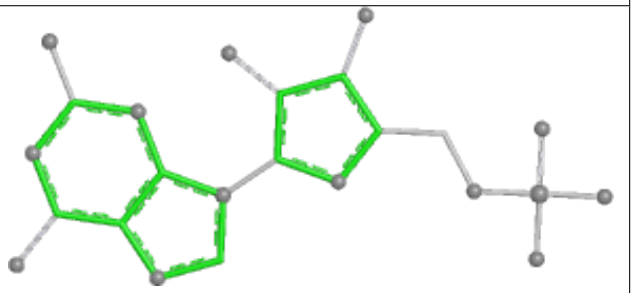

Rings

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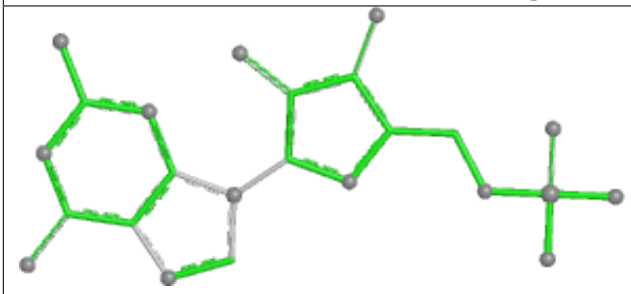	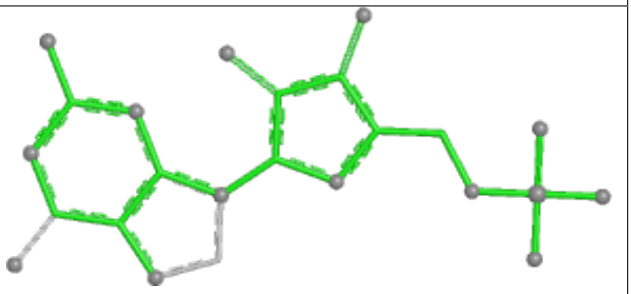
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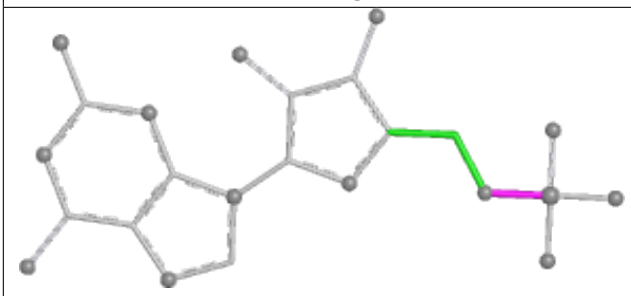	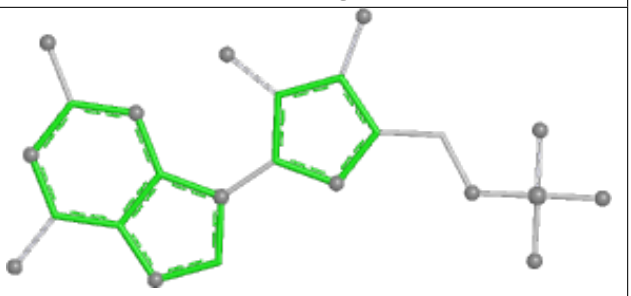
Torsions	**Rings**

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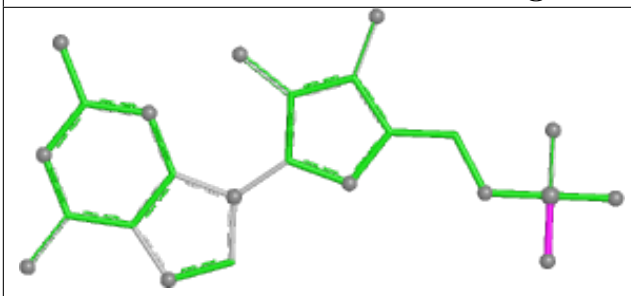	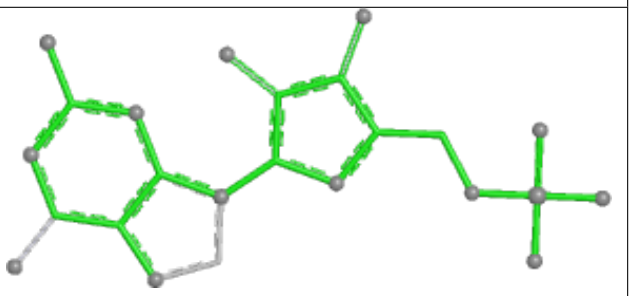
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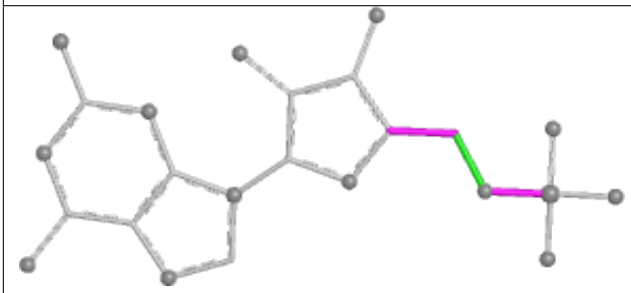	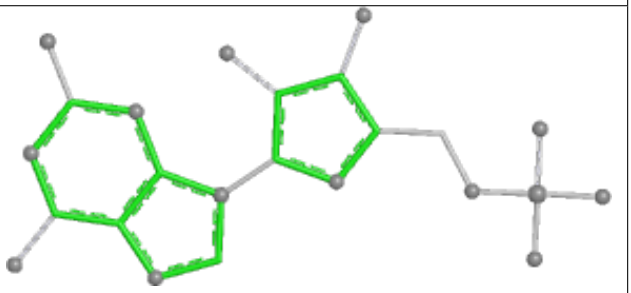
Torsions	**Rings**

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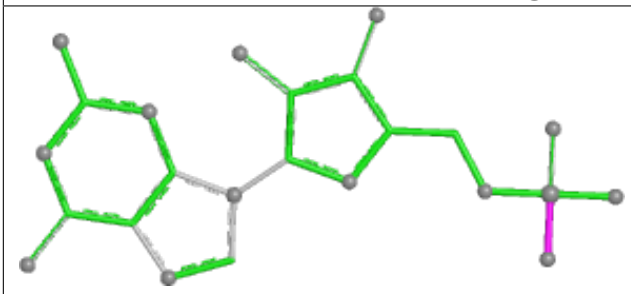
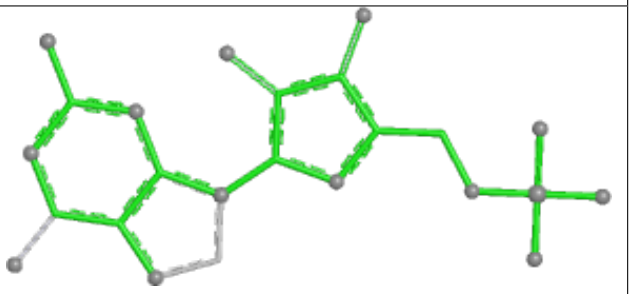
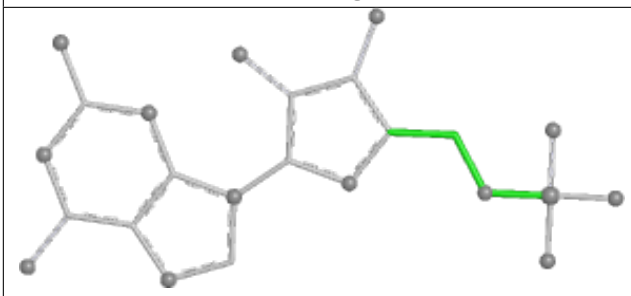
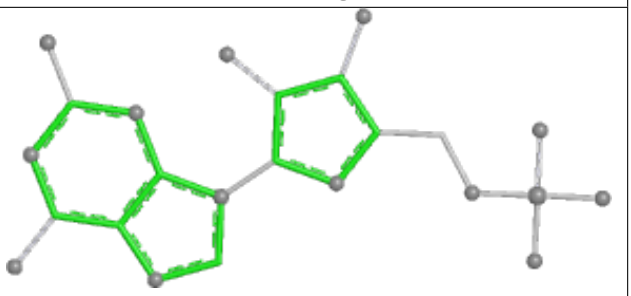
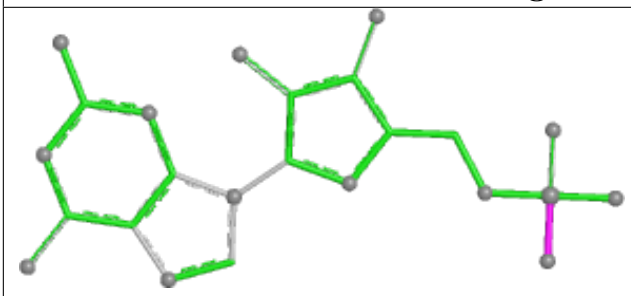
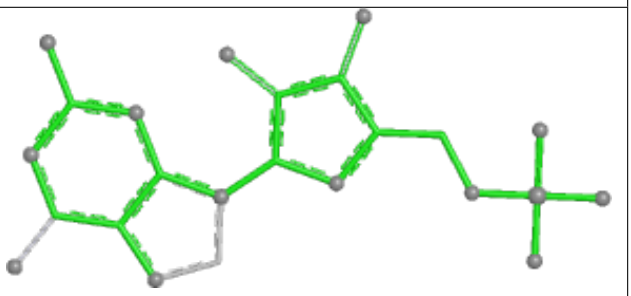
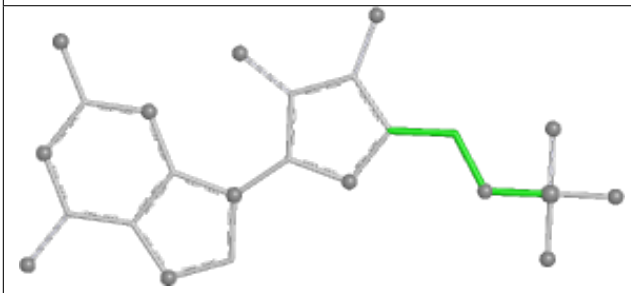
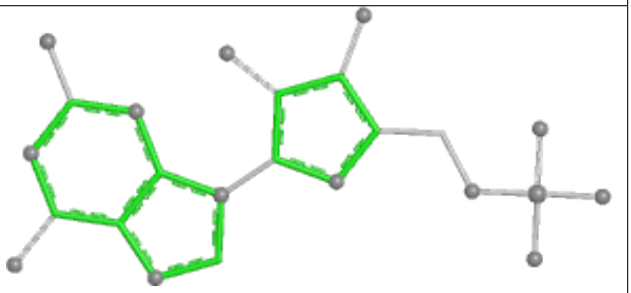
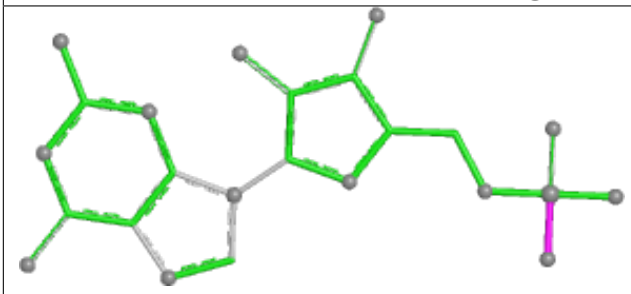
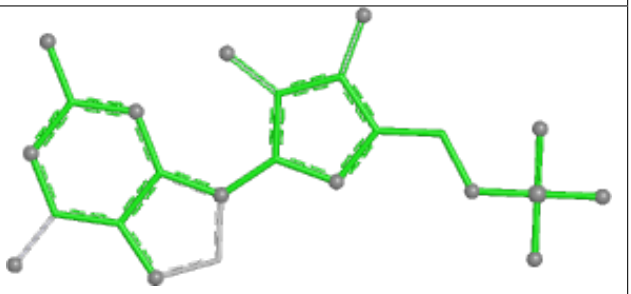
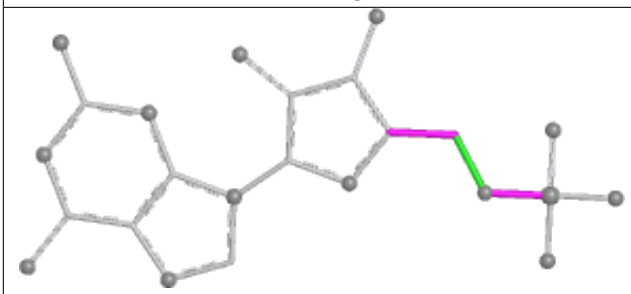
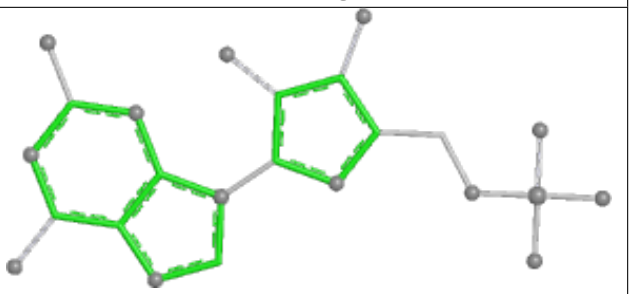
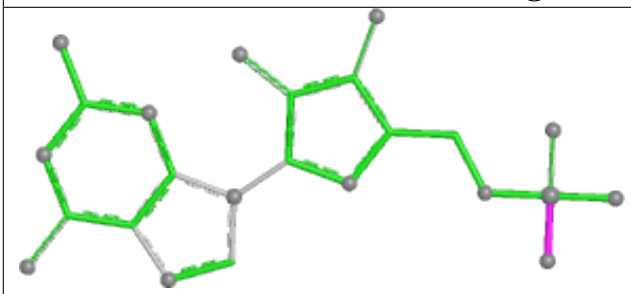
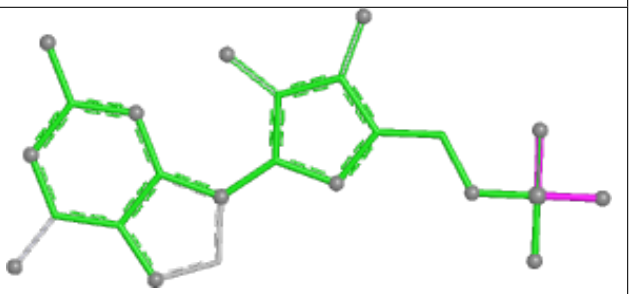
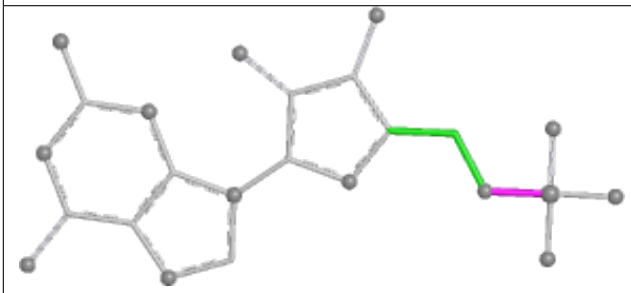
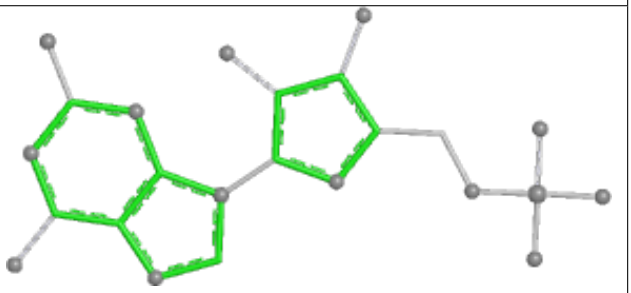
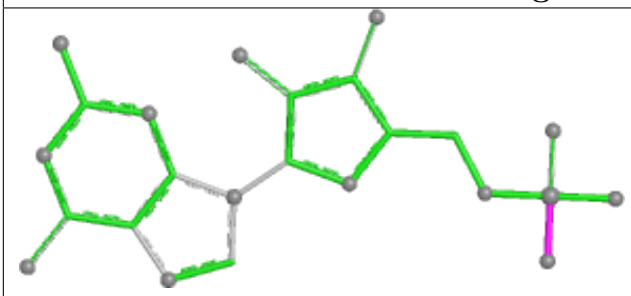
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand 5GP F 501	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

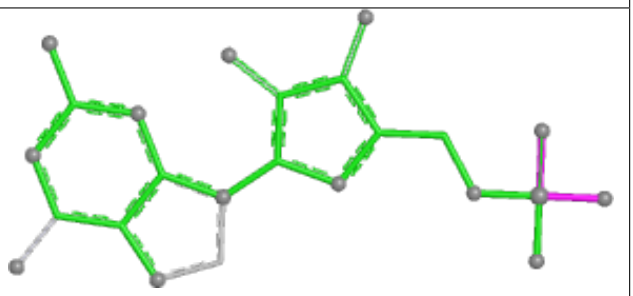
Ligand 5GP B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 5GP O 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

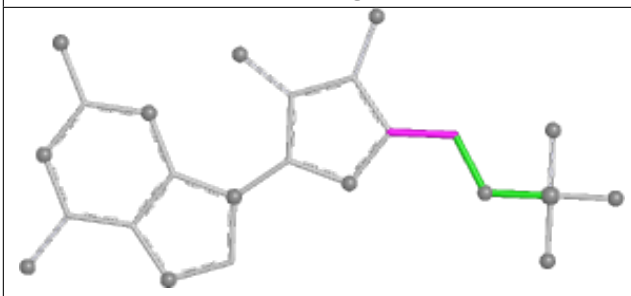
Ligand 5GP I 501



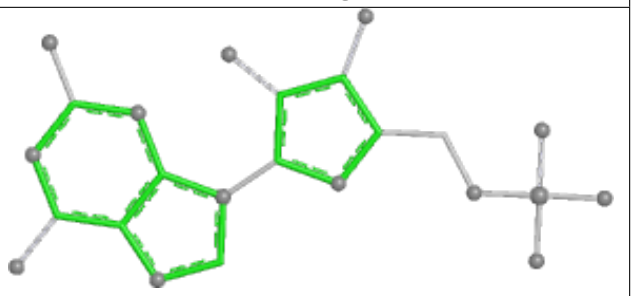
Bond lengths



Bond angles

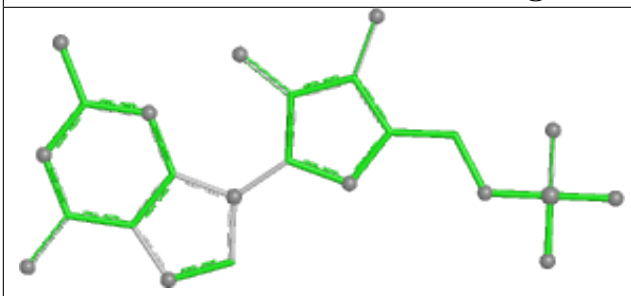


Torsions

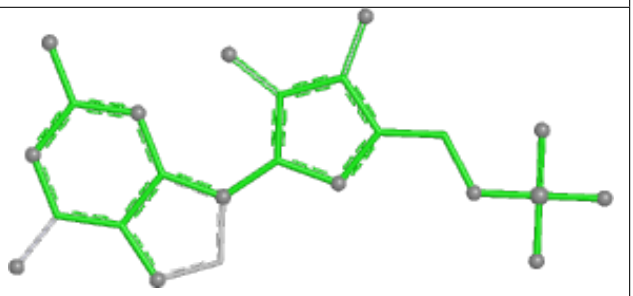


Rings

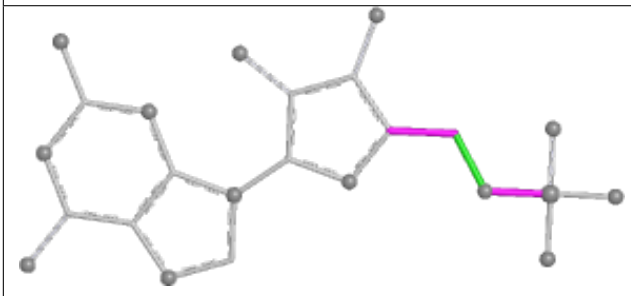
Ligand 5GP P 501



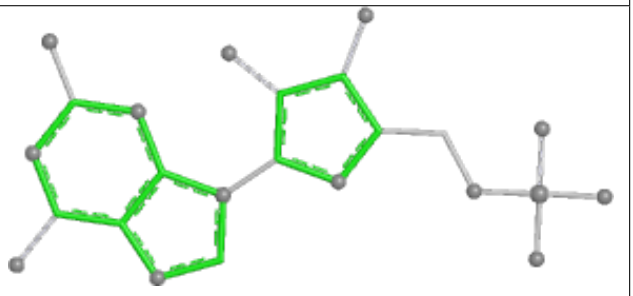
Bond lengths



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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	473/496 (95%)	0.04	11 (2%)	60	63	33, 47, 78, 105	0
1	B	447/496 (90%)	0.15	12 (2%)	54	58	38, 51, 83, 104	0
1	C	446/496 (89%)	0.00	8 (1%)	68	71	34, 53, 75, 95	0
1	D	468/496 (94%)	-0.09	2 (0%)	92	93	35, 48, 64, 91	0
1	E	468/496 (94%)	0.06	9 (1%)	66	69	37, 55, 71, 91	0
1	F	440/496 (88%)	0.24	18 (4%)	37	40	42, 61, 90, 107	0
1	G	424/496 (85%)	0.45	37 (8%)	10	10	48, 68, 88, 103	0
1	H	468/496 (94%)	0.08	8 (1%)	70	72	39, 54, 77, 96	0
1	I	466/496 (93%)	0.13	13 (2%)	53	56	43, 57, 73, 98	1 (0%)
1	J	440/496 (88%)	0.22	16 (3%)	42	46	40, 61, 84, 97	1 (0%)
1	K	450/496 (90%)	0.20	22 (4%)	29	31	42, 56, 86, 103	0
1	L	465/496 (93%)	0.03	6 (1%)	77	79	40, 57, 77, 88	0
1	M	471/496 (94%)	0.05	14 (2%)	50	53	35, 53, 80, 94	0
1	N	461/496 (92%)	0.14	22 (4%)	30	32	33, 56, 79, 107	0
1	O	455/496 (91%)	0.09	9 (1%)	65	68	37, 55, 80, 95	0
1	P	465/496 (93%)	-0.02	7 (1%)	73	75	39, 54, 73, 86	0
All	All	7307/7936 (92%)	0.11	214 (2%)	51	55	33, 56, 80, 107	2 (0%)

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	123	ALA	6.0
1	G	135	LEU	5.6
1	K	299	PRO	5.6
1	I	401	SER	5.1
1	A	176	HIS	5.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

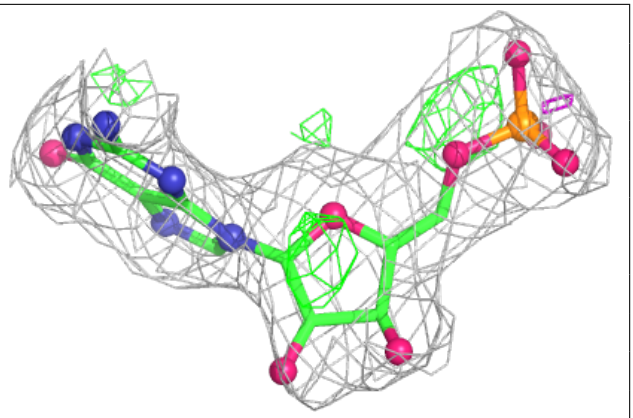
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

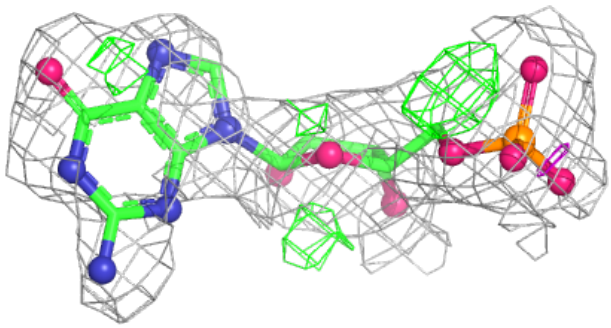
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5GP	F	501	24/24	0.86	0.18	61,79,87,92	0
2	5GP	G	501	24/24	0.90	0.14	56,68,76,80	0
2	5GP	A	501	24/24	0.92	0.15	34,48,53,54	0
2	5GP	I	501	24/24	0.93	0.11	41,56,62,67	0
2	5GP	K	501	24/24	0.93	0.13	53,66,82,85	0
2	5GP	L	501	24/24	0.93	0.13	44,59,66,68	0
2	5GP	P	501	24/24	0.93	0.14	47,53,60,64	0
2	5GP	M	501	24/24	0.94	0.14	38,46,54,59	0
2	5GP	N	501	24/24	0.94	0.13	45,56,65,69	0
2	5GP	C	501	24/24	0.94	0.12	43,50,57,64	0
2	5GP	J	501	24/24	0.95	0.11	46,53,61,62	0
2	5GP	D	501	24/24	0.95	0.14	34,43,49,58	0
2	5GP	O	501	24/24	0.96	0.11	41,54,62,66	0
2	5GP	H	501	24/24	0.97	0.11	37,50,54,59	0
2	5GP	B	501	24/24	0.97	0.11	38,55,64,66	0
2	5GP	E	501	24/24	0.97	0.09	28,48,55,64	0

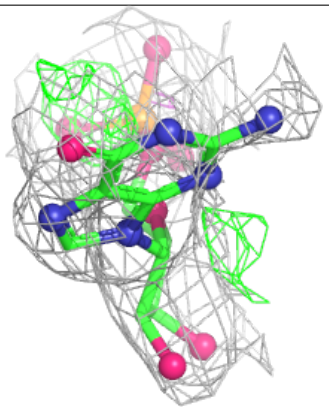
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 5GP F 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

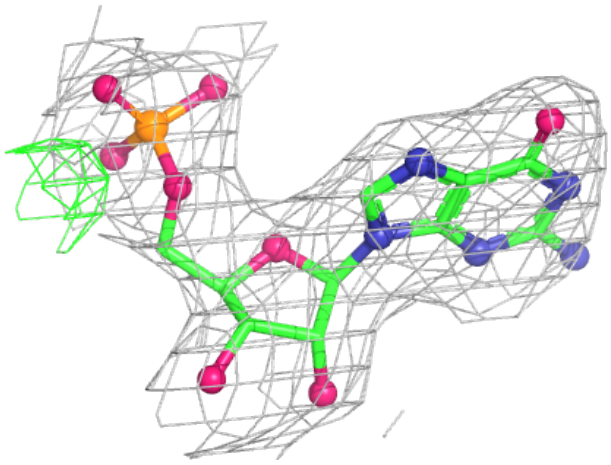


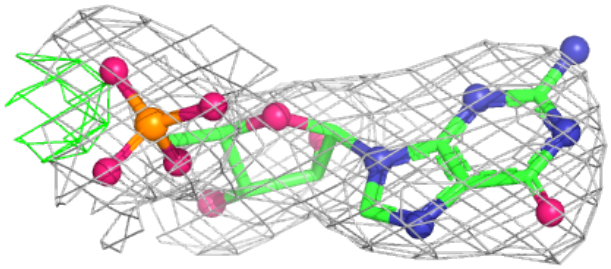


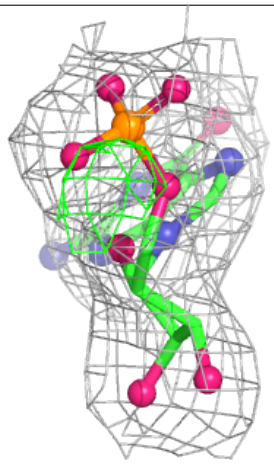


Electron density around 5GP G 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

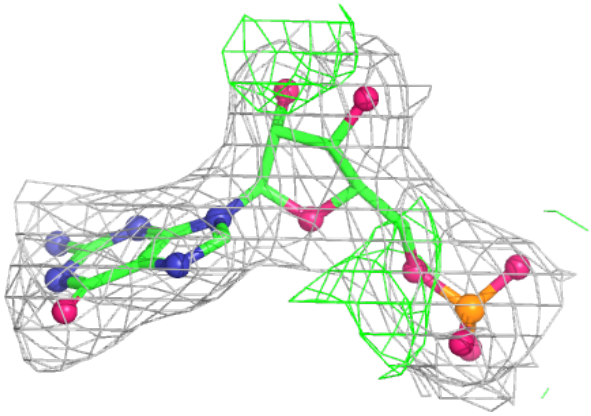


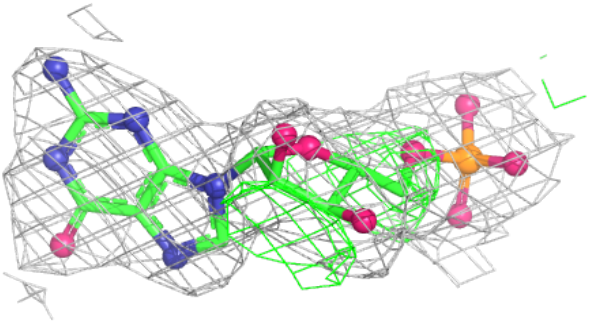


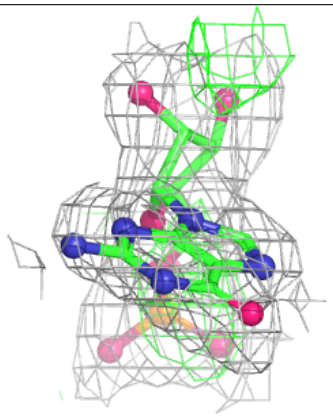


Electron density around 5GP A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

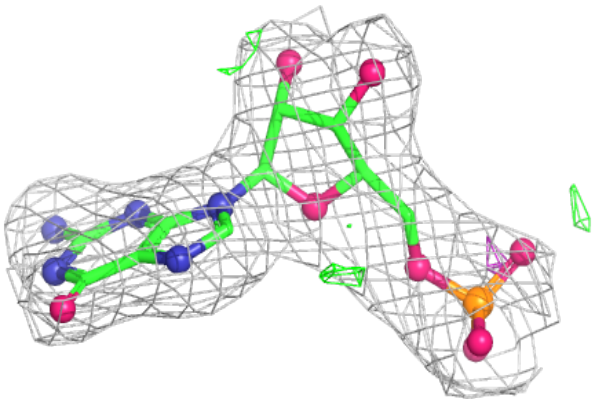


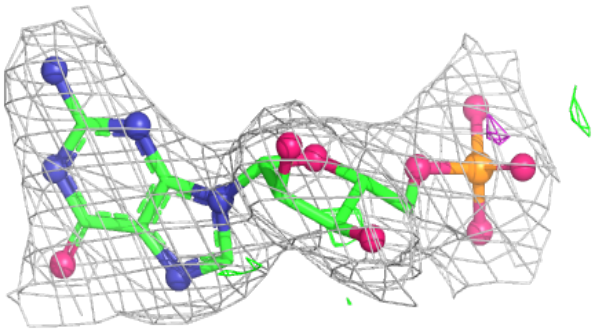


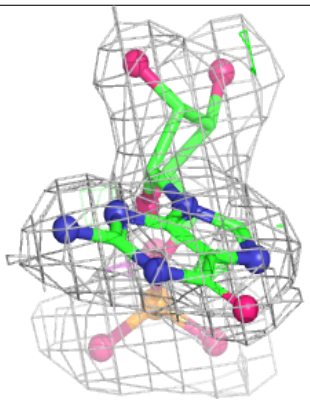


Electron density around 5GP I 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

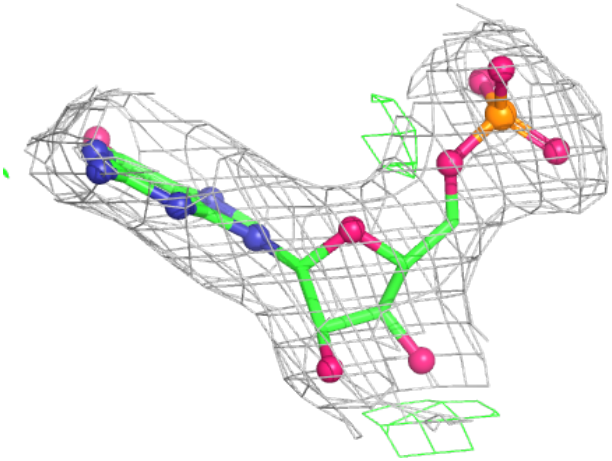


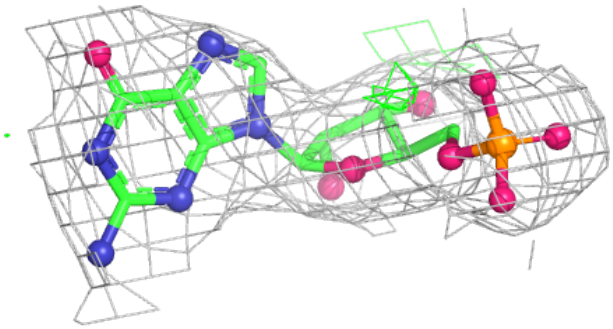


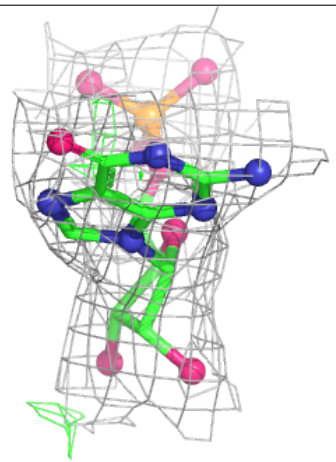


Electron density around 5GP K 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

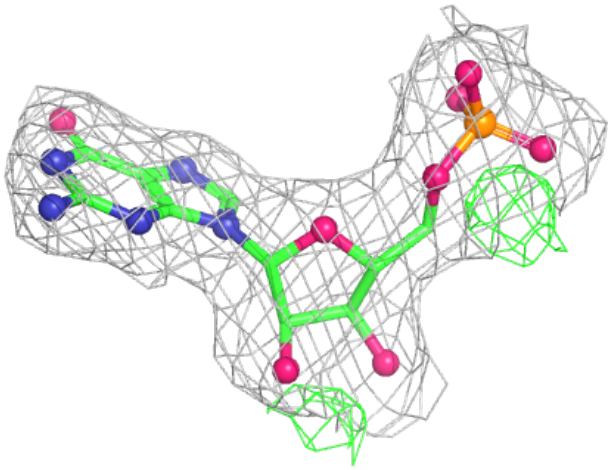


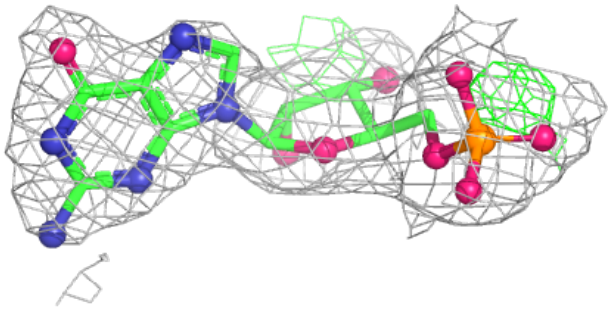


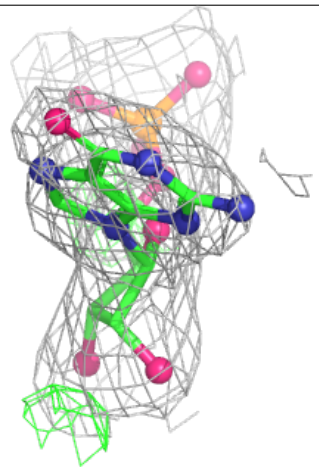


Electron density around 5GP L 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

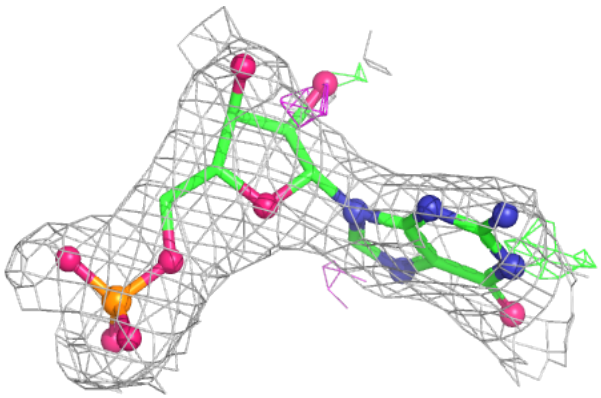


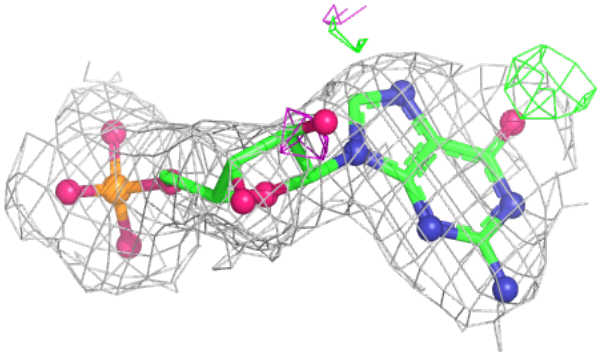


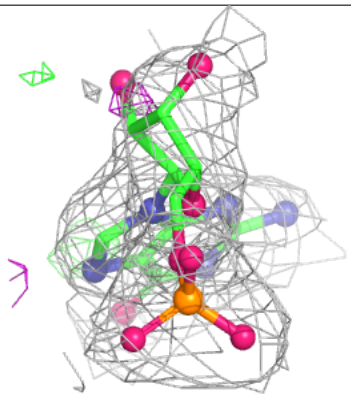


Electron density around 5GP P 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

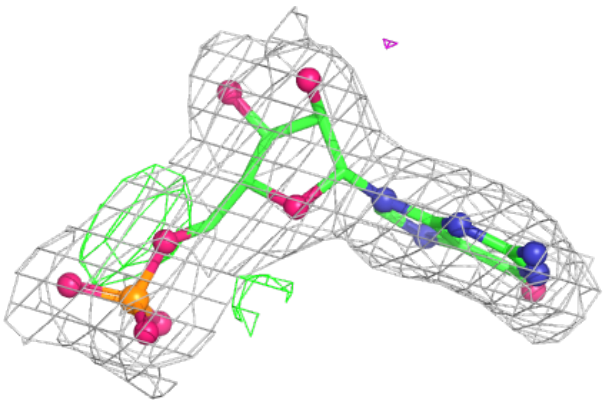


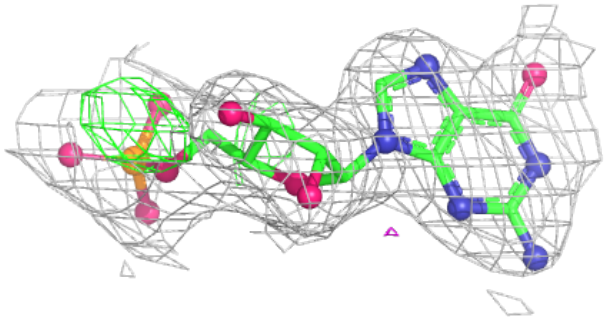


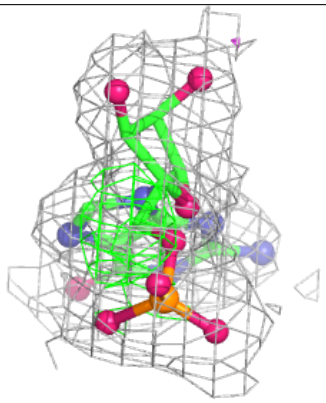


Electron density around 5GP M 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

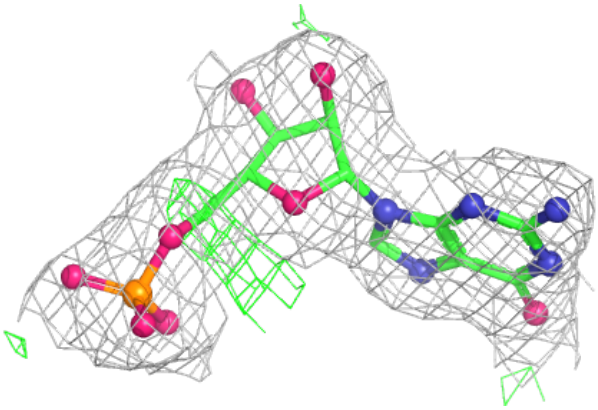


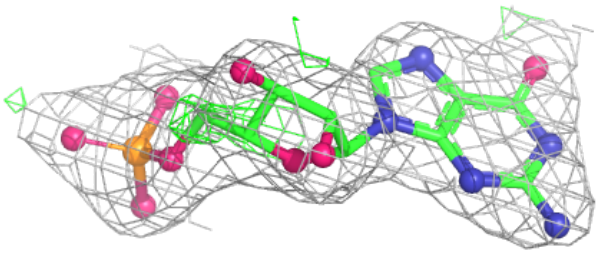


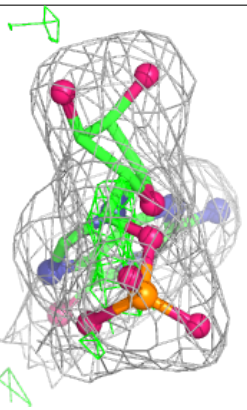


Electron density around 5GP N 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

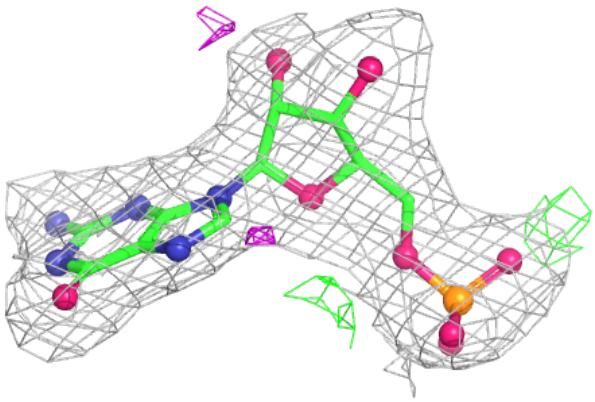


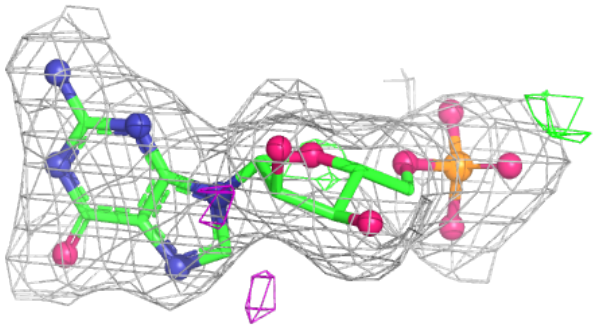


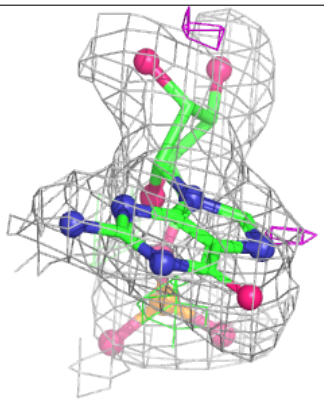


Electron density around 5GP C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

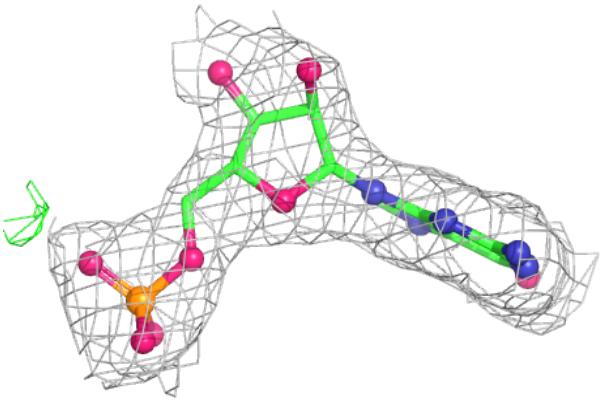


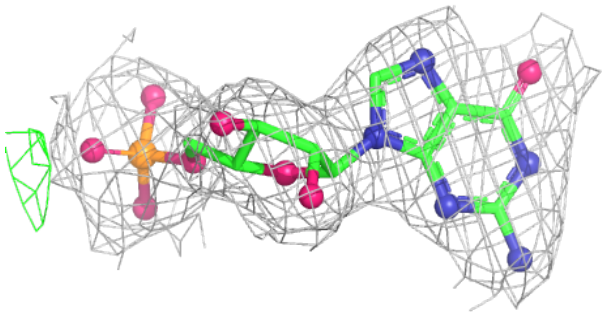


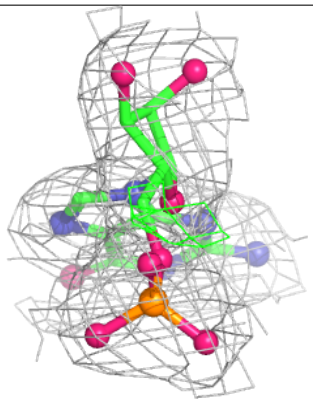


Electron density around 5GP J 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

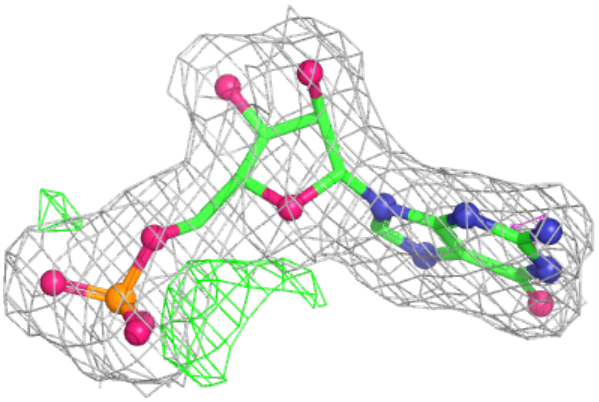


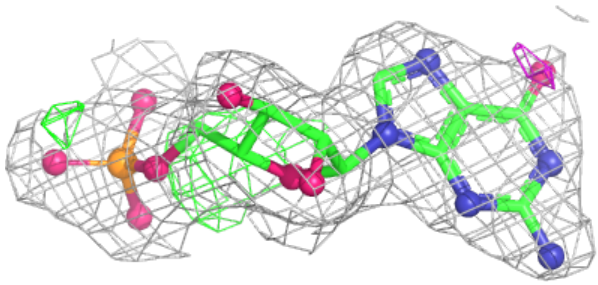


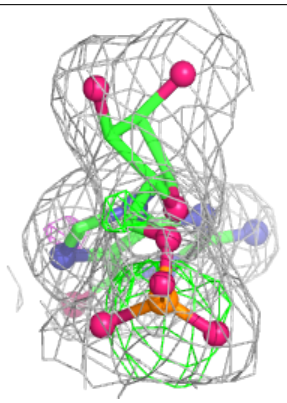


Electron density around 5GP D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

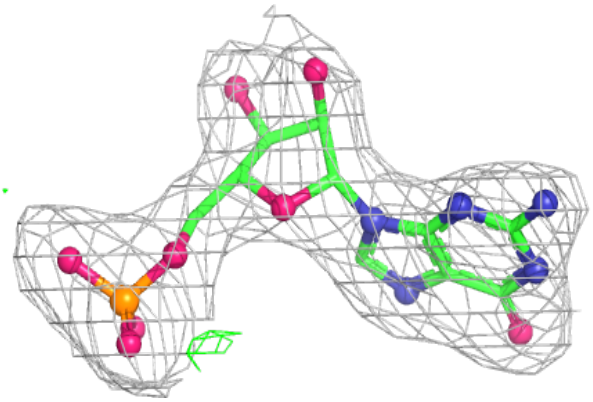


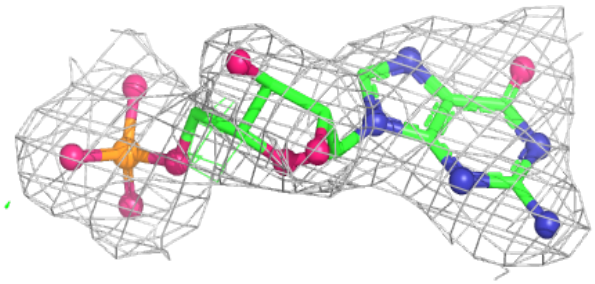


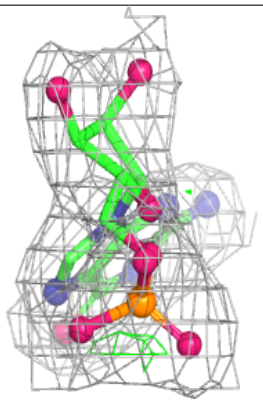


Electron density around 5GP O 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

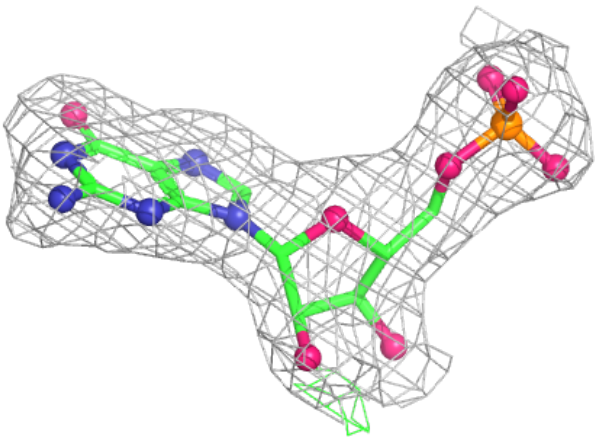


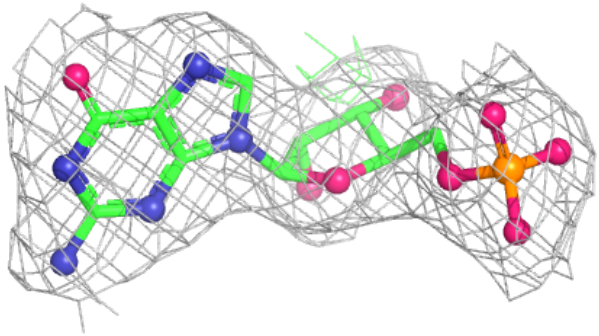


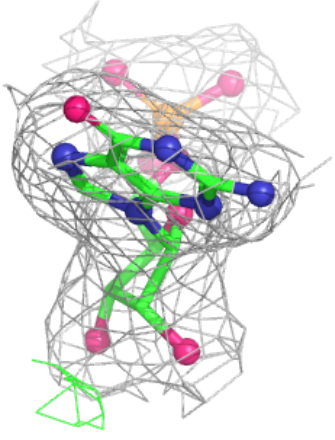


Electron density around 5GP H 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

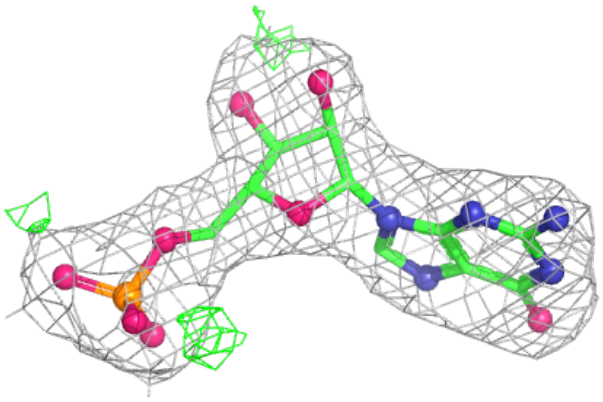


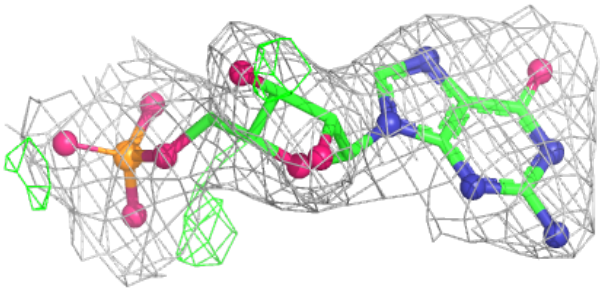


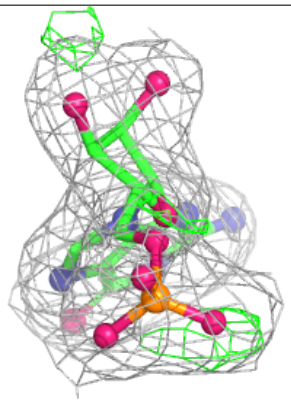


Electron density around 5GP B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

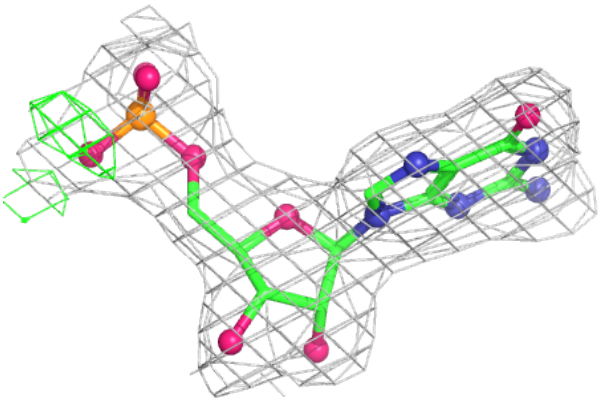


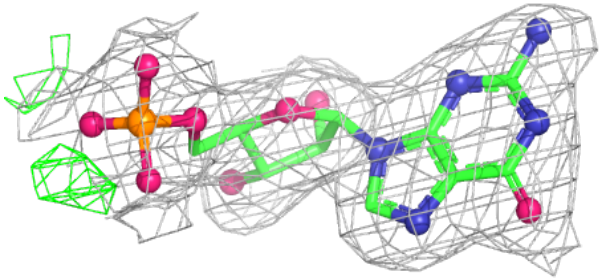


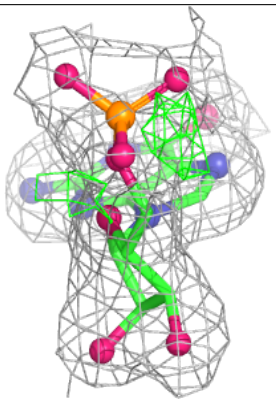


Electron density around 5GP E 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.