wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 12:02 pm GMT

PDB ID	:	6TGE
Title	:	NADP dependent methylene-tetrahydromethanopterin dehydrogenase-NADP +-methenyl-H4MPT+ complex
Authors	:	Ermler, U.; Shima, S.
Deposited on	:	2019-11-15
Resolution	:	1.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

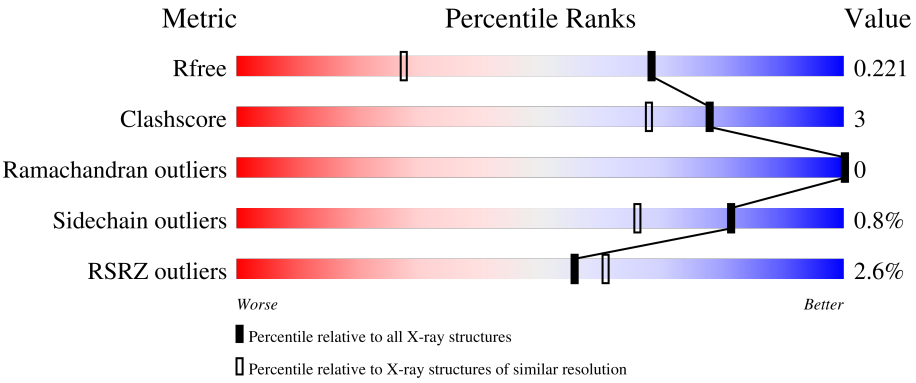
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	288	97%
1	B	288	97%
1	C	288	96%
1	D	288	97%
1	E	288	96%

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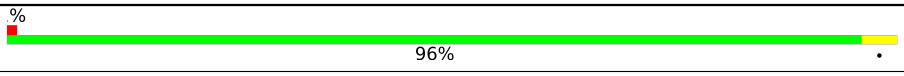
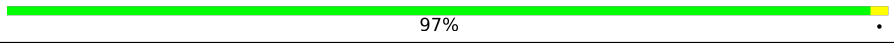
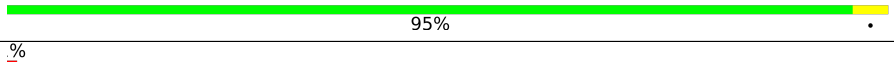
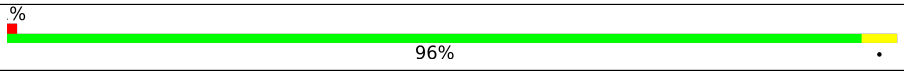
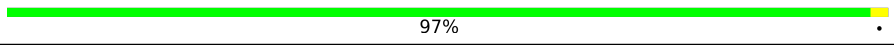
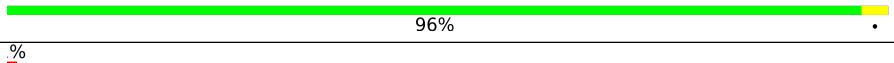
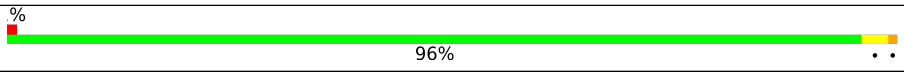
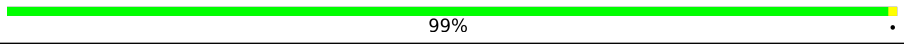
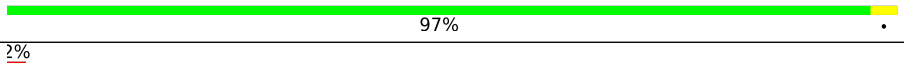
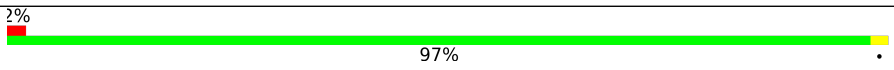
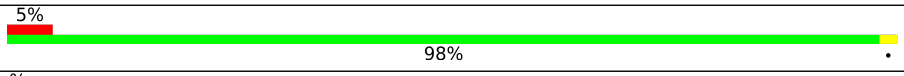
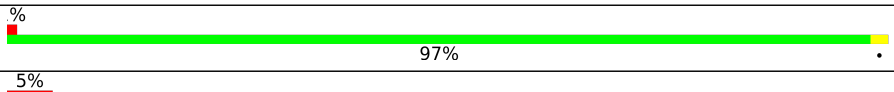
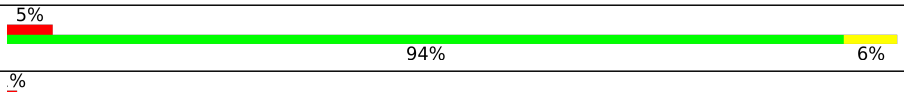
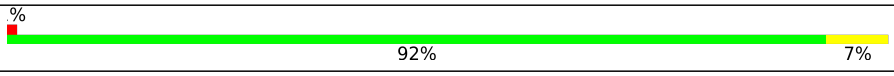
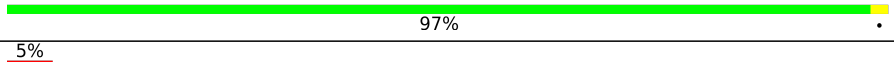
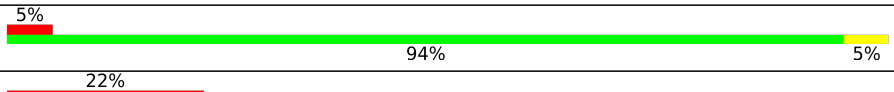
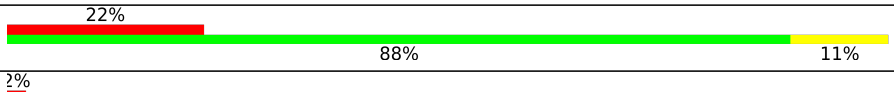
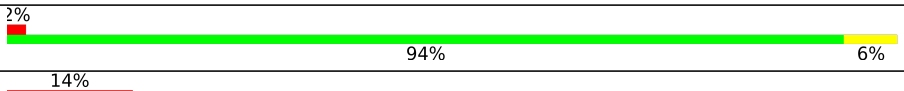
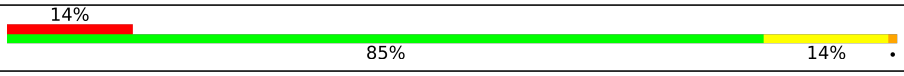
Mol	Chain	Length	Quality of chain
1	F	288	
1	G	288	
1	H	288	
1	I	288	
1	J	288	
1	K	288	
1	L	288	
1	M	288	
1	N	288	
1	O	288	
1	P	288	
1	Q	288	
1	R	288	
1	S	288	
1	T	288	
1	U	288	
1	V	288	
1	W	288	
1	X	288	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 60219 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 Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase/methylenetetrahydrofolate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	B	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	C	287	Total	C	N	O	S	0	1	0
			2091	1317	362	405	7			
1	D	287	Total	C	N	O	S	0	1	0
			2092	1317	363	405	7			
1	E	287	Total	C	N	O	S	0	1	0
			2091	1317	362	405	7			
1	F	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	G	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	H	287	Total	C	N	O	S	0	4	0
			2113	1328	365	413	7			
1	I	287	Total	C	N	O	S	0	1	0
			2091	1317	362	405	7			
1	J	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	K	287	Total	C	N	O	S	0	1	0
			2090	1316	362	405	7			
1	L	287	Total	C	N	O	S	0	3	0
			2105	1324	364	410	7			
1	M	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	N	287	Total	C	N	O	S	0	3	0
			2105	1325	365	408	7			
1	O	287	Total	C	N	O	S	0	1	0
			2093	1319	363	404	7			
1	P	287	Total	C	N	O	S	0	1	0
			2090	1316	362	405	7			

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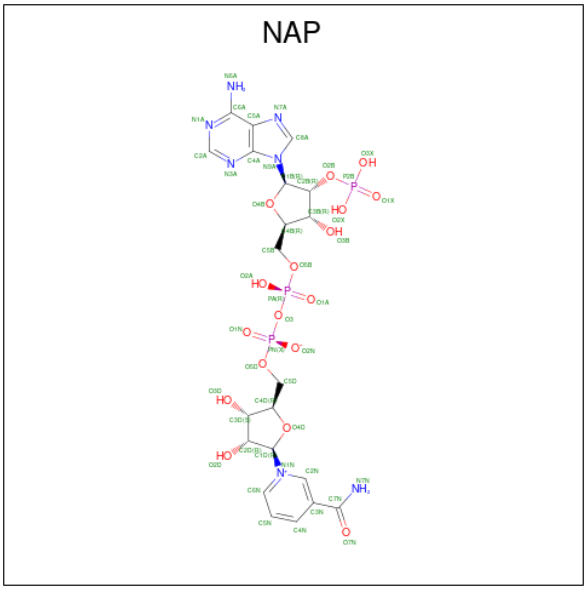
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	R	287	Total	C	N	O	S	0	3	0
			2104	1323	364	410	7			
1	S	287	Total	C	N	O	S	0	1	0
			2093	1319	363	404	7			
1	T	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			
1	U	287	Total	C	N	O	S	0	1	0
			2095	1319	365	404	7			
1	V	287	Total	C	N	O	S	0	2	0
			2099	1321	363	408	7			
1	W	287	Total	C	N	O	S	0	2	0
			2096	1319	363	407	7			
1	X	287	Total	C	N	O	S	0	0	0
			2084	1313	361	403	7			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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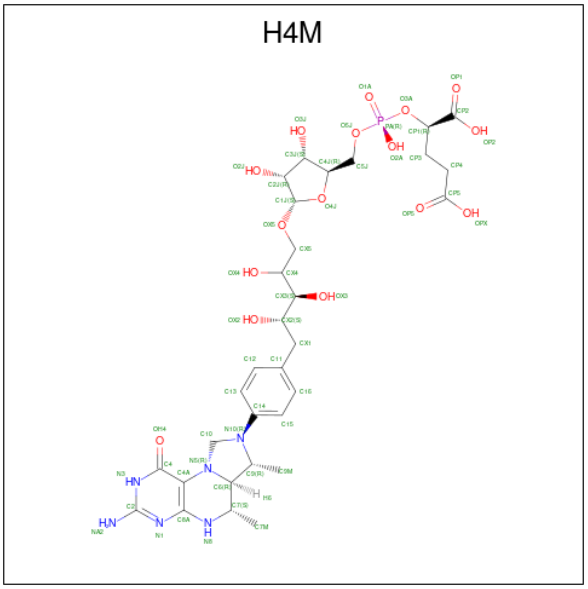
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	Q	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	R	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	S	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	T	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	U	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	V	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	W	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	X	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5,10-DIMETHYLENE TETRAHYDROMETHANOPTERIN (three-letter code: H4M) (formula: $C_{31}H_{45}N_6O_{16}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	B	1	Total	C	N	O	P	14	0
			45	26	6	12	1		
3	C	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	D	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	E	1	Total	C	N	O	P	14	0
			45	26	6	12	1		
3	F	1	Total	C	N	O	P	14	0
			45	26	6	12	1		
3	G	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	H	1	Total	C	N	O	P	14	0
			45	26	6	12	1		
3	I	1	Total	C	N	O	P	13	0
			45	26	6	12	1		
3	J	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	K	1	Total	C	N	O	P	13	0
			45	26	6	12	1		
3	L	1	Total	C	N	O	P	13	0
			45	26	6	12	1		

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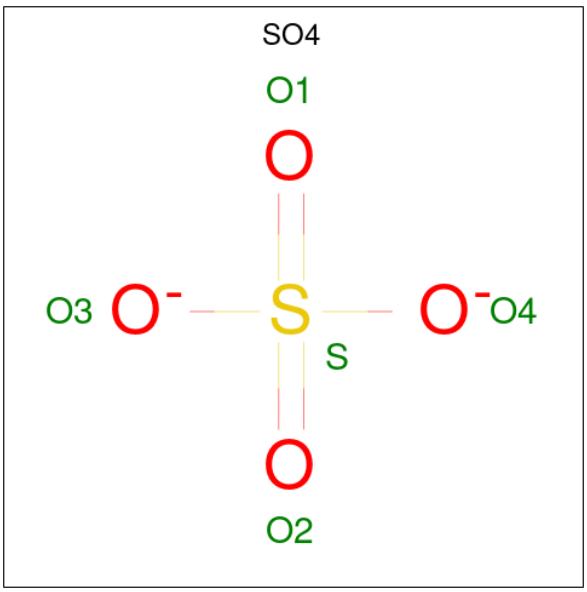
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	M	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	N	1	Total	C	N	O	P	13	0
			45	26	6	12	1		
3	O	1	Total	C	N	O	P	13	0
			45	26	6	12	1		
3	P	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	Q	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	R	1	Total	C	N	O	P	13	0
			45	26	6	12	1		
3	S	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	T	1	Total	C	N	O	P	13	0
			45	26	6	12	1		
3	U	1	Total	C	N	O	P	13	0
			45	26	6	12	1		
3	V	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	W	1	Total	C	N	O	P	0	0
			45	26	6	12	1		
3	X	1	Total	C	N	O	P	13	0
			45	26	6	12	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	P	1	Total O S 5 4 1	0	0
4	S	1	Total O S 5 4 1	0	0
4	V	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	386	Total O 387 387	0	1
5	B	349	Total O 354 354	0	5
5	C	339	Total O 341 341	0	2
5	D	329	Total O 331 331	0	2
5	E	387	Total O 390 390	0	3
5	F	365	Total O 368 368	0	3
5	G	379	Total O 385 385	0	6
5	H	401	Total O 404 404	0	3
5	I	347	Total O 350 350	0	3
5	J	349	Total O 352 352	0	3
5	K	348	Total O 352 352	0	4
5	L	308	Total O 309 309	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	381	Total O 382 382	0	1
5	N	362	Total O 363 363	0	1
5	O	331	Total O 334 334	0	3
5	P	310	Total O 310 310	0	0
5	Q	378	Total O 381 381	0	3
5	R	227	Total O 232 232	0	5
5	S	253	Total O 257 257	0	4
5	T	328	Total O 330 330	0	2
5	U	194	Total O 194 194	0	0
5	V	197	Total O 197 197	0	0
5	W	320	Total O 323 323	0	3
5	X	116	Total O 117 117	0	1

3 Residue-property plots (i)

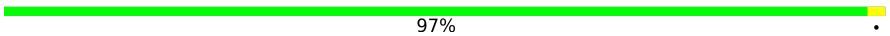
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

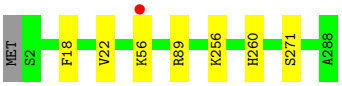
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain A:

• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

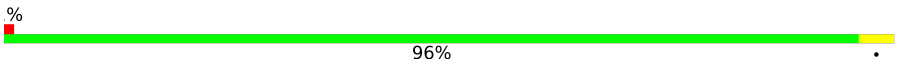
Chain B:

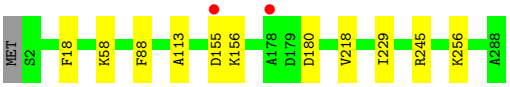




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

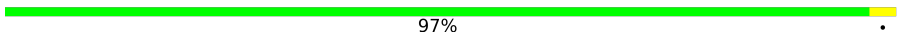
Chain C:

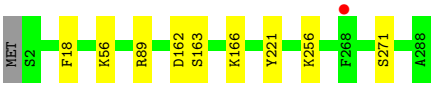




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

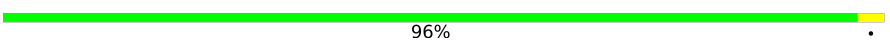
Chain D:





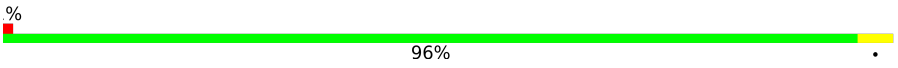
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

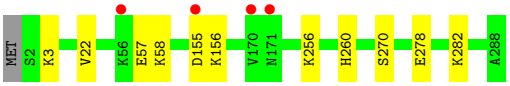
Chain E:



• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

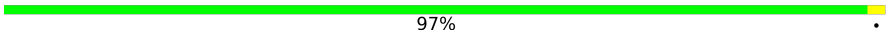
Chain F:





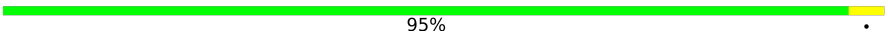
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

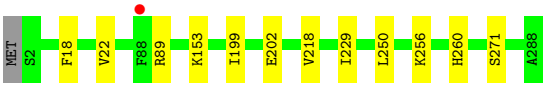
Chain G:



• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

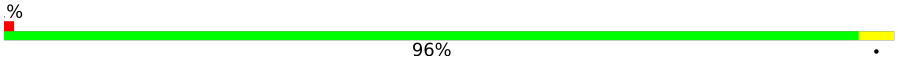
Chain H:

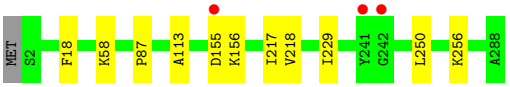




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

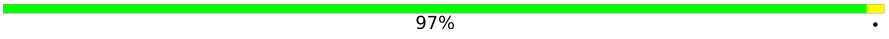
Chain I:





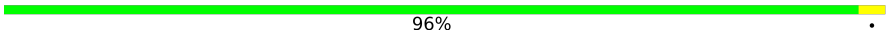
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

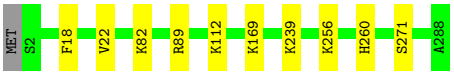
Chain J:



• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

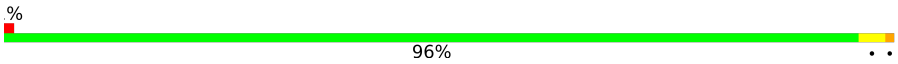
Chain K:

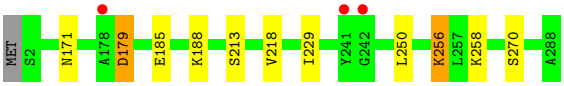




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

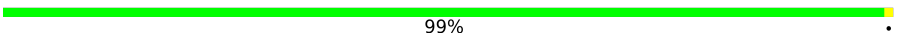
Chain L:

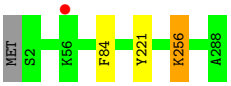




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

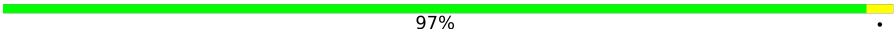
Chain M:





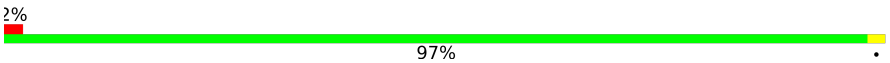
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

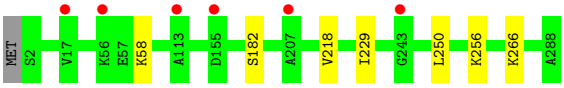
Chain N:



• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

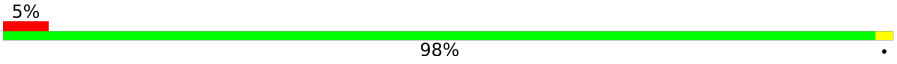
Chain O:

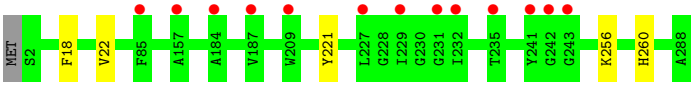




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

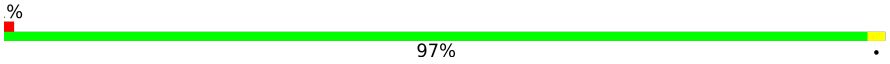
Chain P:

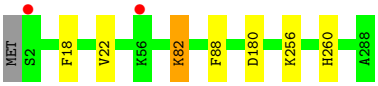




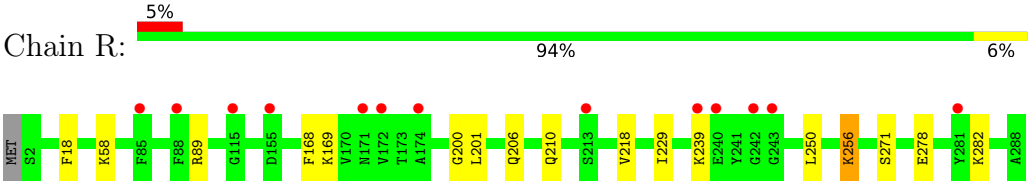
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain Q:

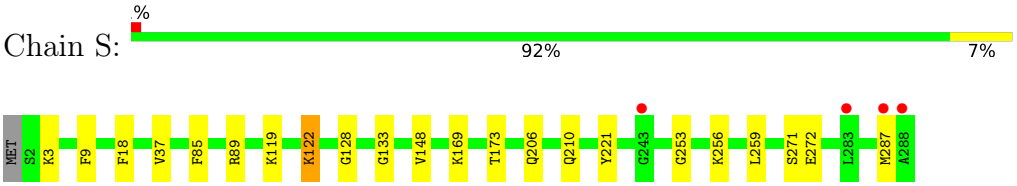




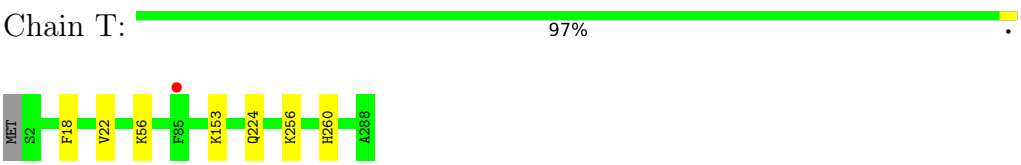
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



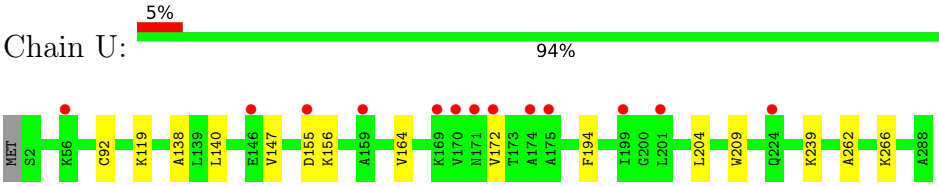
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



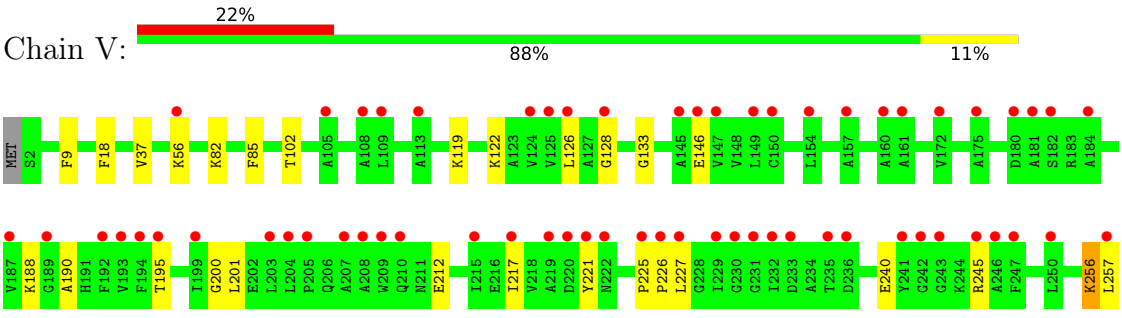
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

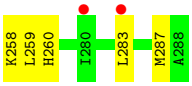


• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



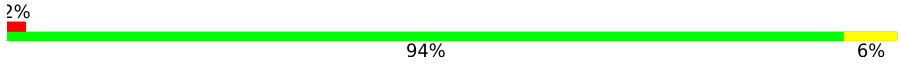
• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

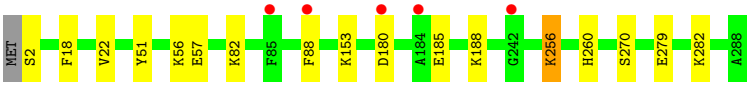




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

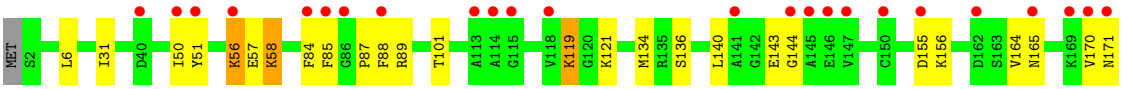
Chain W:

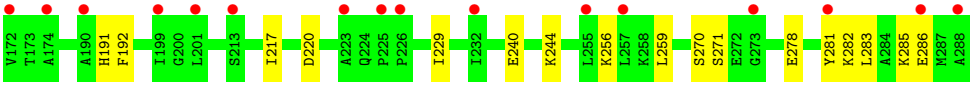




• Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	98.64Å 123.50Å 167.30Å 94.79° 100.39° 108.97°	Depositor
Resolution (Å)	48.76 – 1.50 48.76 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.76-1.50) 95.5 (48.76-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.186 , 0.216 0.192 , 0.221	Depositor DCC
R_{free} test set	55363 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	60219	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7090e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NAP, H4M, SO4

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	0.39	0/2116	0.57	0/2850
1	B	0.38	0/2116	0.55	0/2850
1	C	0.34	0/2123	0.53	0/2860
1	D	0.37	0/2124	0.57	0/2861
1	E	0.38	0/2123	0.56	0/2860
1	F	0.36	0/2116	0.56	0/2850
1	G	0.41	0/2116	0.58	0/2850
1	H	0.39	0/2145	0.58	0/2889
1	I	0.35	0/2123	0.55	0/2860
1	J	0.35	0/2116	0.55	0/2850
1	K	0.35	0/2122	0.55	0/2858
1	L	0.33	0/2137	0.55	1/2878 (0.0%)
1	M	0.39	0/2116	0.61	0/2850
1	N	0.38	0/2137	0.57	0/2877
1	O	0.34	0/2125	0.53	0/2861
1	P	0.37	0/2122	0.55	0/2858
1	Q	0.37	0/2116	0.55	0/2850
1	R	0.34	0/2136	0.53	0/2877
1	S	0.32	0/2125	0.52	0/2861
1	T	0.32	0/2116	0.54	0/2850
1	U	0.35	1/2127 (0.0%)	0.51	0/2864
1	V	0.35	0/2131	0.53	0/2870
1	W	0.33	0/2128	0.53	0/2866
1	X	0.32	0/2116	0.51	0/2850
All	All	0.36	1/50972 (0.0%)	0.55	1/68650 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	92	CYS	CB-SG	-5.59	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	179	ASP	CB-CA-C	-6.62	97.15	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2084	0	2086	4	0
1	B	2084	0	2086	5	0
1	C	2091	0	2092	8	0
1	D	2092	0	2091	9	0
1	E	2091	0	2092	9	0
1	F	2084	0	2086	10	0
1	G	2084	0	2086	4	0
1	H	2113	0	2102	11	0
1	I	2091	0	2092	8	0
1	J	2084	0	2086	6	0
1	K	2090	0	2090	8	0
1	L	2105	0	2099	7	0
1	M	2084	0	2086	5	0
1	N	2105	0	2106	4	0
1	O	2093	0	2098	6	0
1	P	2090	0	2090	4	0
1	Q	2084	0	2086	7	0
1	R	2104	0	2097	11	0
1	S	2093	0	2098	21	0
1	T	2084	0	2086	5	0
1	U	2095	0	2098	7	0
1	V	2099	0	2095	34	0
1	W	2096	0	2094	14	0
1	X	2084	0	2086	31	0
2	A	48	0	25	8	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	48	0	25	5	0
2	E	48	0	25	1	0
2	F	48	0	25	2	0
2	G	48	0	25	6	0
2	H	48	0	25	1	0
2	I	48	0	25	1	0
2	J	48	0	25	5	0
2	K	48	0	25	1	0
2	L	48	0	25	2	0
2	M	48	0	25	6	0
2	N	48	0	25	1	0
2	O	48	0	25	1	0
2	P	48	0	25	4	0
2	Q	48	0	25	1	0
2	R	48	0	25	1	0
2	S	48	0	25	7	0
2	T	48	0	25	1	0
2	U	48	0	25	2	0
2	V	48	0	25	3	0
2	W	48	0	25	1	0
2	X	48	0	25	1	0
3	A	45	0	37	8	0
3	B	45	0	37	5	0
3	C	45	0	37	4	0
3	D	45	0	37	6	0
3	E	45	0	37	3	0
3	F	45	0	37	3	0
3	G	45	0	37	7	0
3	H	45	0	37	6	0
3	I	45	0	37	3	0
3	J	45	0	37	7	0
3	K	45	0	37	5	0
3	L	45	0	37	4	0
3	M	45	0	37	5	0
3	N	45	0	37	3	0
3	O	45	0	37	4	0
3	P	45	0	37	8	0
3	Q	45	0	37	3	0
3	R	45	0	37	7	0
3	S	45	0	37	8	0
3	T	45	0	37	3	0
3	U	45	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	45	0	37	7	0
3	W	45	0	37	3	0
3	X	45	0	37	4	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
4	H	5	0	0	0	0
4	J	5	0	0	0	0
4	M	5	0	0	0	0
4	P	5	0	0	0	0
4	S	5	0	0	0	0
4	V	5	0	0	0	0
5	A	387	0	0	1	0
5	B	354	0	0	0	0
5	C	341	0	0	2	0
5	D	331	0	0	1	0
5	E	390	0	0	3	0
5	F	368	0	0	4	0
5	G	385	0	0	0	0
5	H	404	0	0	3	0
5	I	350	0	0	0	0
5	J	352	0	0	0	0
5	K	352	0	0	2	0
5	L	309	0	0	2	0
5	M	382	0	0	1	0
5	N	363	0	0	0	0
5	O	334	0	0	1	0
5	P	310	0	0	1	0
5	Q	381	0	0	0	0
5	R	232	0	0	0	0
5	S	257	0	0	3	0
5	T	330	0	0	2	0
5	U	194	0	0	0	0
5	V	197	0	0	5	0
5	W	323	0	0	2	0
5	X	117	0	0	3	0
All	All	60219	0	51696	302	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 3.

The worst 5 of 302 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)
2:A:301:NAP:C4N	3:A:302:H4M:H16	1.36	1.51
2:M:301:NAP:C4N	3:M:302:H4M:H16	1.54	1.38
2:G:301:NAP:C4N	3:G:302:H4M:H16	1.61	1.29
2:P:301:NAP:C4N	3:P:302:H4M:H16	1.72	1.19
2:S:301:NAP:C4N	3:S:302:H4M:H16	1.73	1.17

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 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	285/288 (99%)	280 (98%)	5 (2%)	0	100	100
1	B	285/288 (99%)	281 (99%)	4 (1%)	0	100	100
1	C	286/288 (99%)	281 (98%)	5 (2%)	0	100	100
1	D	286/288 (99%)	281 (98%)	5 (2%)	0	100	100
1	E	286/288 (99%)	281 (98%)	5 (2%)	0	100	100
1	F	285/288 (99%)	281 (99%)	4 (1%)	0	100	100
1	G	285/288 (99%)	279 (98%)	6 (2%)	0	100	100
1	H	289/288 (100%)	285 (99%)	4 (1%)	0	100	100
1	I	286/288 (99%)	282 (99%)	4 (1%)	0	100	100
1	J	285/288 (99%)	279 (98%)	6 (2%)	0	100	100
1	K	286/288 (99%)	282 (99%)	4 (1%)	0	100	100
1	L	288/288 (100%)	284 (99%)	4 (1%)	0	100	100
1	M	285/288 (99%)	279 (98%)	6 (2%)	0	100	100
1	N	288/288 (100%)	284 (99%)	4 (1%)	0	100	100
1	O	286/288 (99%)	281 (98%)	5 (2%)	0	100	100
1	P	286/288 (99%)	279 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	285/288 (99%)	280 (98%)	5 (2%)	0	100	100
1	R	288/288 (100%)	284 (99%)	4 (1%)	0	100	100
1	S	286/288 (99%)	280 (98%)	6 (2%)	0	100	100
1	T	285/288 (99%)	280 (98%)	5 (2%)	0	100	100
1	U	286/288 (99%)	281 (98%)	5 (2%)	0	100	100
1	V	287/288 (100%)	278 (97%)	9 (3%)	0	100	100
1	W	287/288 (100%)	282 (98%)	5 (2%)	0	100	100
1	X	285/288 (99%)	278 (98%)	7 (2%)	0	100	100
All	All	6866/6912 (99%)	6742 (98%)	124 (2%)	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	204/205 (100%)	203 (100%)	1 (0%)	88	78
1	B	204/205 (100%)	203 (100%)	1 (0%)	88	78
1	C	205/205 (100%)	204 (100%)	1 (0%)	88	78
1	D	205/205 (100%)	204 (100%)	1 (0%)	88	78
1	E	205/205 (100%)	205 (100%)	0	100	100
1	F	204/205 (100%)	202 (99%)	2 (1%)	76	57
1	G	204/205 (100%)	203 (100%)	1 (0%)	88	78
1	H	208/205 (102%)	207 (100%)	1 (0%)	88	78
1	I	205/205 (100%)	204 (100%)	1 (0%)	88	78
1	J	204/205 (100%)	202 (99%)	2 (1%)	76	57
1	K	205/205 (100%)	204 (100%)	1 (0%)	88	78
1	L	207/205 (101%)	202 (98%)	5 (2%)	49	19
1	M	204/205 (100%)	203 (100%)	1 (0%)	88	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	207/205 (101%)	205 (99%)	2 (1%)	76 57
1	O	205/205 (100%)	204 (100%)	1 (0%)	88 78
1	P	205/205 (100%)	204 (100%)	1 (0%)	88 78
1	Q	204/205 (100%)	202 (99%)	2 (1%)	76 57
1	R	207/205 (101%)	204 (99%)	3 (1%)	67 42
1	S	205/205 (100%)	204 (100%)	1 (0%)	88 78
1	T	204/205 (100%)	203 (100%)	1 (0%)	88 78
1	U	205/205 (100%)	204 (100%)	1 (0%)	88 78
1	V	206/205 (100%)	204 (99%)	2 (1%)	76 57
1	W	206/205 (100%)	203 (98%)	3 (2%)	65 39
1	X	204/205 (100%)	199 (98%)	5 (2%)	47 18
All	All	4922/4920 (100%)	4882 (99%)	40 (1%)	81 66

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	224	GLN
1	X	56	LYS
1	U	239	LYS
1	W	2	SER
1	X	119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	171	ASN
1	X	206	GLN
1	X	260	HIS
1	Q	206	GLN
1	T	171	ASN

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)

56 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	303	-	4,4,4	0.11	0	6,6,6	0.12	0
4	SO4	P	303	-	4,4,4	0.13	0	6,6,6	0.15	0
3	H4M	G	302	-	47,49,58	5.79	9 (19%)	62,74,86	1.85	8 (12%)
3	H4M	E	302	-	47,49,58	5.66	6 (12%)	62,74,86	1.45	10 (16%)
2	NAP	S	301	-	45,52,52	1.86	14 (31%)	56,80,80	1.48	6 (10%)
3	H4M	H	302	-	47,49,58	5.81	7 (14%)	62,74,86	1.69	11 (17%)
2	NAP	E	301	-	45,52,52	1.97	13 (28%)	56,80,80	1.39	6 (10%)
3	H4M	L	302	-	47,49,58	5.90	6 (12%)	62,74,86	1.66	13 (20%)
3	H4M	C	302	-	47,49,58	5.62	6 (12%)	62,74,86	1.62	10 (16%)
3	H4M	J	302	-	47,49,58	5.70	7 (14%)	62,74,86	1.87	11 (17%)
3	H4M	O	302	-	47,49,58	5.84	7 (14%)	62,74,86	1.81	11 (17%)
3	H4M	S	302	-	47,49,58	5.79	7 (14%)	62,74,86	1.84	10 (16%)
2	NAP	L	301	-	45,52,52	1.84	12 (26%)	56,80,80	1.60	7 (12%)
4	SO4	D	303	-	4,4,4	0.18	0	6,6,6	0.14	0
3	H4M	B	302	-	47,49,58	5.81	7 (14%)	62,74,86	1.72	11 (17%)
3	H4M	Q	302	-	47,49,58	5.70	6 (12%)	62,74,86	1.49	8 (12%)
2	NAP	P	301	-	45,52,52	1.86	12 (26%)	56,80,80	1.52	8 (14%)
2	NAP	B	301	-	45,52,52	1.76	11 (24%)	56,80,80	1.39	6 (10%)
4	SO4	V	303	-	4,4,4	0.16	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	H4M	R	302	-	47,49,58	5.61	7 (14%)	62,74,86	1.83	10 (16%)
3	H4M	T	302	-	47,49,58	5.66	6 (12%)	62,74,86	1.45	8 (12%)
3	H4M	M	302	-	47,49,58	5.68	6 (12%)	62,74,86	1.92	13 (20%)
3	H4M	U	302	-	47,49,58	6.14	6 (12%)	62,74,86	1.66	12 (19%)
3	H4M	W	302	-	47,49,58	5.68	6 (12%)	62,74,86	1.47	9 (14%)
3	H4M	N	302	-	47,49,58	5.98	7 (14%)	62,74,86	1.70	9 (14%)
2	NAP	D	302	-	45,52,52	1.79	12 (26%)	56,80,80	1.59	7 (12%)
3	H4M	V	302	-	47,49,58	5.37	7 (14%)	62,74,86	2.10	13 (20%)
2	NAP	K	301	-	45,52,52	1.73	10 (22%)	56,80,80	1.50	7 (12%)
2	NAP	V	301	-	45,52,52	1.93	13 (28%)	56,80,80	1.60	5 (8%)
2	NAP	H	301	-	45,52,52	1.72	12 (26%)	56,80,80	1.41	7 (12%)
3	H4M	A	302	-	47,49,58	5.58	7 (14%)	62,74,86	1.70	11 (17%)
2	NAP	X	301	-	45,52,52	1.92	13 (28%)	56,80,80	1.51	5 (8%)
3	H4M	I	302	-	47,49,58	5.73	6 (12%)	62,74,86	1.55	8 (12%)
2	NAP	Q	301	-	45,52,52	1.81	13 (28%)	56,80,80	1.42	8 (14%)
3	H4M	F	302	-	47,49,58	6.08	6 (12%)	62,74,86	1.64	13 (20%)
2	NAP	F	301	-	45,52,52	1.82	14 (31%)	56,80,80	1.62	7 (12%)
2	NAP	I	301	-	45,52,52	1.82	13 (28%)	56,80,80	1.63	8 (14%)
2	NAP	T	301	-	45,52,52	1.91	13 (28%)	56,80,80	1.52	8 (14%)
4	SO4	J	303	-	4,4,4	0.16	0	6,6,6	0.15	0
4	SO4	S	303	-	4,4,4	0.17	0	6,6,6	0.10	0
2	NAP	M	301	-	45,52,52	1.72	10 (22%)	56,80,80	1.32	8 (14%)
2	NAP	O	301	-	45,52,52	1.87	12 (26%)	56,80,80	1.59	8 (14%)
2	NAP	A	301	-	45,52,52	1.87	13 (28%)	56,80,80	1.48	7 (12%)
3	H4M	P	302	-	47,49,58	5.56	7 (14%)	62,74,86	1.98	10 (16%)
2	NAP	R	301	-	45,52,52	1.88	15 (33%)	56,80,80	1.51	6 (10%)
2	NAP	C	301	-	45,52,52	1.84	11 (24%)	56,80,80	1.59	7 (12%)
2	NAP	J	301	-	45,52,52	1.92	14 (31%)	56,80,80	1.47	6 (10%)
2	NAP	U	301	-	45,52,52	1.93	13 (28%)	56,80,80	1.66	7 (12%)
3	H4M	K	302	-	47,49,58	5.85	7 (14%)	62,74,86	1.70	8 (12%)
3	H4M	D	301	-	47,49,58	5.55	7 (14%)	62,74,86	1.73	8 (12%)
3	H4M	X	302	-	47,49,58	5.84	7 (14%)	62,74,86	1.82	13 (20%)
2	NAP	W	301	-	45,52,52	1.97	14 (31%)	56,80,80	1.48	8 (14%)
4	SO4	H	303	-	4,4,4	0.13	0	6,6,6	0.12	0
2	NAP	N	301	-	45,52,52	1.78	11 (24%)	56,80,80	1.52	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	G	301	-	45,52,52	1.84	12 (26%)	56,80,80	1.44	8 (14%)
4	SO4	M	303	-	4,4,4	0.19	0	6,6,6	0.25	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
3	H4M	G	302	-	-	16/27/71/85	0/5/5/5
3	H4M	E	302	-	-	10/27/71/85	0/5/5/5
2	NAP	S	301	-	-	7/31/67/67	0/5/5/5
3	H4M	H	302	-	-	18/27/71/85	0/5/5/5
2	NAP	E	301	-	-	3/31/67/67	0/5/5/5
3	H4M	L	302	-	-	18/27/71/85	0/5/5/5
3	H4M	C	302	-	-	8/27/71/85	0/5/5/5
3	H4M	J	302	-	-	8/27/71/85	0/5/5/5
3	H4M	O	302	-	-	17/27/71/85	0/5/5/5
3	H4M	S	302	-	-	12/27/71/85	0/5/5/5
2	NAP	L	301	-	-	7/31/67/67	0/5/5/5
3	H4M	B	302	-	-	15/27/71/85	0/5/5/5
3	H4M	Q	302	-	-	8/27/71/85	0/5/5/5
2	NAP	P	301	-	-	7/31/67/67	0/5/5/5
2	NAP	B	301	-	-	3/31/67/67	0/5/5/5
3	H4M	R	302	-	-	12/27/71/85	0/5/5/5
3	H4M	T	302	-	-	6/27/71/85	0/5/5/5
3	H4M	M	302	-	-	5/27/71/85	0/5/5/5
3	H4M	U	302	-	-	15/27/71/85	0/5/5/5
3	H4M	W	302	-	-	12/27/71/85	0/5/5/5
3	H4M	N	302	-	-	18/27/71/85	0/5/5/5
2	NAP	D	302	-	-	7/31/67/67	0/5/5/5
3	H4M	V	302	-	-	10/27/71/85	0/5/5/5
2	NAP	K	301	-	-	2/31/67/67	0/5/5/5
2	NAP	V	301	-	-	8/31/67/67	0/5/5/5
2	NAP	H	301	-	-	4/31/67/67	0/5/5/5
3	H4M	A	302	-	-	7/27/71/85	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	X	301	-	-	4/31/67/67	0/5/5/5
3	H4M	I	302	-	-	14/27/71/85	0/5/5/5
2	NAP	Q	301	-	-	4/31/67/67	0/5/5/5
3	H4M	F	302	-	-	15/27/71/85	0/5/5/5
2	NAP	F	301	-	-	5/31/67/67	0/5/5/5
2	NAP	I	301	-	-	3/31/67/67	0/5/5/5
2	NAP	T	301	-	-	4/31/67/67	0/5/5/5
2	NAP	M	301	-	-	7/31/67/67	0/5/5/5
2	NAP	O	301	-	-	3/31/67/67	0/5/5/5
2	NAP	A	301	-	-	6/31/67/67	0/5/5/5
3	H4M	P	302	-	-	19/27/71/85	0/5/5/5
2	NAP	R	301	-	-	4/31/67/67	0/5/5/5
2	NAP	C	301	-	-	3/31/67/67	0/5/5/5
2	NAP	J	301	-	-	8/31/67/67	0/5/5/5
2	NAP	U	301	-	-	4/31/67/67	0/5/5/5
3	H4M	K	302	-	-	18/27/71/85	0/5/5/5
3	H4M	D	301	-	-	12/27/71/85	0/5/5/5
3	H4M	X	302	-	-	21/27/71/85	0/5/5/5
2	NAP	W	301	-	-	4/31/67/67	0/5/5/5
2	NAP	N	301	-	-	3/31/67/67	0/5/5/5
2	NAP	G	301	-	-	6/31/67/67	0/5/5/5

The worst 5 of 460 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	302	H4M	C10-N5	-40.53	1.23	1.46
3	F	302	H4M	C10-N5	-40.16	1.23	1.46
3	N	302	H4M	C10-N5	-39.42	1.24	1.46
3	L	302	H4M	C10-N5	-38.96	1.24	1.46
3	K	302	H4M	C10-N5	-38.49	1.24	1.46

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAP	C5A-C6A-N6A	6.99	130.97	120.35
2	L	301	NAP	C5A-C6A-N6A	6.98	130.96	120.35
2	I	301	NAP	C5A-C6A-N6A	6.83	130.73	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	301	NAP	C5A-C6A-N6A	6.80	130.69	120.35
2	O	301	NAP	C5A-C6A-N6A	6.78	130.66	120.35

There are no chirality outliers.

5 of 430 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C2B-O2B-P2B-O1X
2	A	301	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	O4D-C1D-N1N-C6N
2	A	301	NAP	C2D-C1D-N1N-C2N
2	A	301	NAP	C2D-C1D-N1N-C6N

There are no ring outliers.

48 monomers are involved in 131 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	302	H4M	7	0
3	E	302	H4M	3	0
2	S	301	NAP	7	0
3	H	302	H4M	6	0
2	E	301	NAP	1	0
3	L	302	H4M	4	0
3	C	302	H4M	4	0
3	J	302	H4M	7	0
3	O	302	H4M	4	0
3	S	302	H4M	8	0
2	L	301	NAP	2	0
3	B	302	H4M	5	0
3	Q	302	H4M	3	0
2	P	301	NAP	4	0
2	B	301	NAP	1	0
3	R	302	H4M	7	0
3	T	302	H4M	3	0
3	M	302	H4M	5	0
3	U	302	H4M	3	0
3	W	302	H4M	3	0
3	N	302	H4M	3	0
2	D	302	NAP	5	0
3	V	302	H4M	7	0
2	K	301	NAP	1	0

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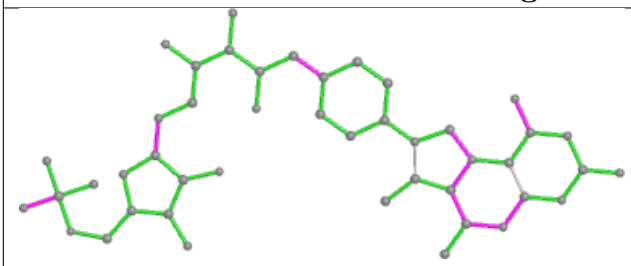
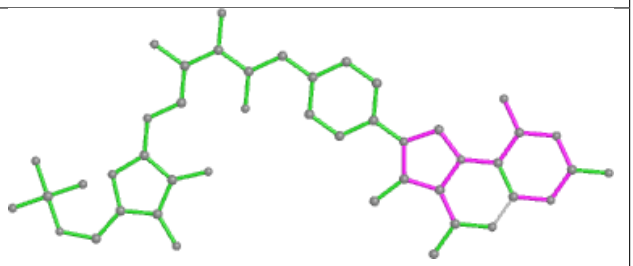
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	V	301	NAP	3	0
2	H	301	NAP	1	0
3	A	302	H4M	8	0
2	X	301	NAP	1	0
3	I	302	H4M	3	0
2	Q	301	NAP	1	0
3	F	302	H4M	3	0
2	F	301	NAP	2	0
2	I	301	NAP	1	0
2	T	301	NAP	1	0
2	M	301	NAP	6	0
2	O	301	NAP	1	0
2	A	301	NAP	8	0
3	P	302	H4M	8	0
2	R	301	NAP	1	0
2	C	301	NAP	1	0
2	J	301	NAP	5	0
2	U	301	NAP	2	0
3	K	302	H4M	5	0
3	D	301	H4M	6	0
3	X	302	H4M	4	0
2	W	301	NAP	1	0
2	N	301	NAP	1	0
2	G	301	NAP	6	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.

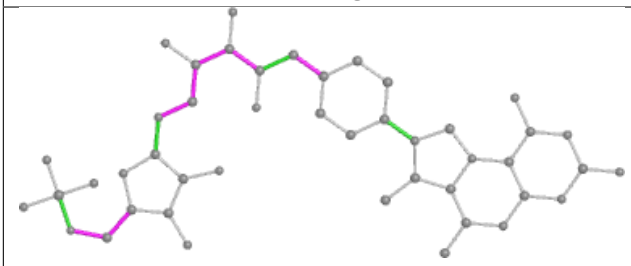
Ligand H4M G 302



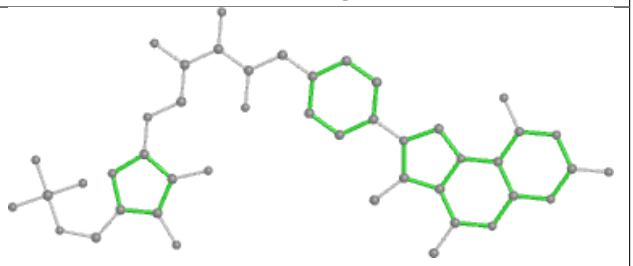
Bond lengths



Bond angles

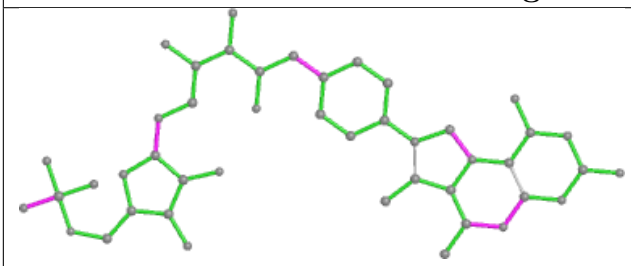


Torsions

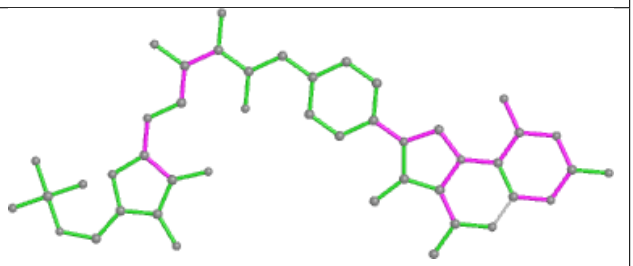


Rings

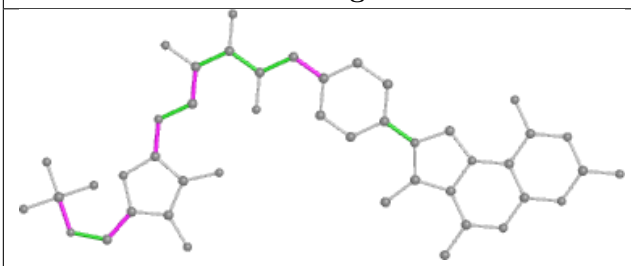
Ligand H4M E 302



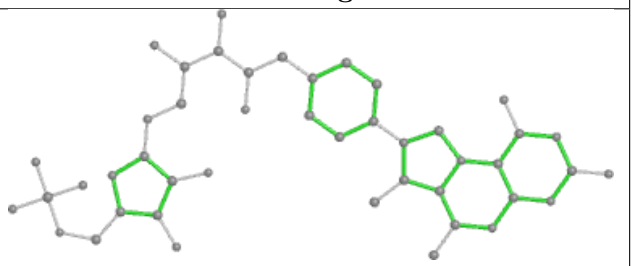
Bond lengths



Bond angles

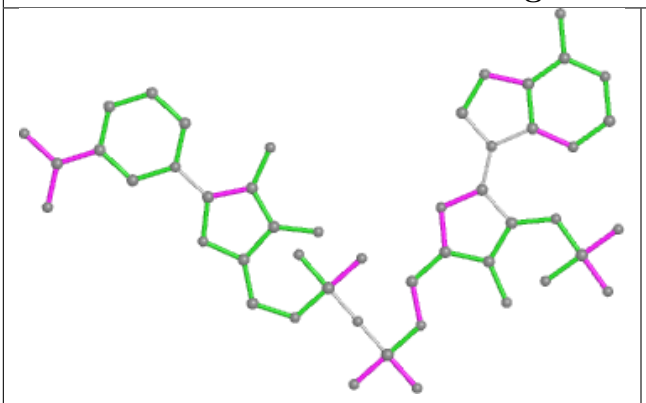


Torsions



Rings

Ligand NAP S 301



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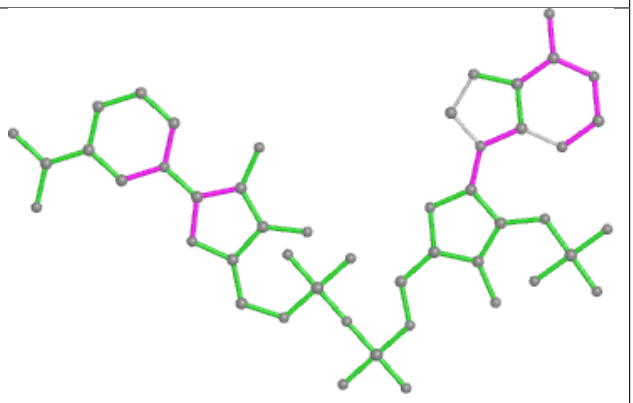
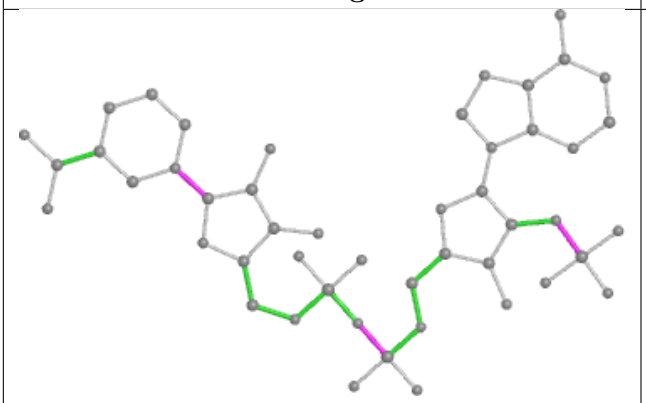


Bond angles



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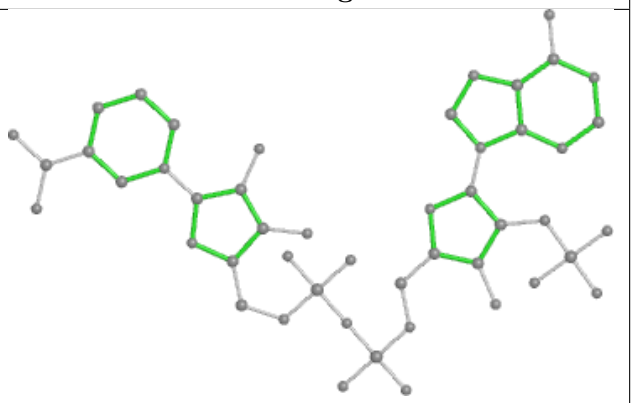
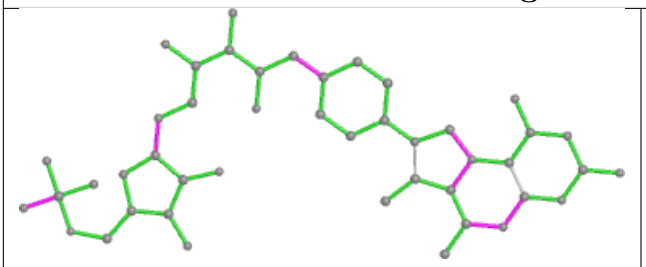


Rings

Ligand H4M H 302



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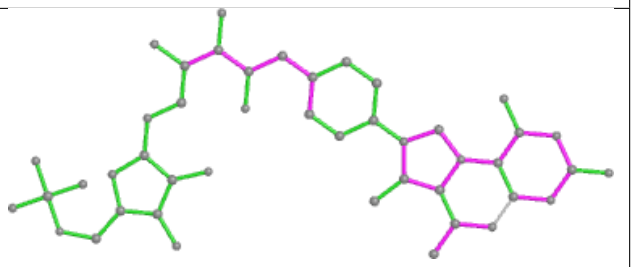
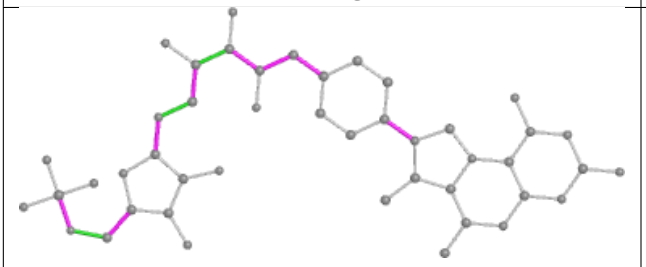
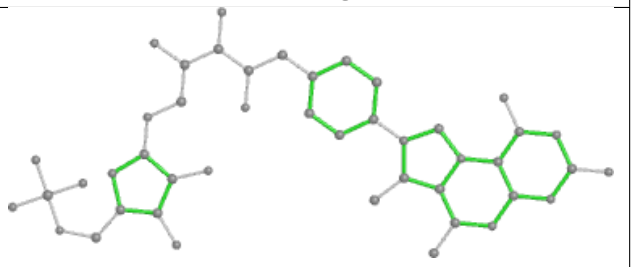


Bond angles

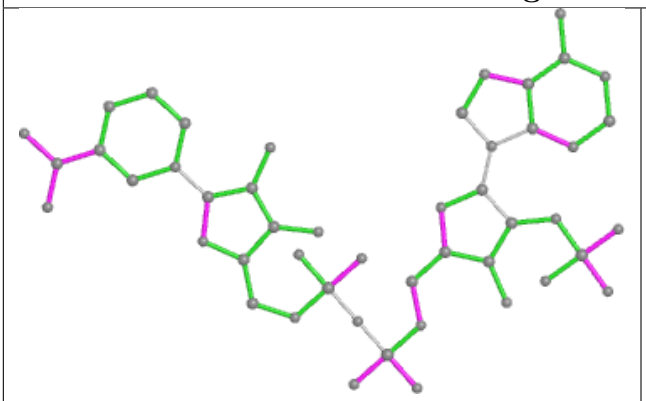


Torsions



Rings

Ligand NAP E 301



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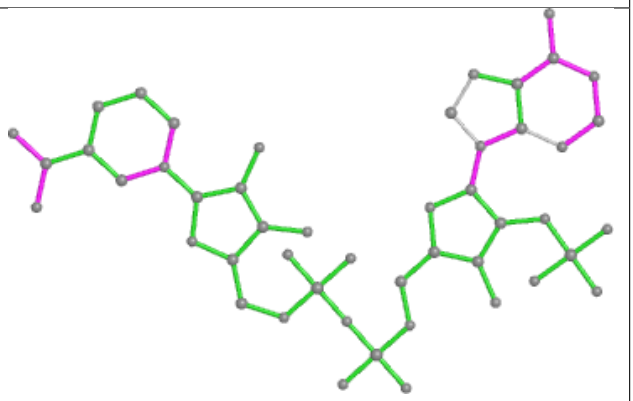
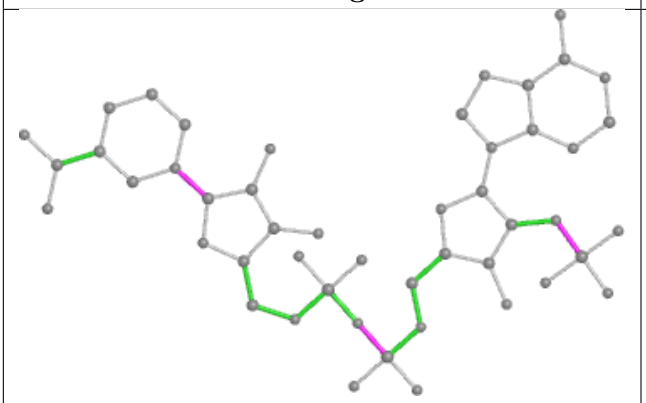


Bond angles



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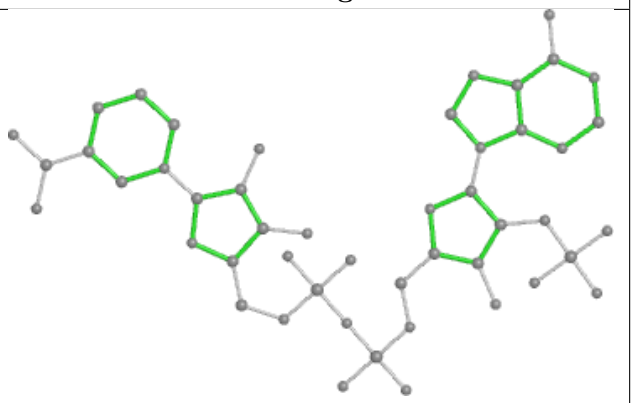
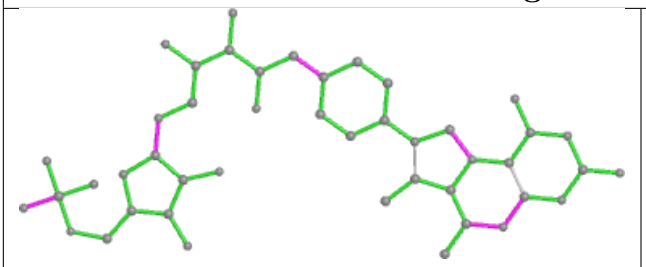


Rings

Ligand H4M L 302



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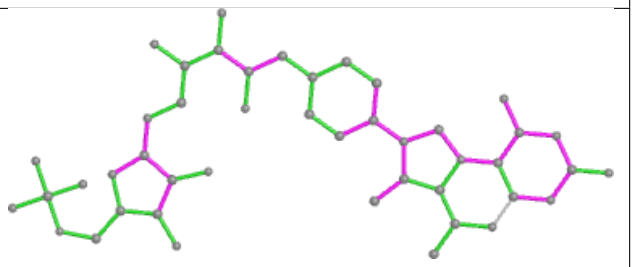

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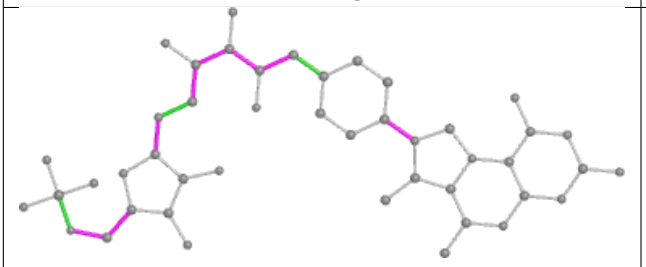

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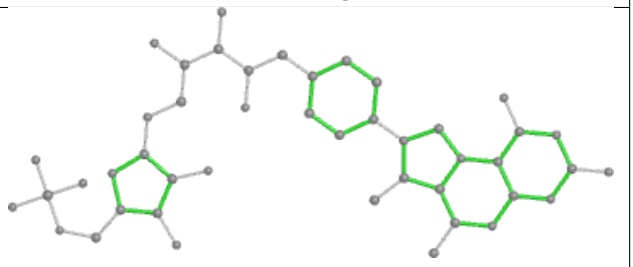
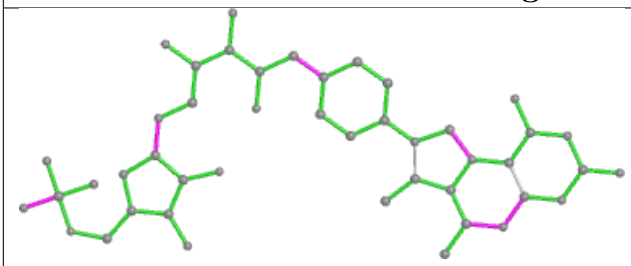


Rings

Ligand H4M C 302



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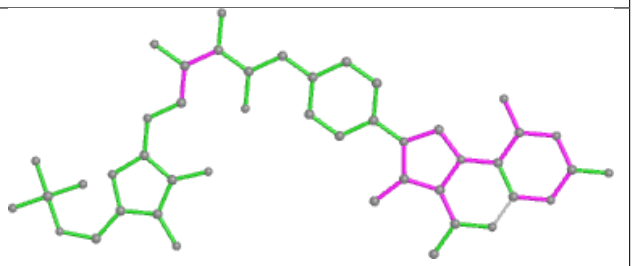

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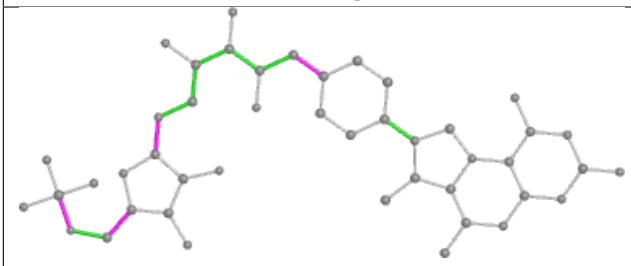

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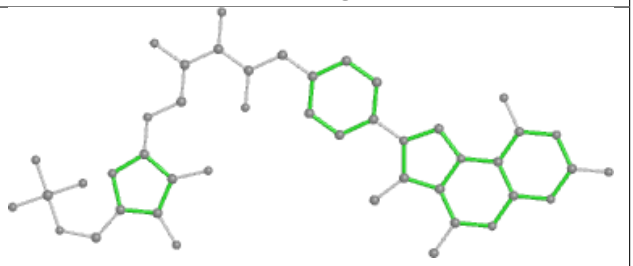
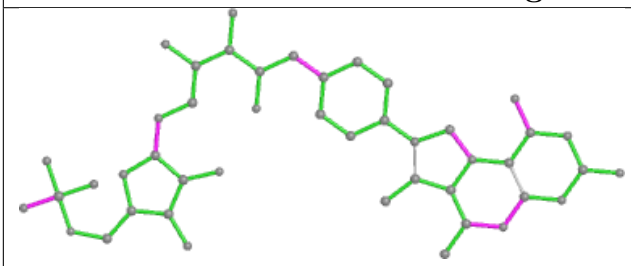


Rings

Ligand H4M J 302



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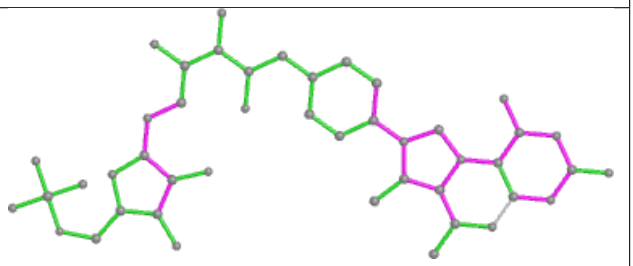
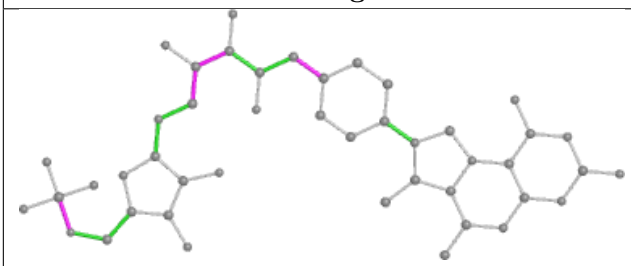
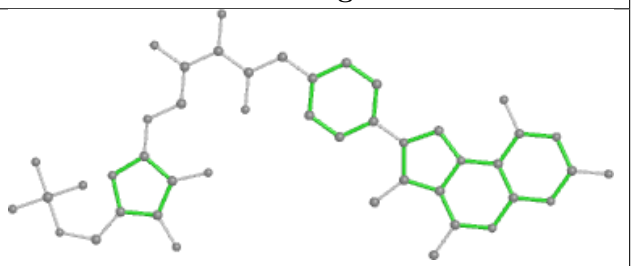


Bond angles

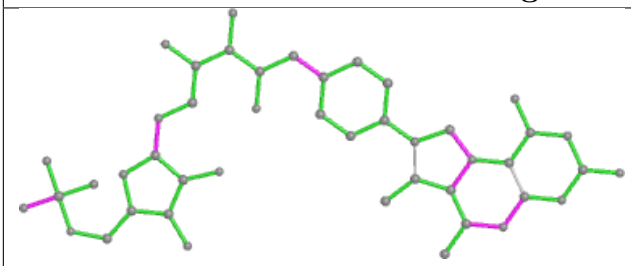


Torsions



Rings

Ligand H4M O 302



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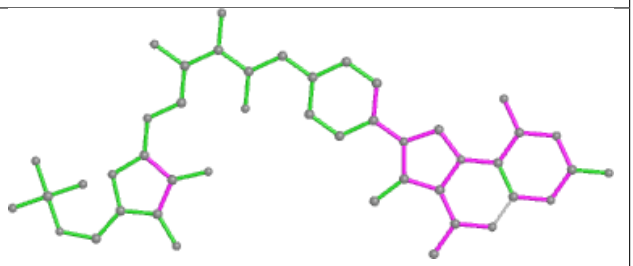

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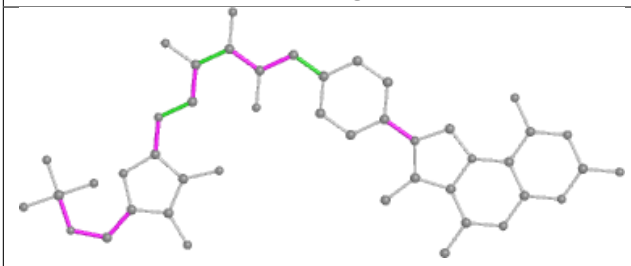

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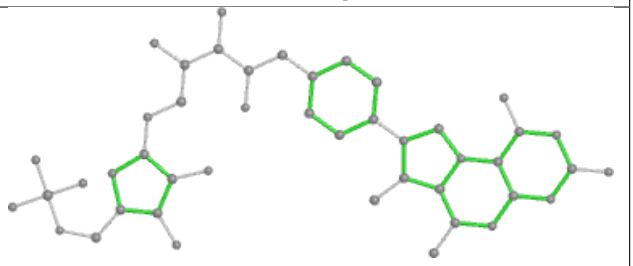
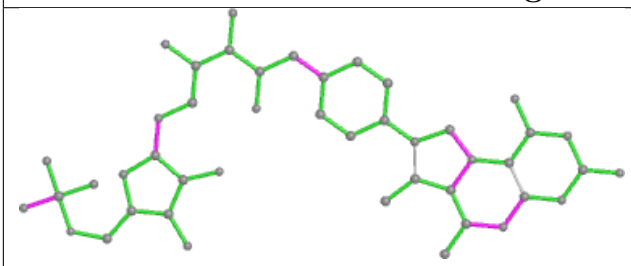


Rings

Ligand H4M S 302



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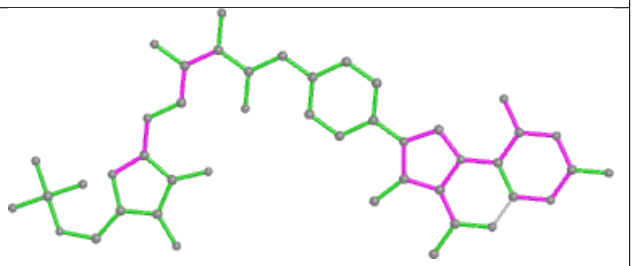
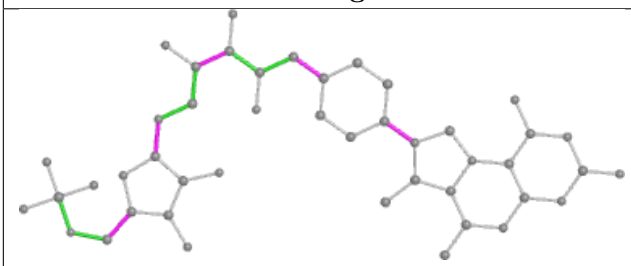


Bond angles



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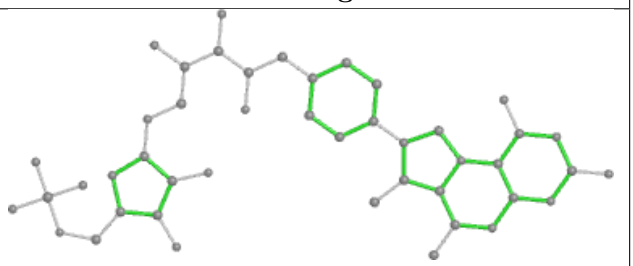
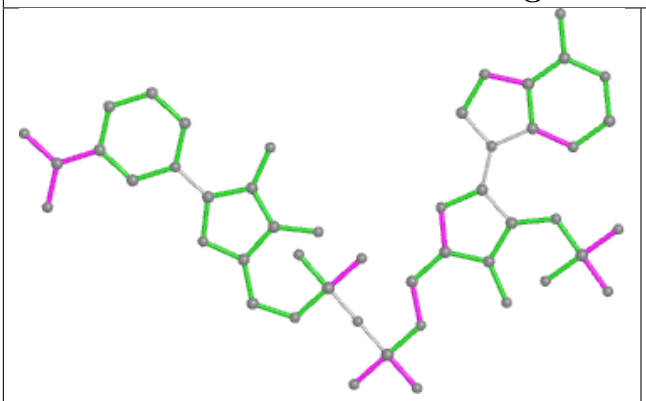


Rings

Ligand NAP L 301



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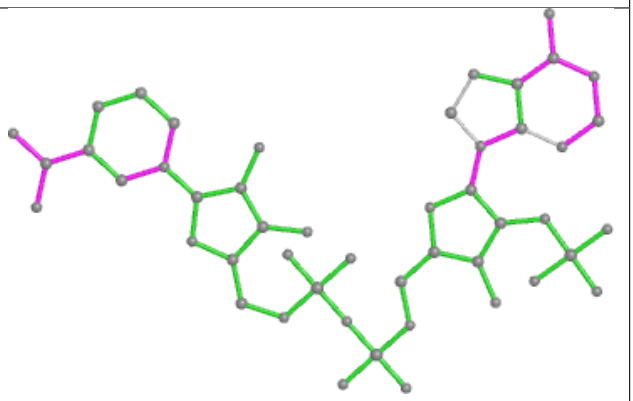
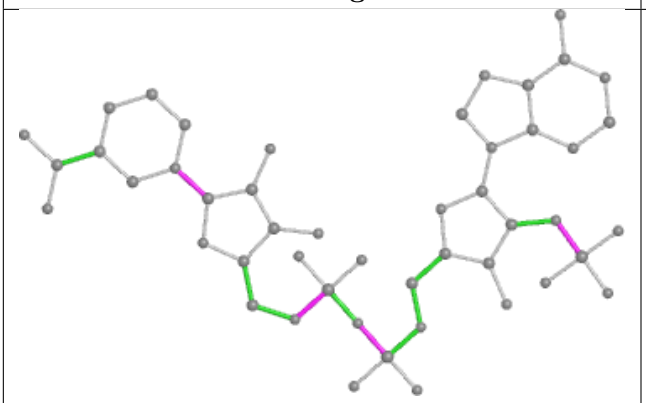


Bond angles



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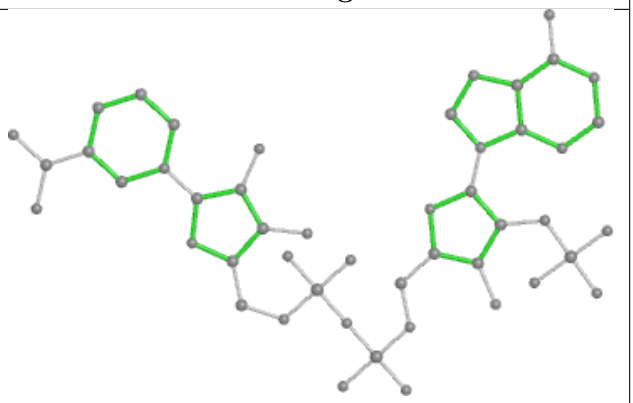
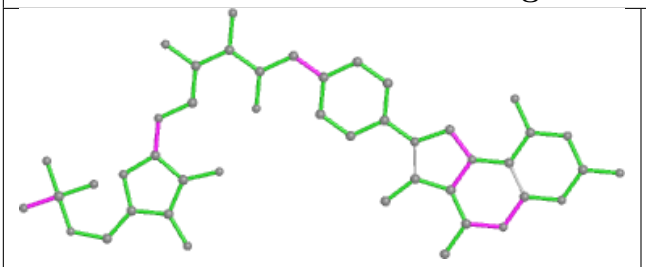
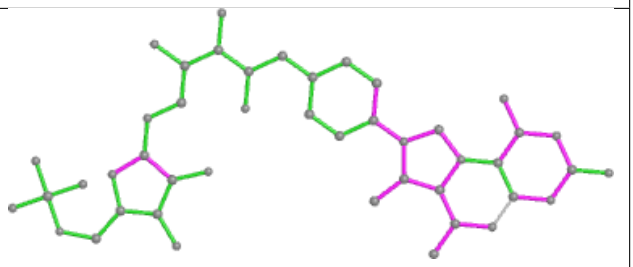


Rings

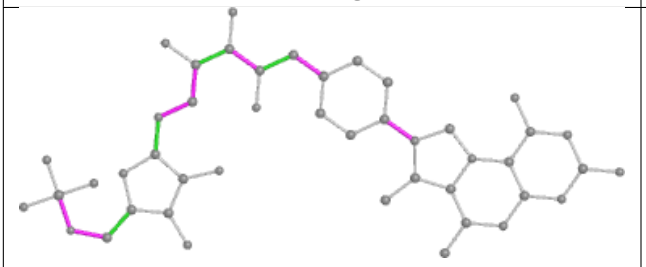
Ligand H4M B 302



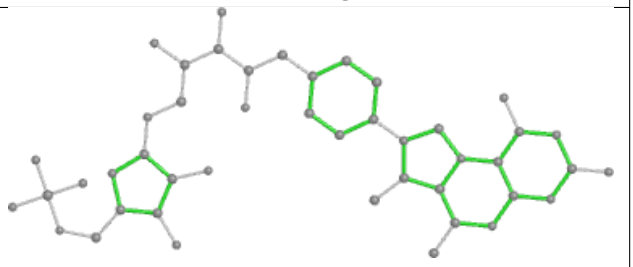
Bond lengths



Bond angles

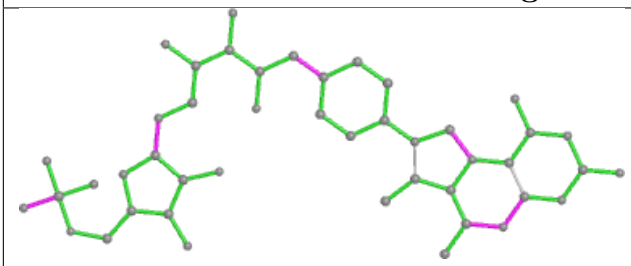


Torsions

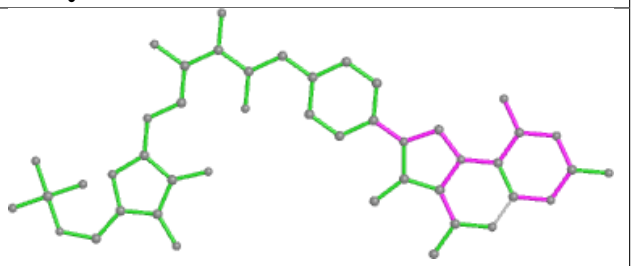


Rings

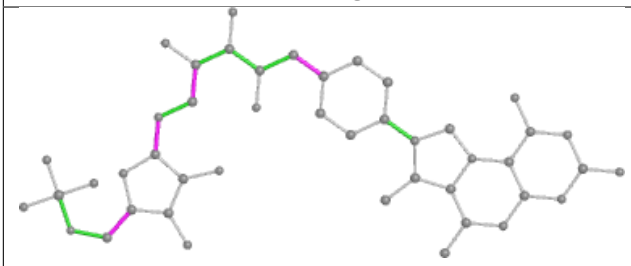
Ligand H4M Q 302



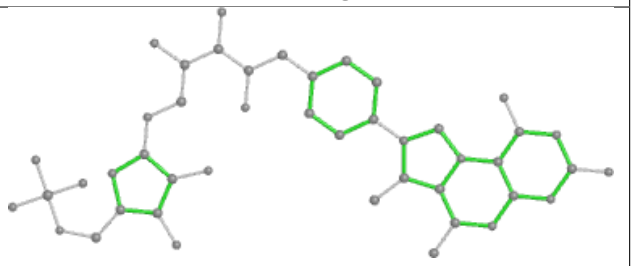
Bond lengths



Bond angles

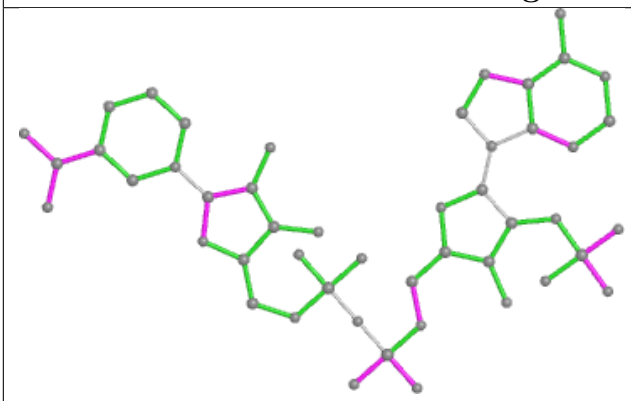


Torsions

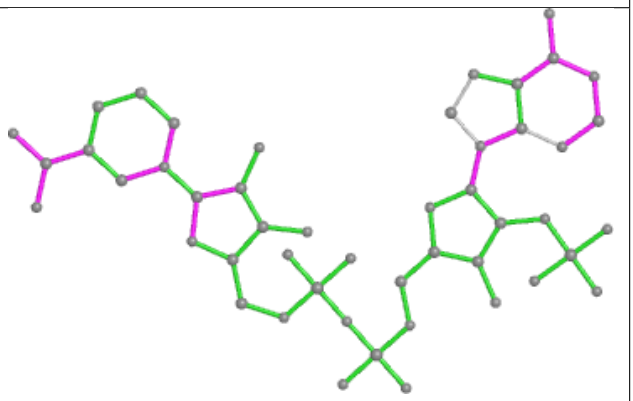


Rings

Ligand NAP P 301



Bond lengths



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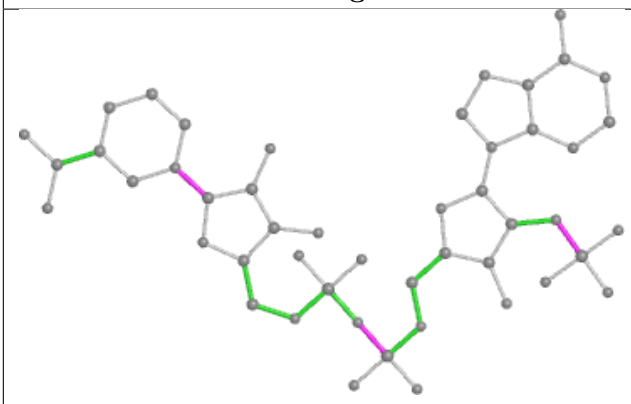
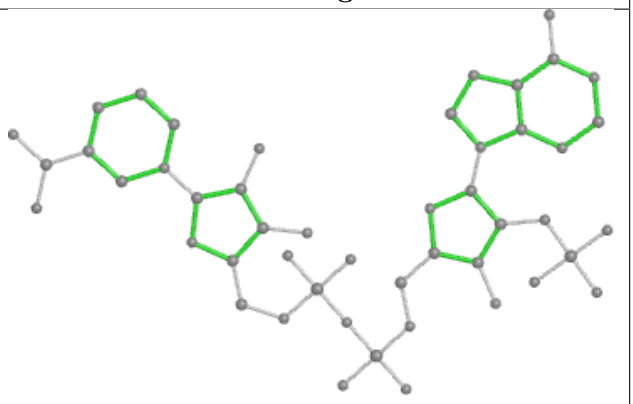
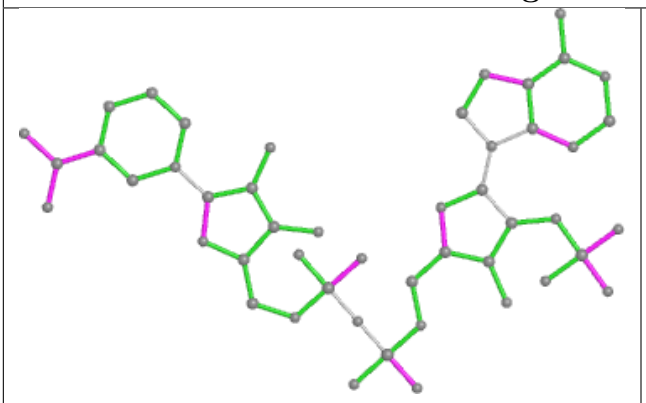


Torsions



Rings

Ligand NAP B 301



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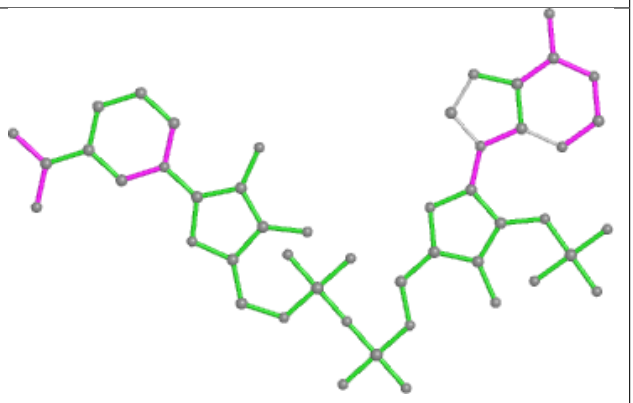

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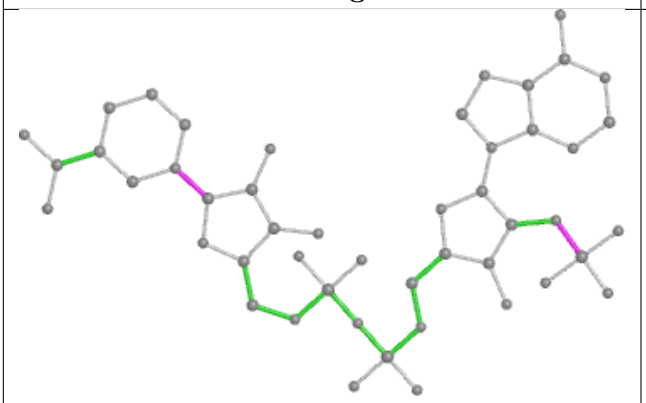

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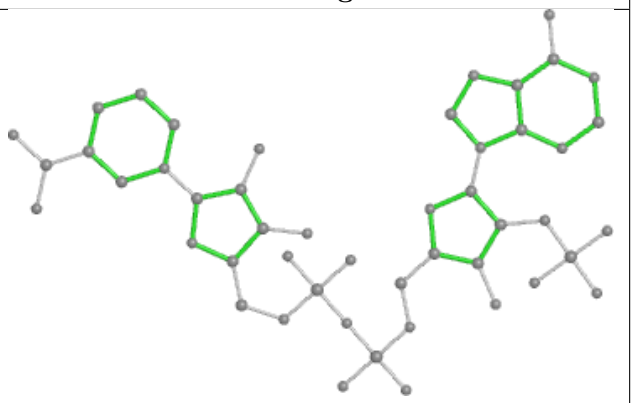
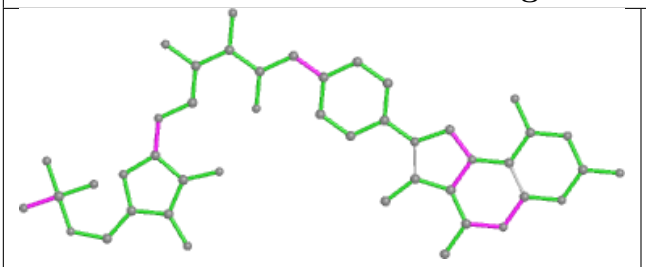


Rings

Ligand H4M R 302



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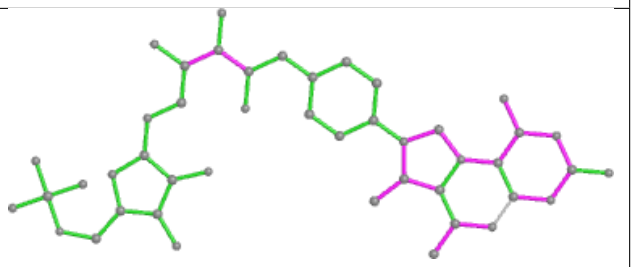

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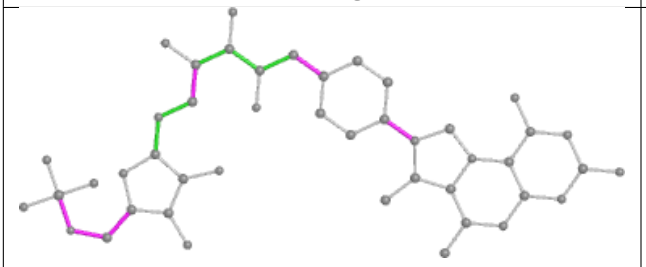

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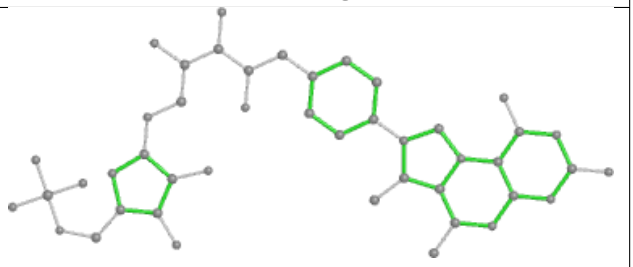
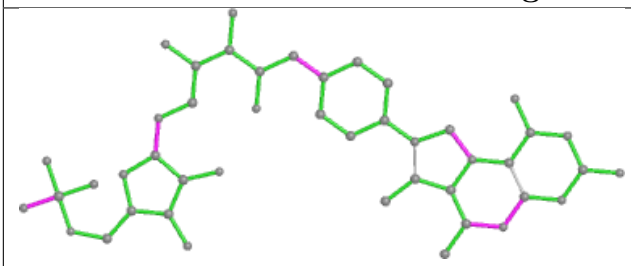


Rings

Ligand H4M T 302



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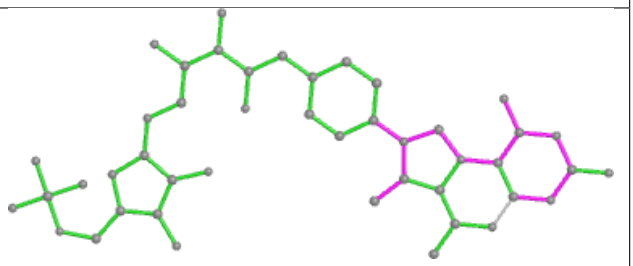

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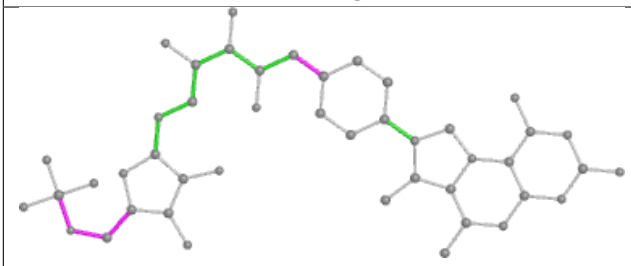

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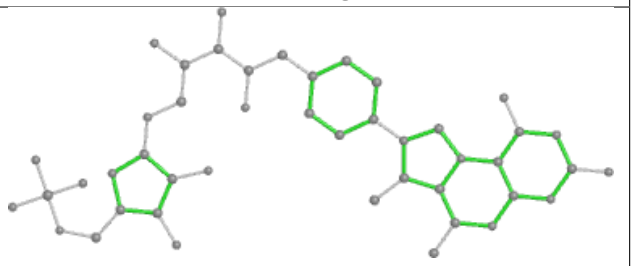
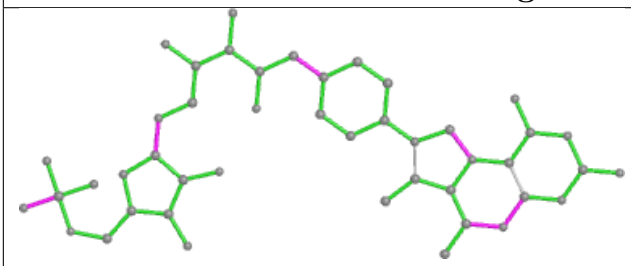


Rings

Ligand H4M M 302



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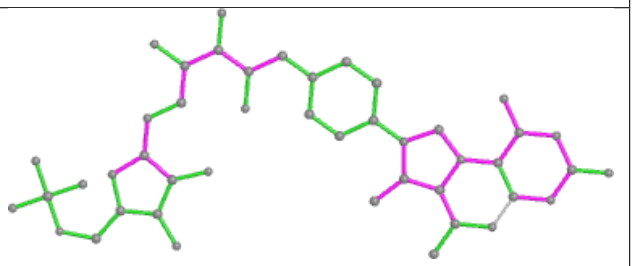

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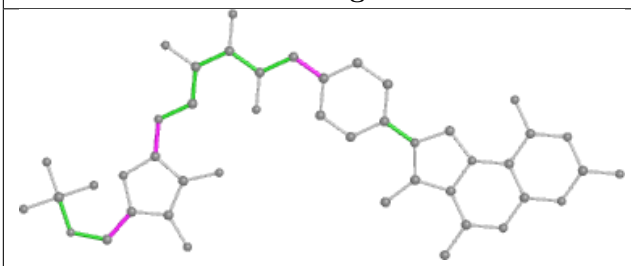

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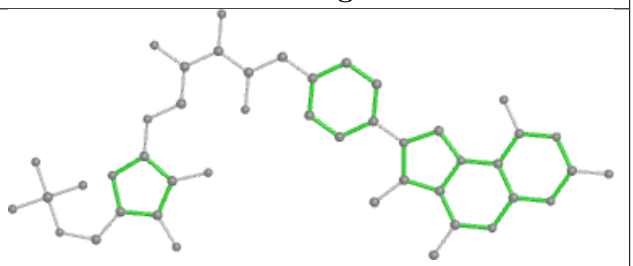
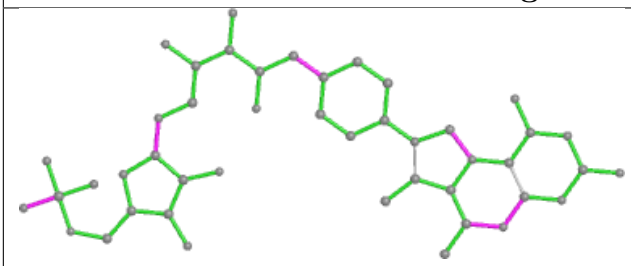


Rings

Ligand H4M U 302



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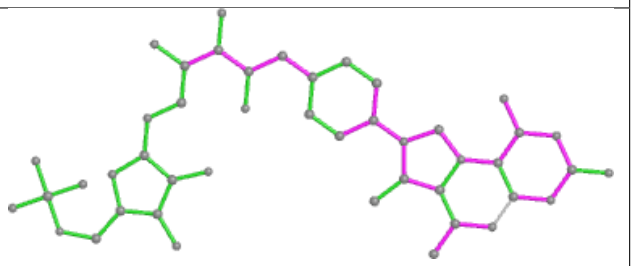
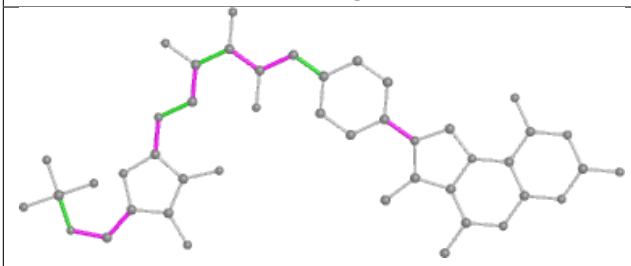


Bond angles



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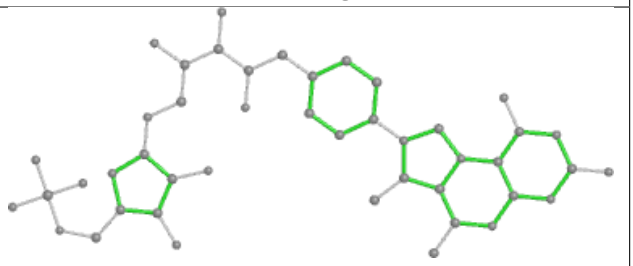
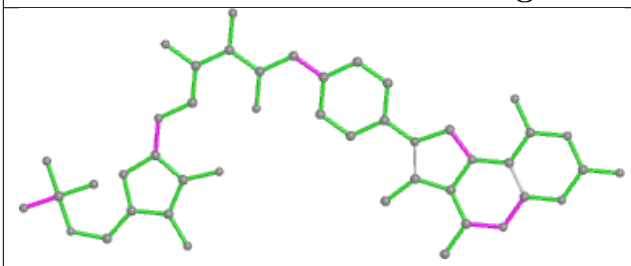


Rings

Ligand H4M W 302



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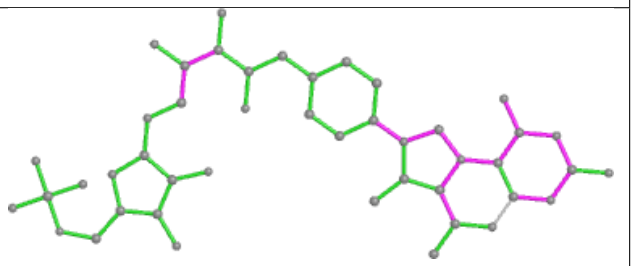

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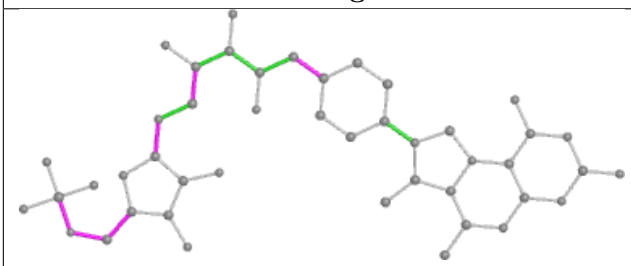

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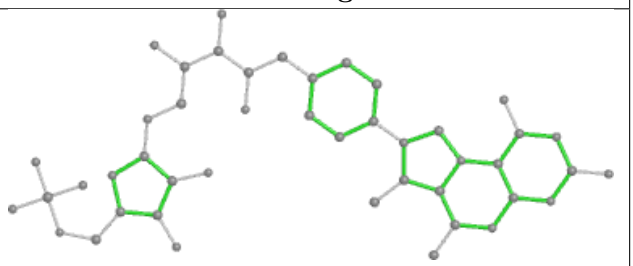
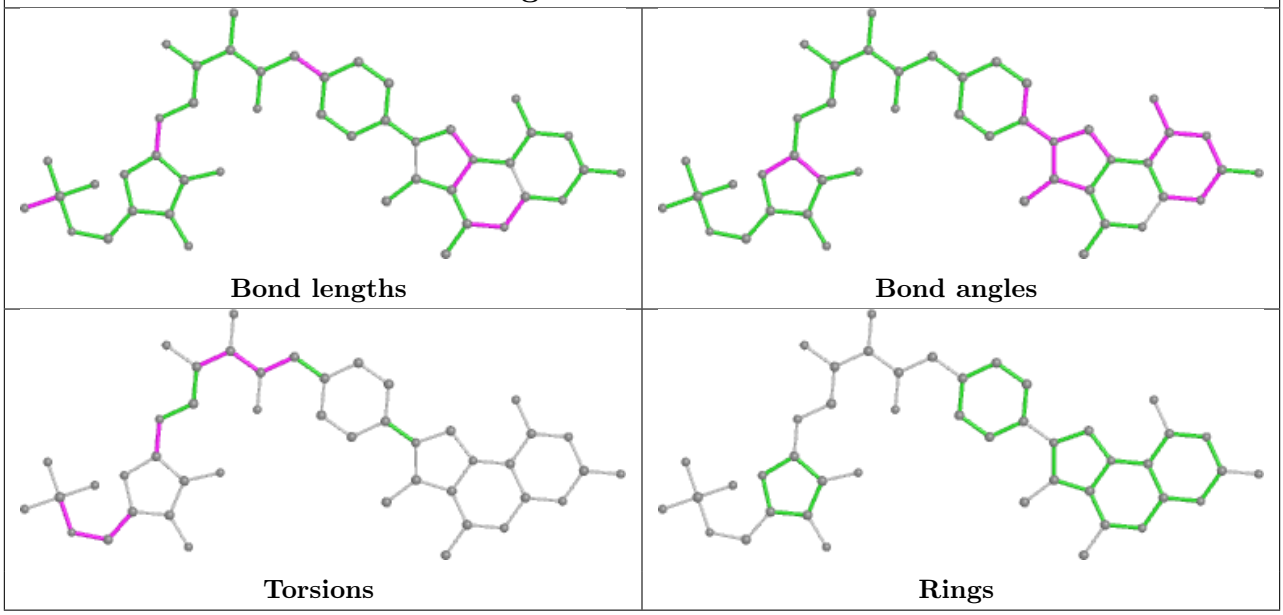
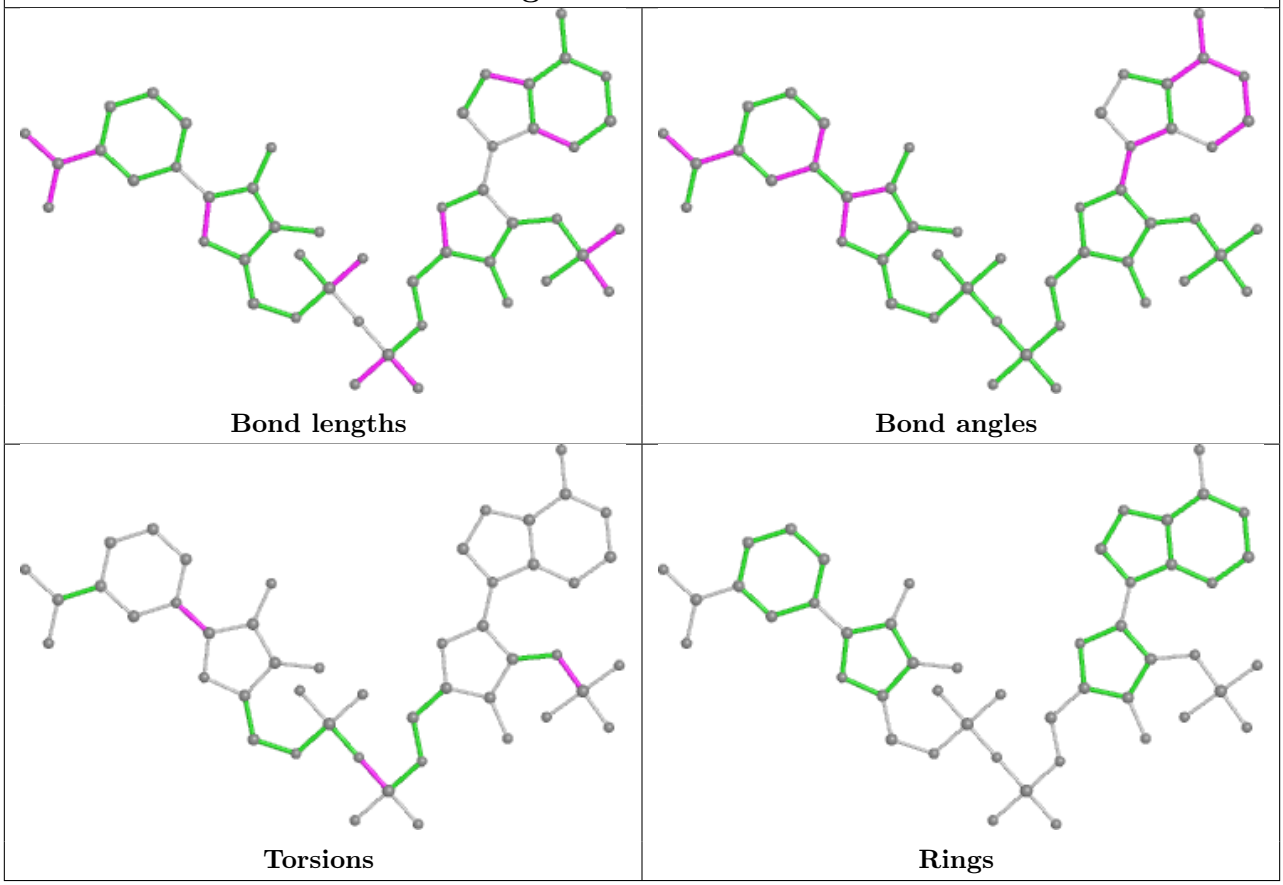


Rings

Ligand H4M N 302



Ligand NAP D 302



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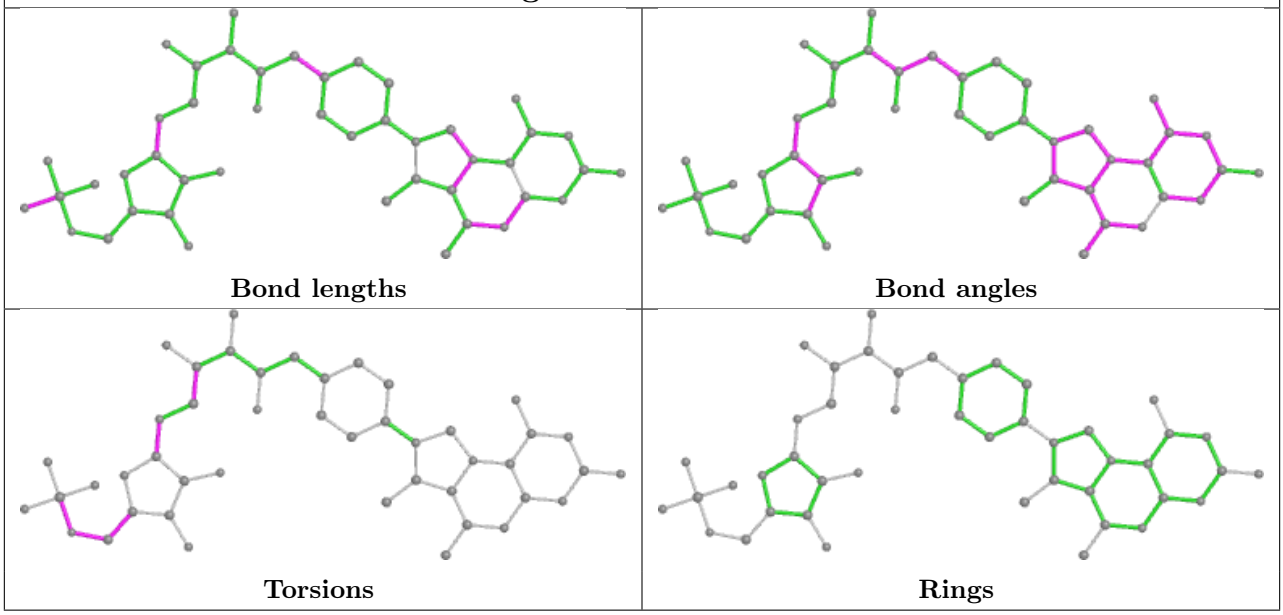

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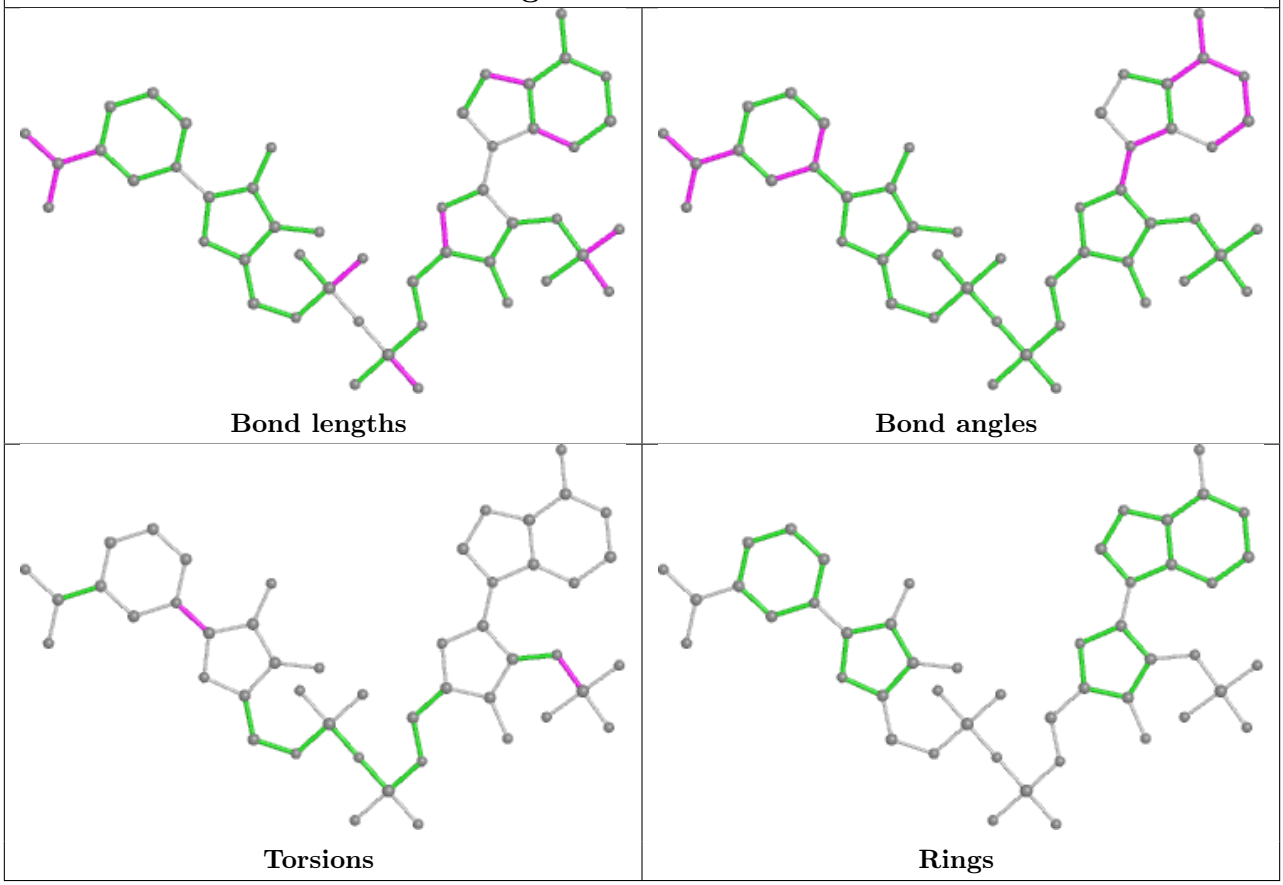

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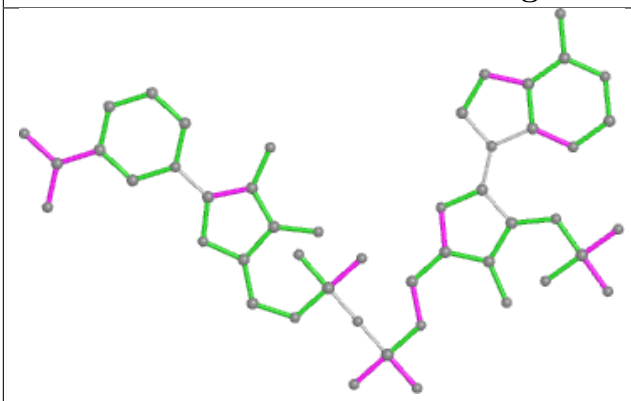
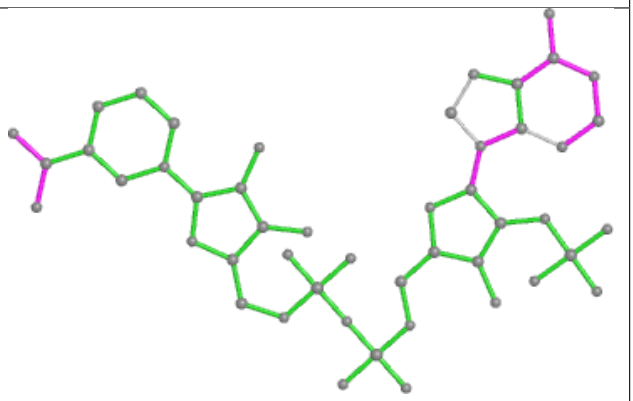
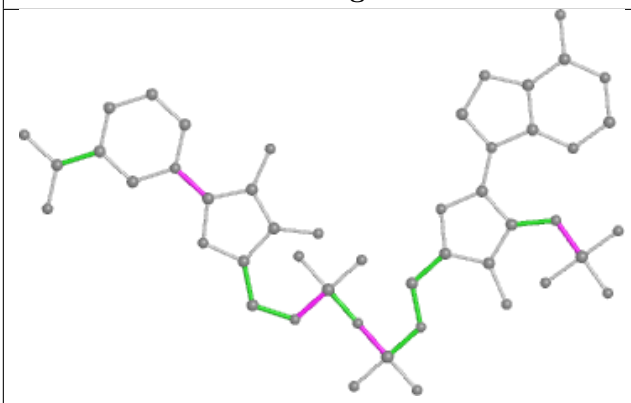


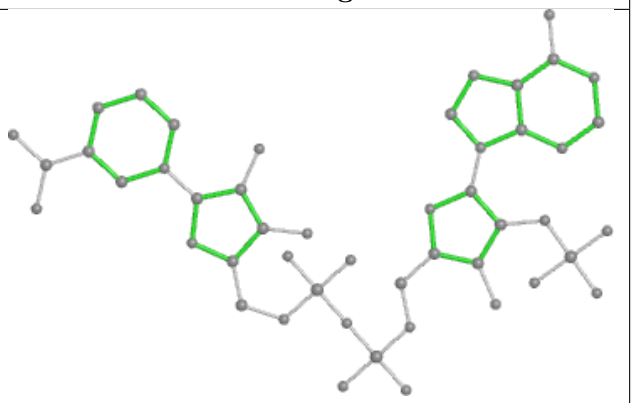
Bond lengths



Bond angles

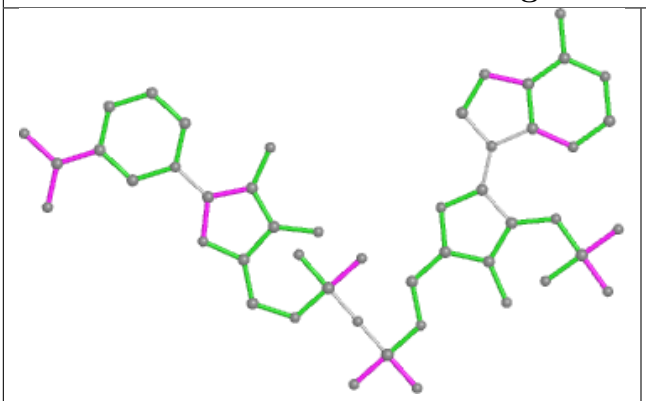


Torsions



Rings

Ligand NAP H 301



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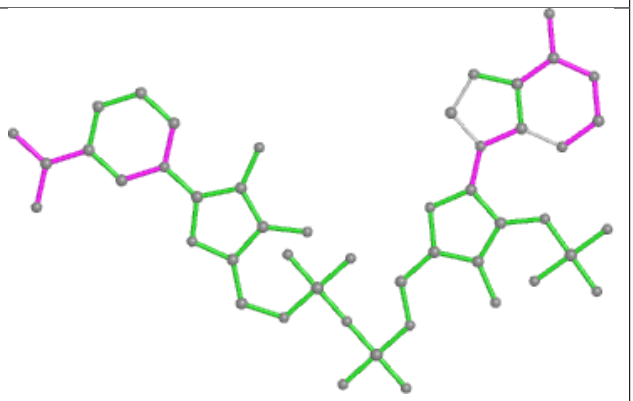
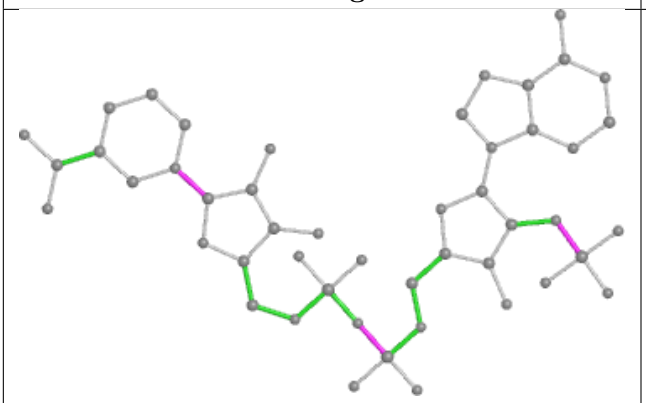


Bond angles



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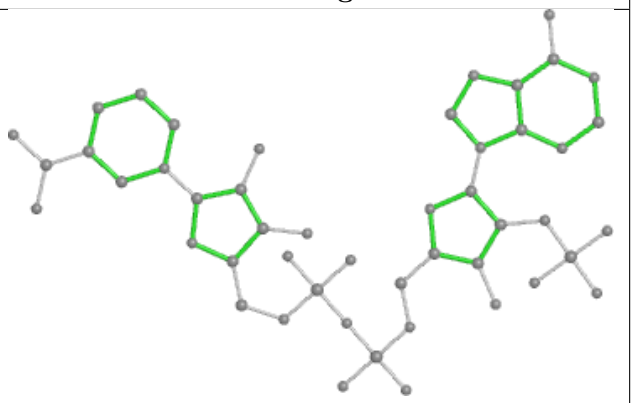
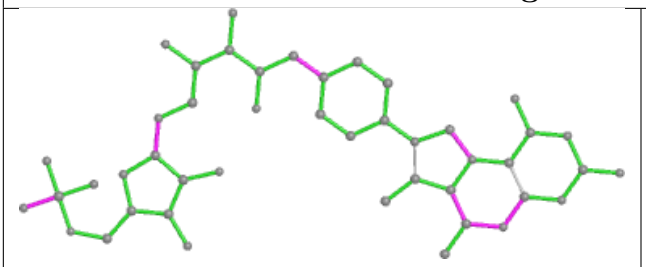


Rings

Ligand H4M A 302



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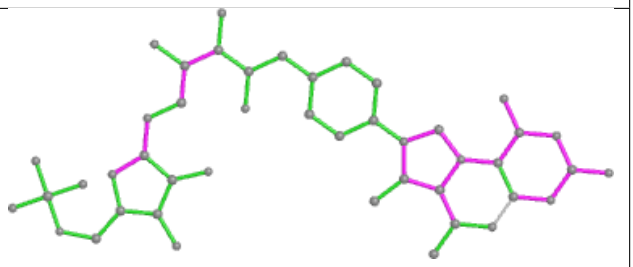
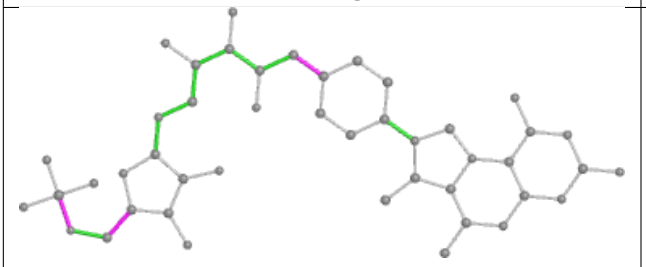


Bond angles



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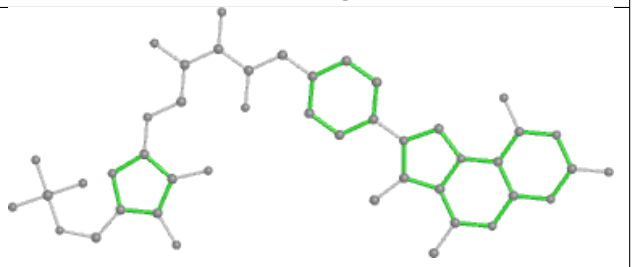
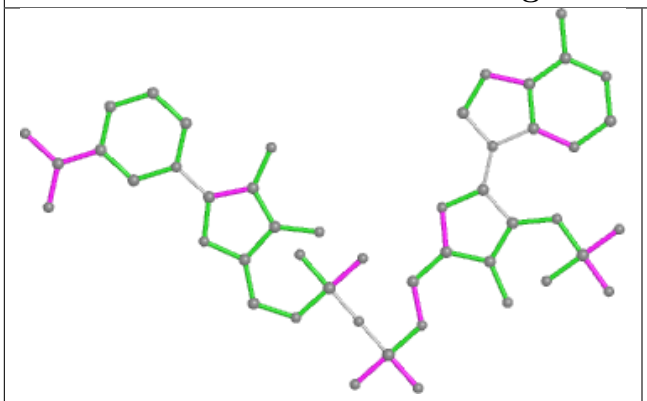


Rings

Ligand NAP X 301



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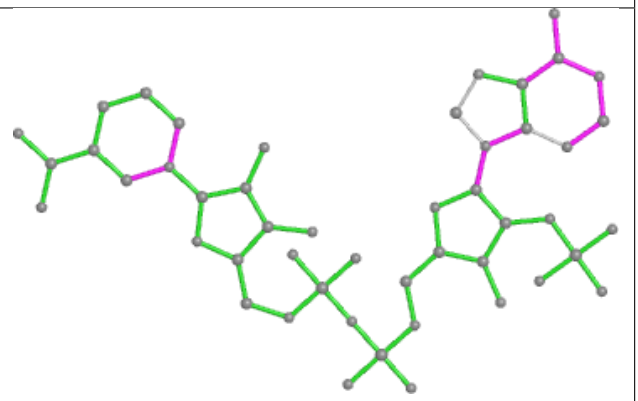
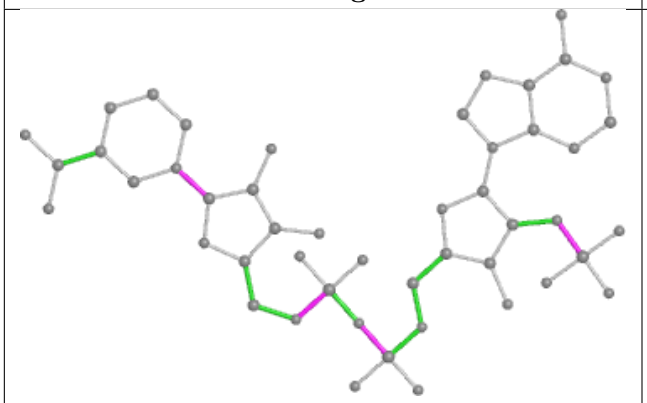


Bond angles



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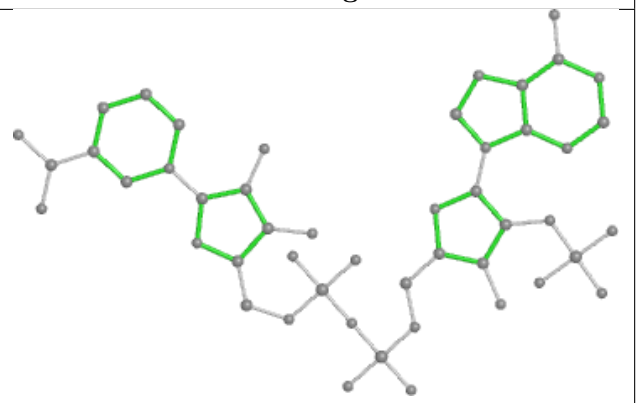
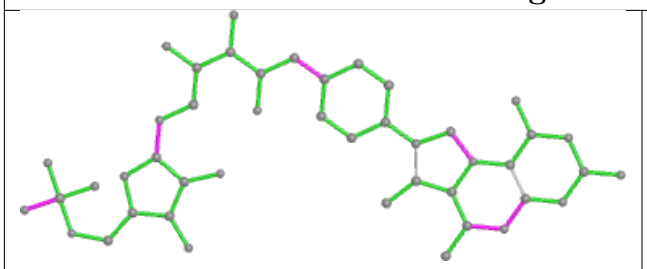


Rings

Ligand H4M I 302



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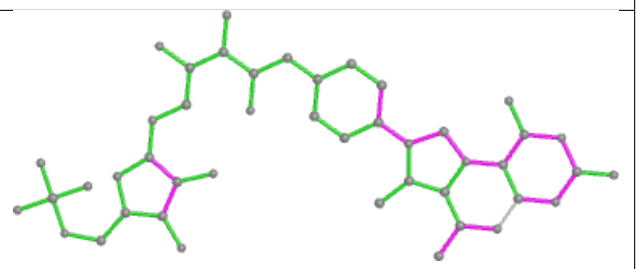
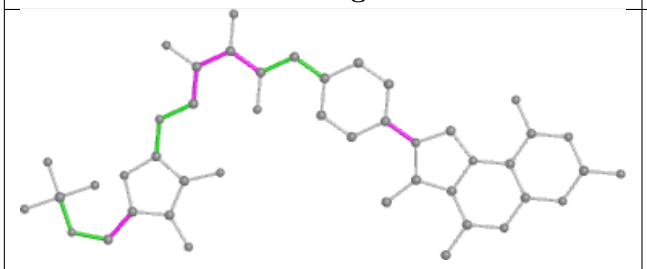


Bond angles



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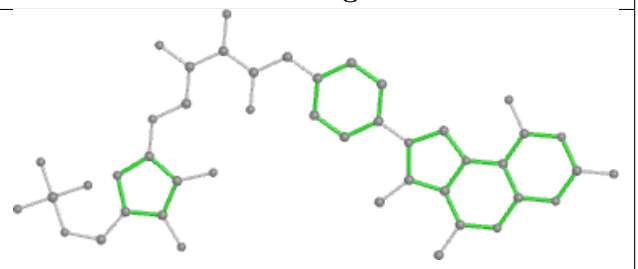
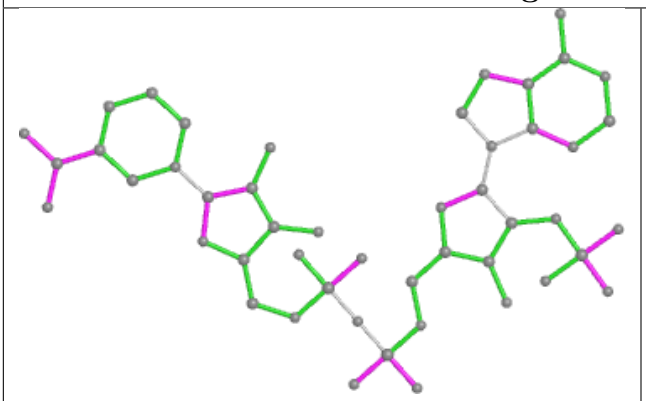


Rings

Ligand NAP Q 301



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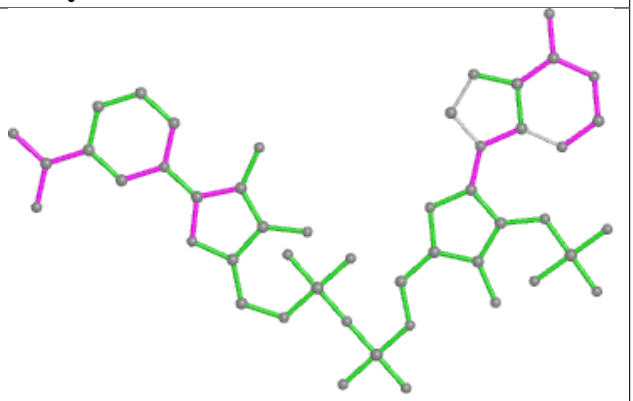
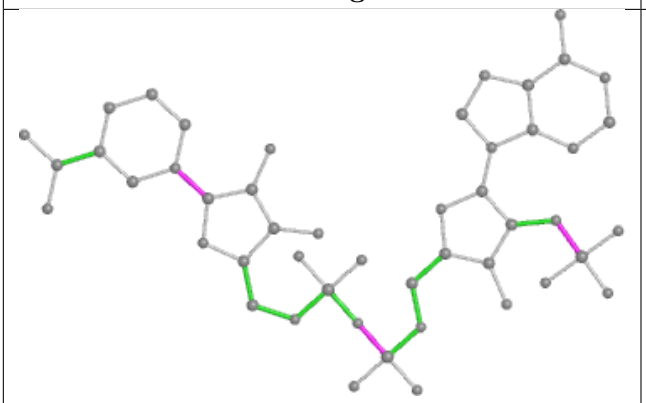


Bond angles



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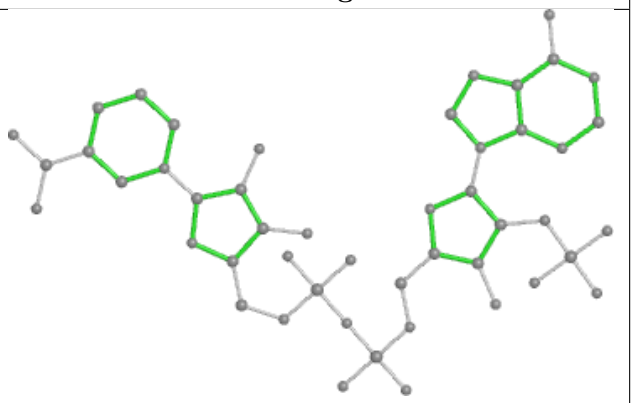
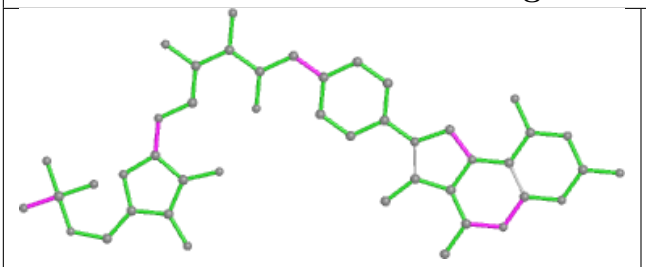


Rings

Ligand H4M F 302



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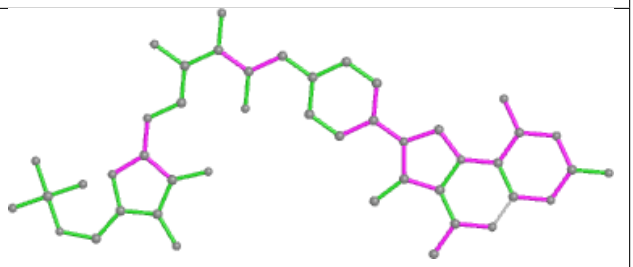
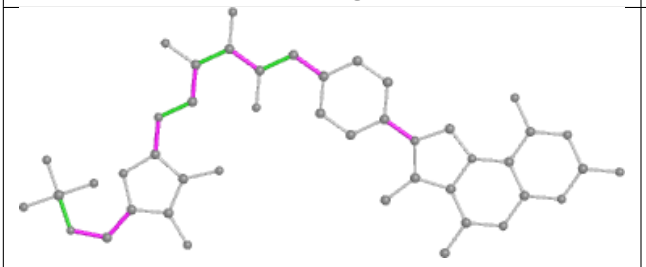
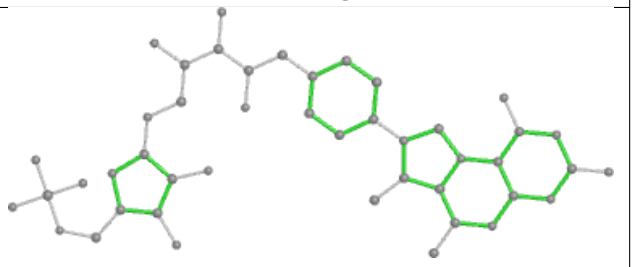


Bond angles

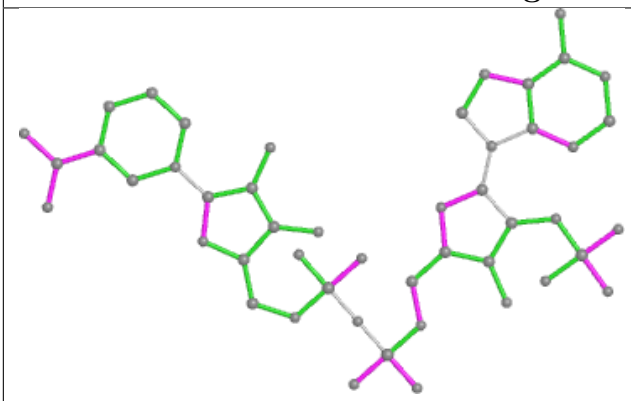


Torsions



Rings

Ligand NAP F 301



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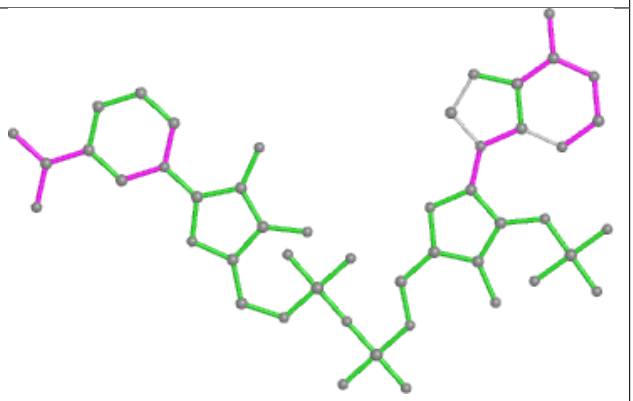

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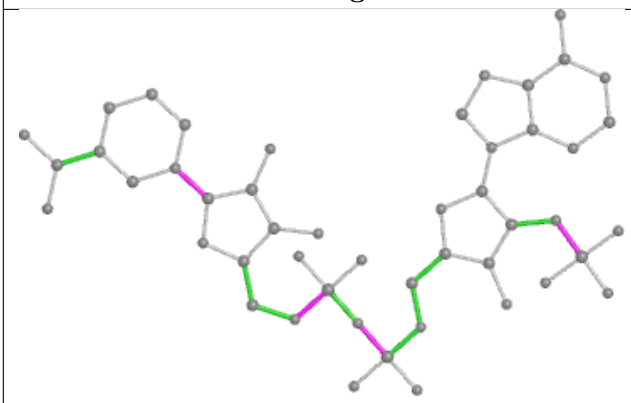

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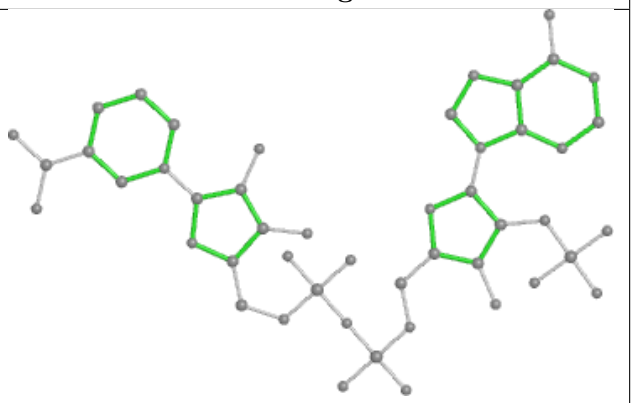
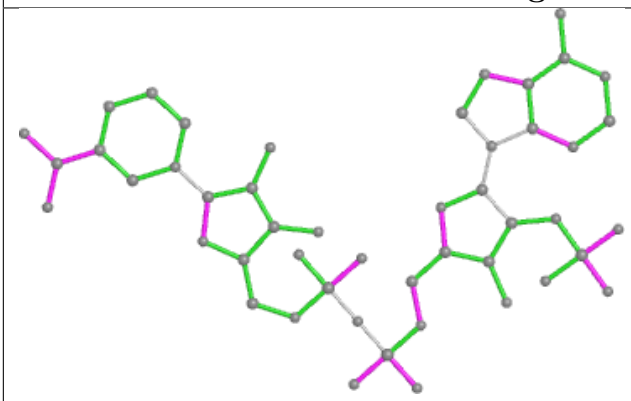


Rings

Ligand NAP I 301



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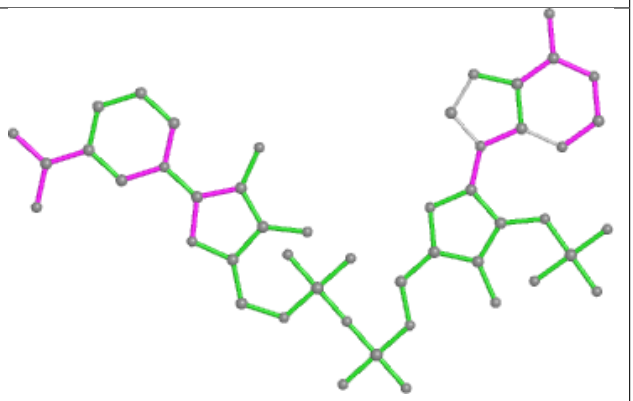

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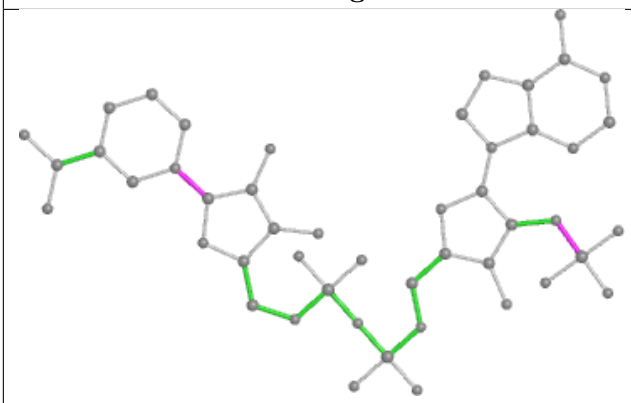

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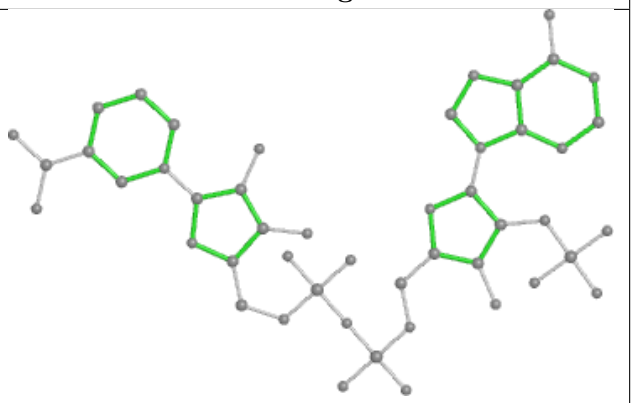
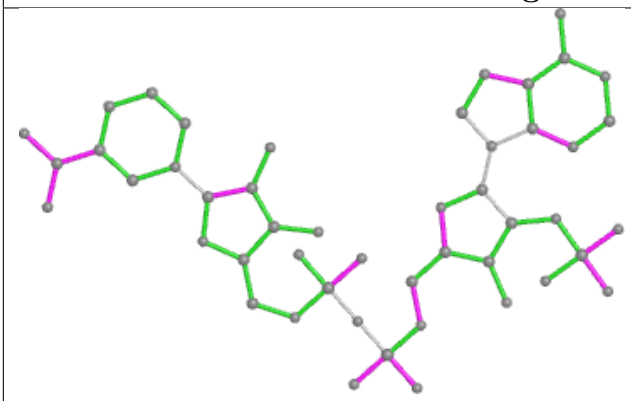


Rings

Ligand NAP T 301



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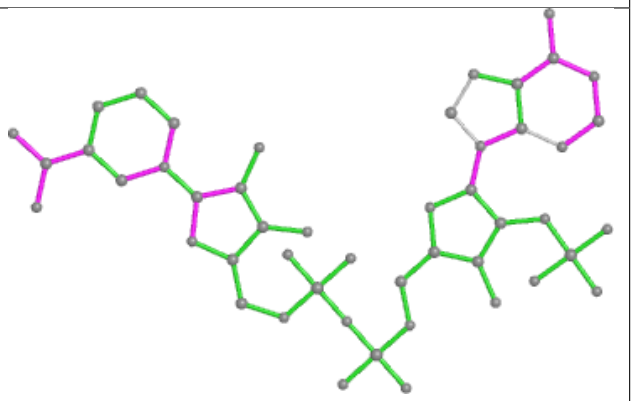

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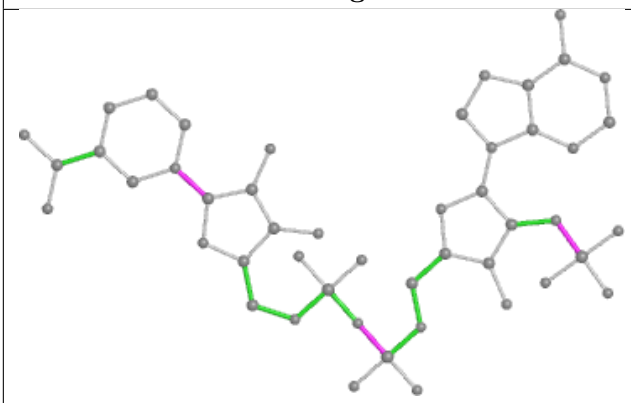

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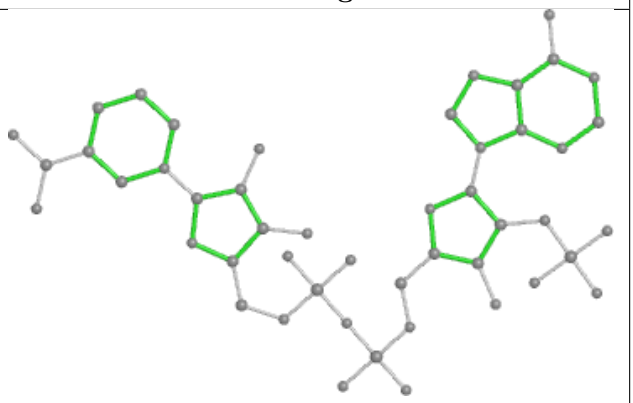
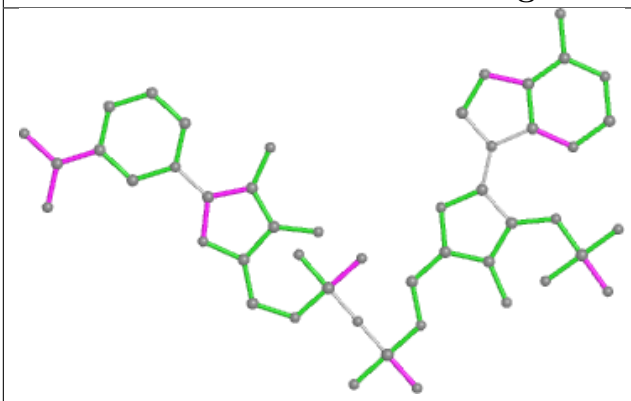


Rings

Ligand NAP M 301



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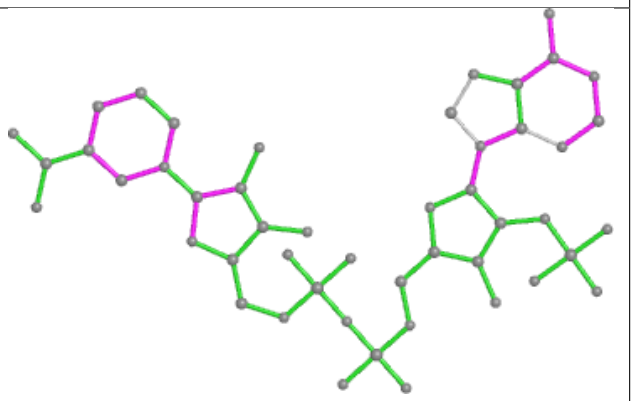

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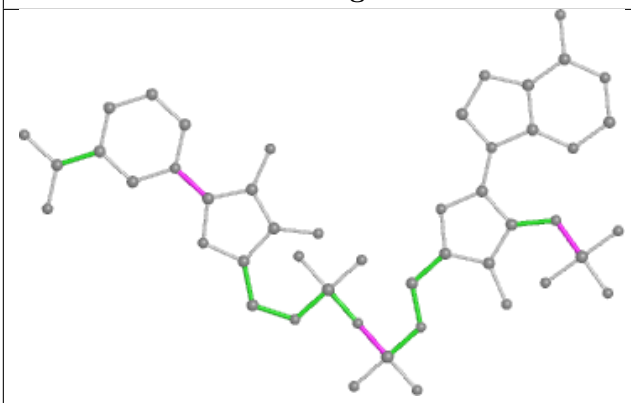

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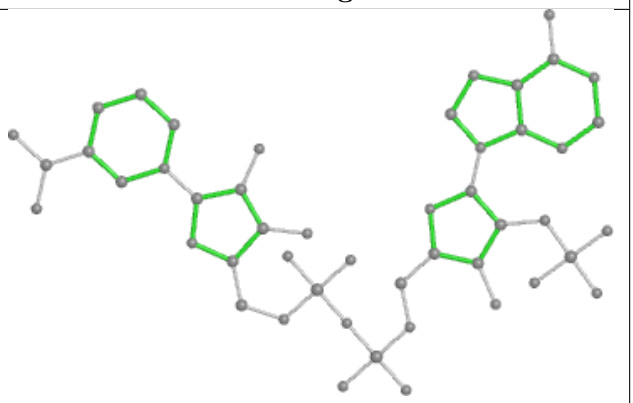
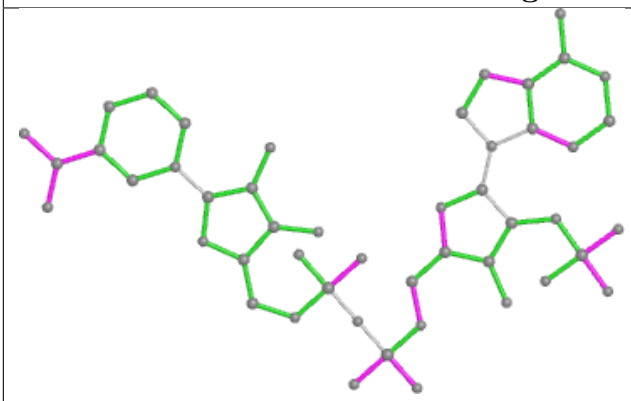


Rings

Ligand NAP O 301



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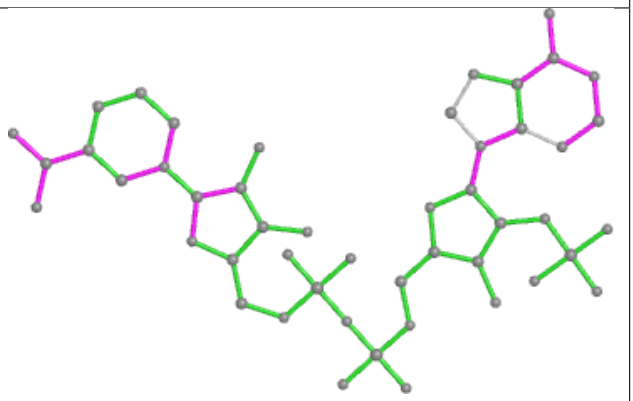

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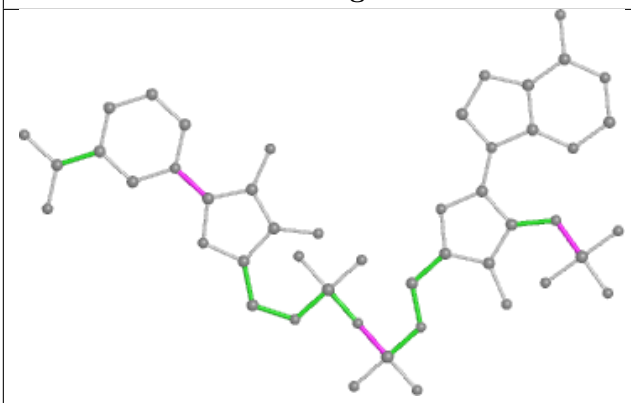

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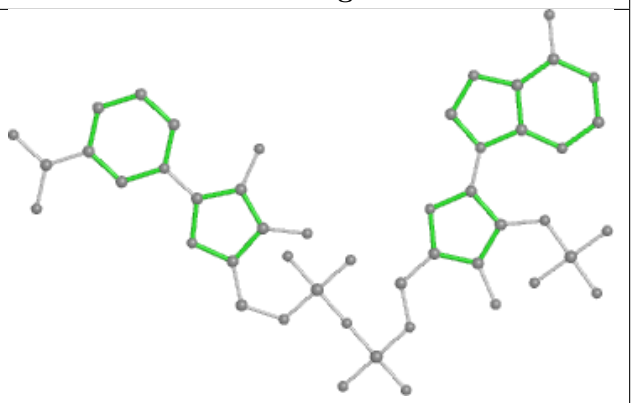
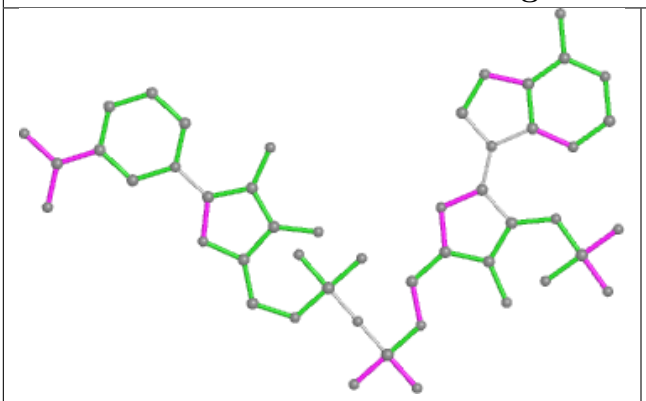


Rings

Ligand NAP A 301



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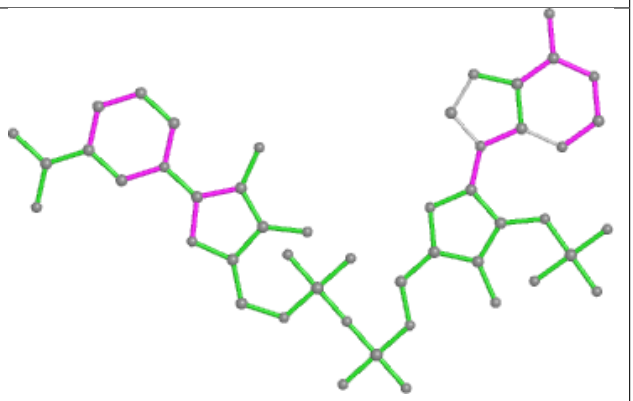

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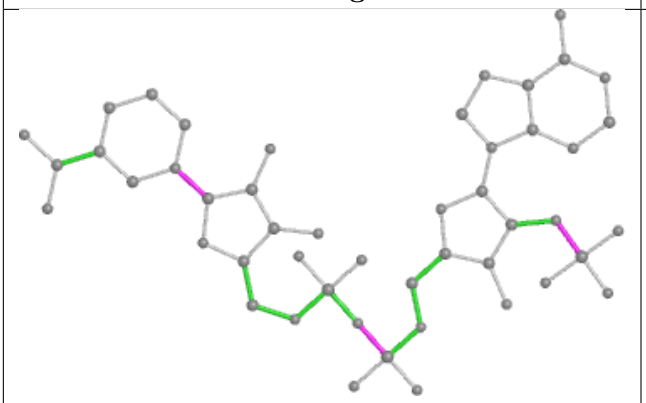

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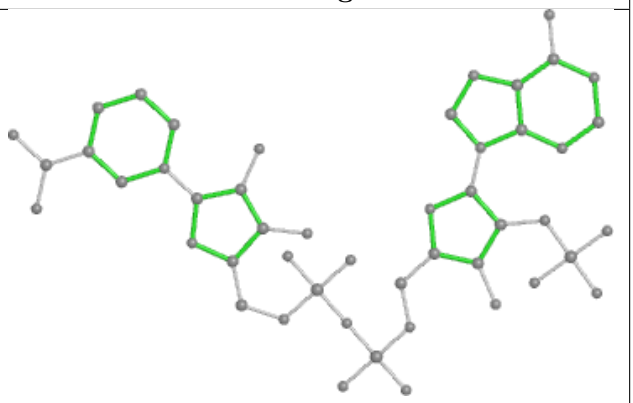
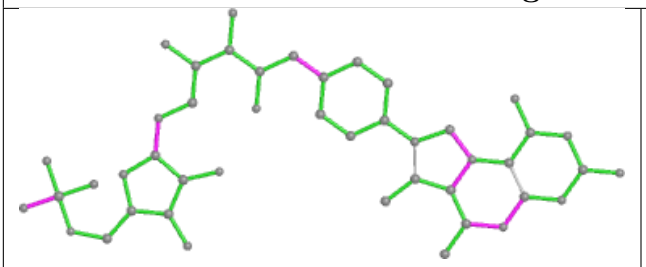


Rings

Ligand H4M P 302



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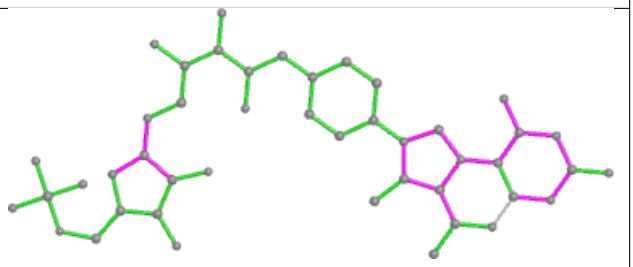

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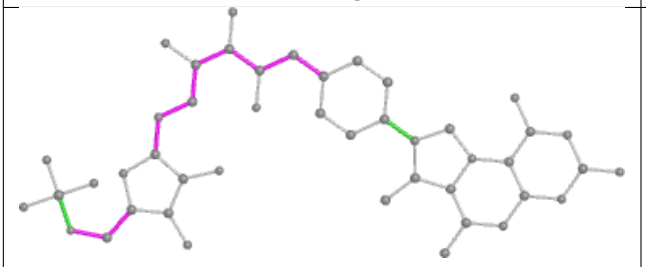

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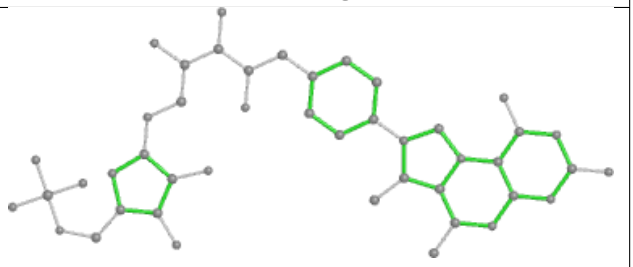
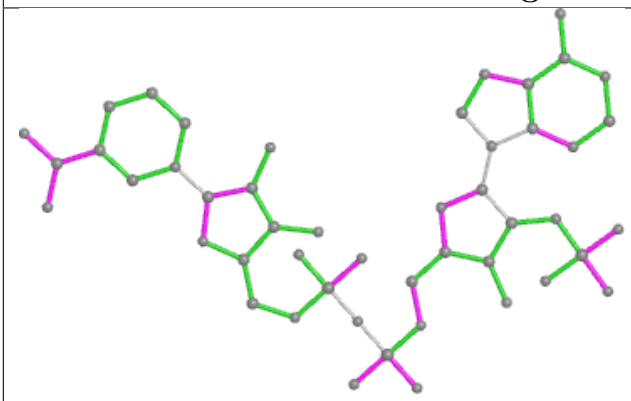


Rings

Ligand NAP R 301



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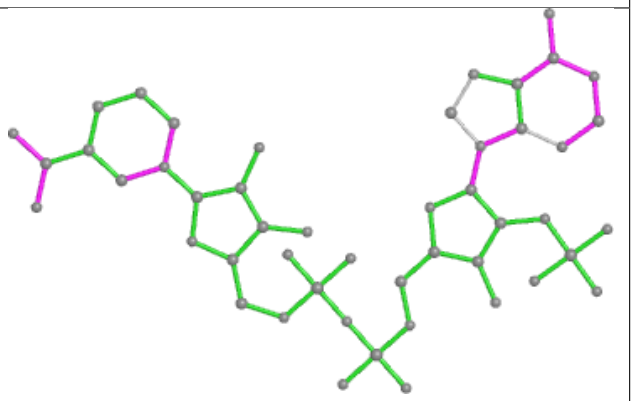

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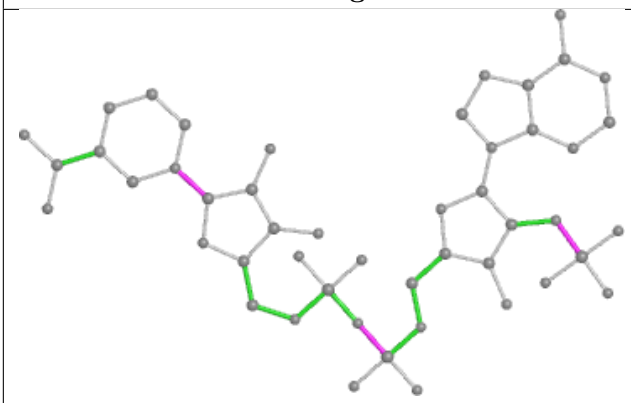

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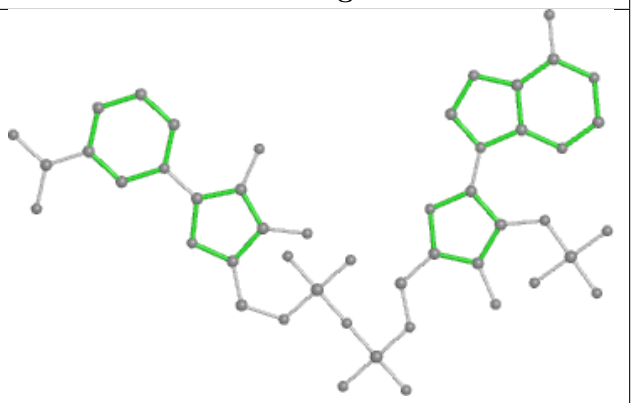
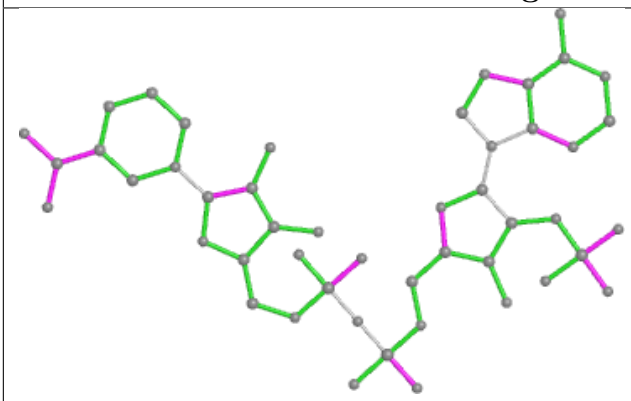


Rings

Ligand NAP C 301



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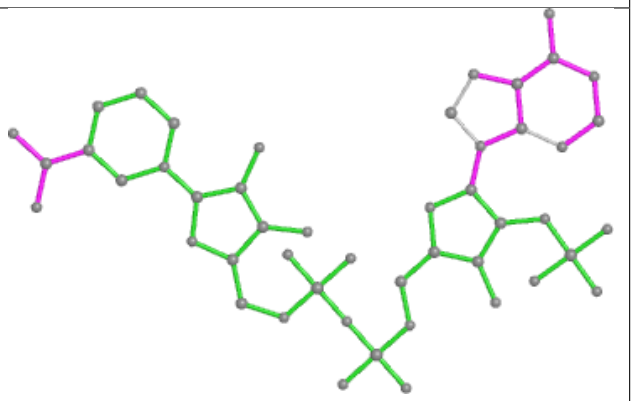

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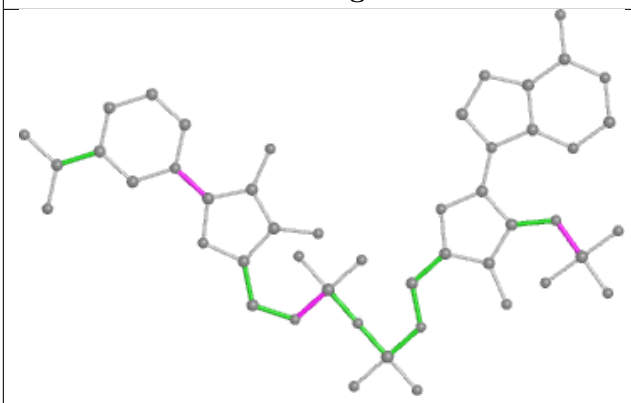

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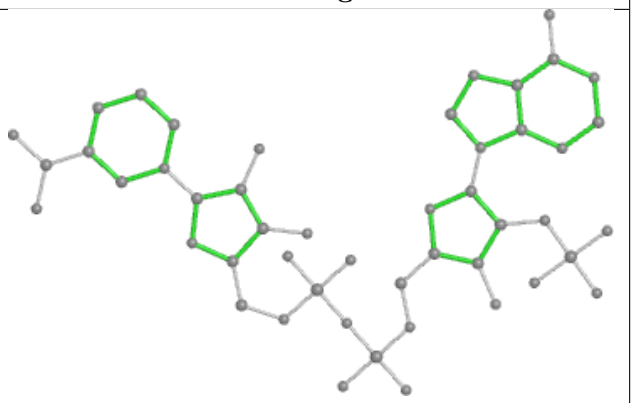
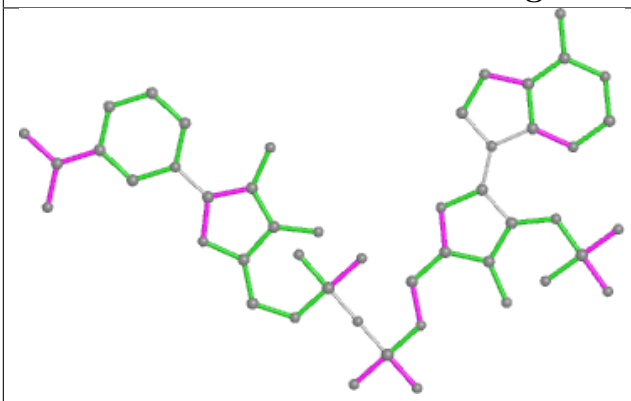


Rings

Ligand NAP J 301



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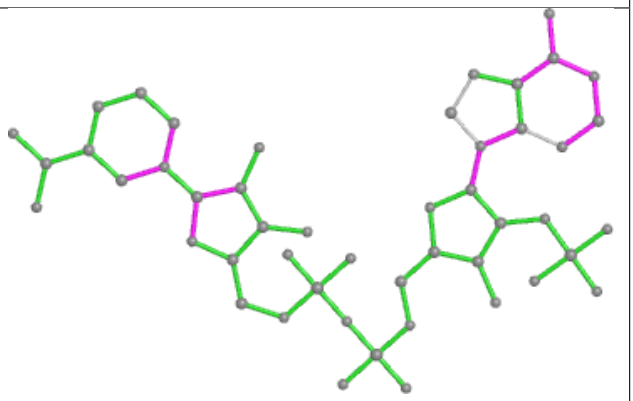

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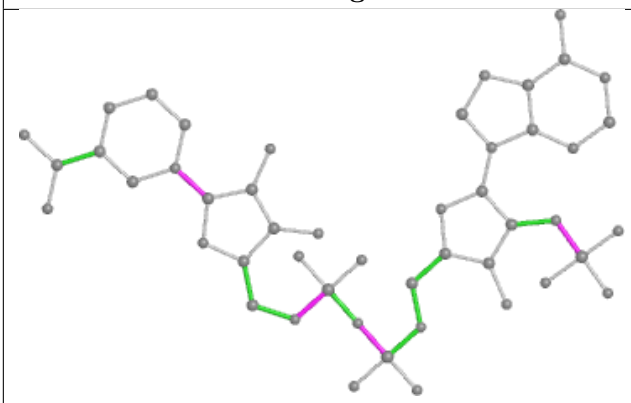

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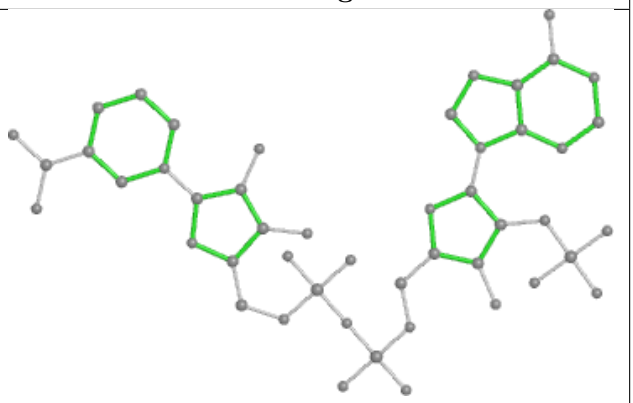
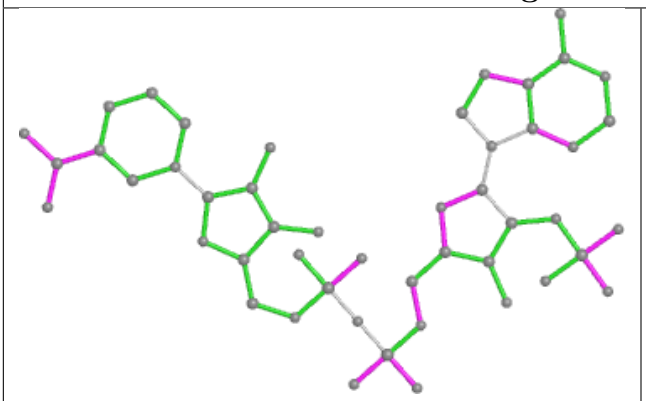


Rings

Ligand NAP U 301



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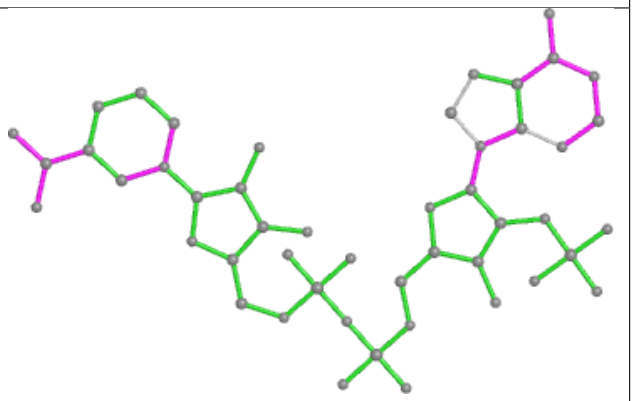

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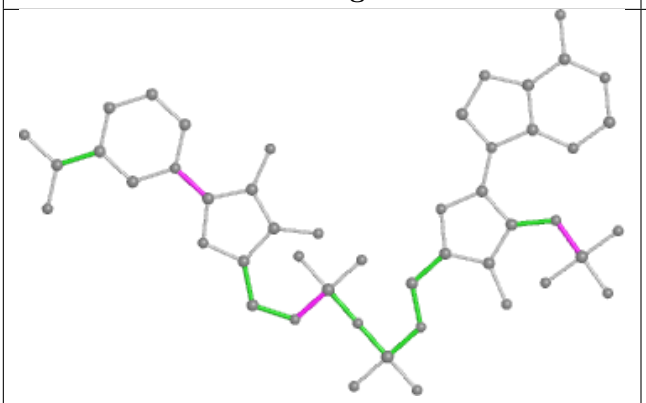

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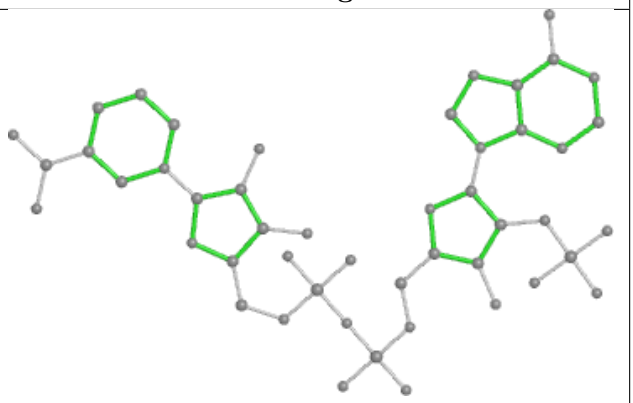
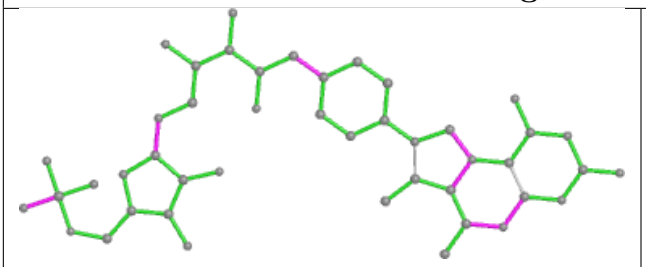


Rings

Ligand H4M K 302



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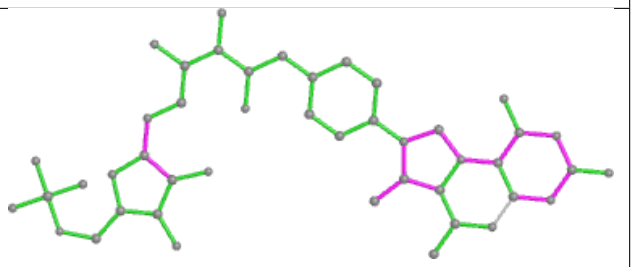

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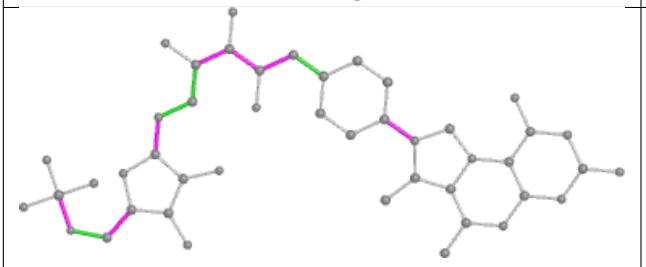

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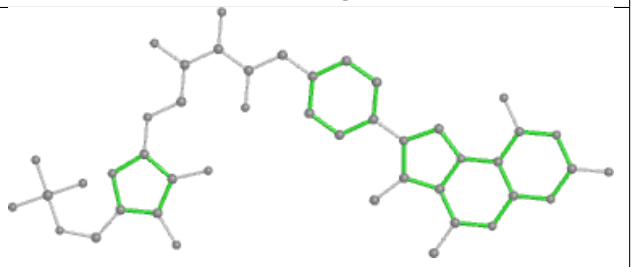
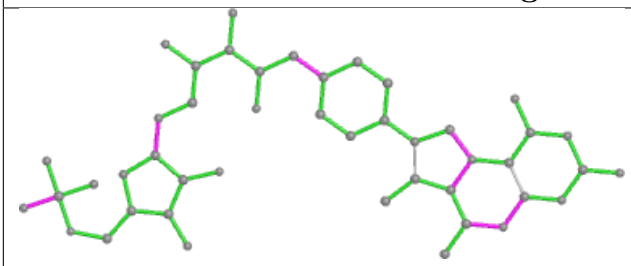


Rings

Ligand H4M D 301



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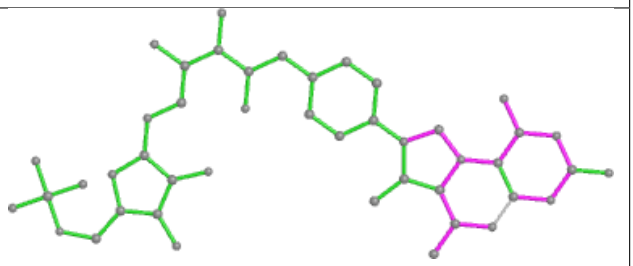
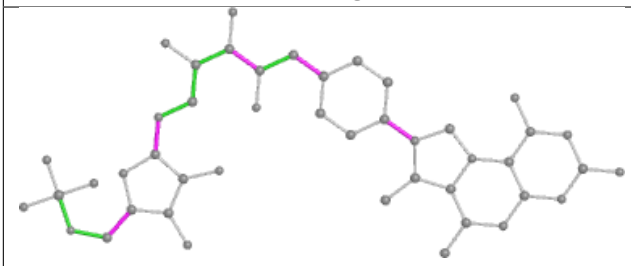


Bond angles



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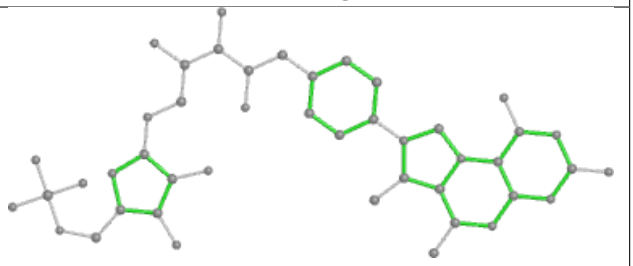
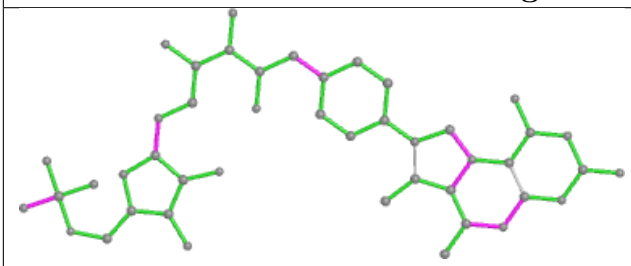


Rings

Ligand H4M X 302



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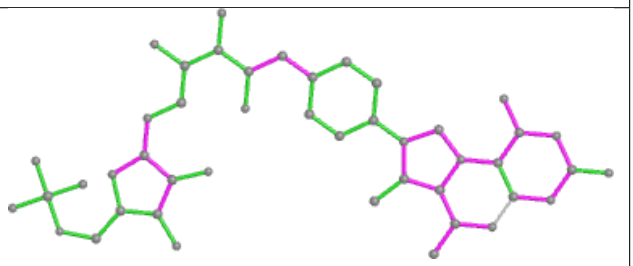
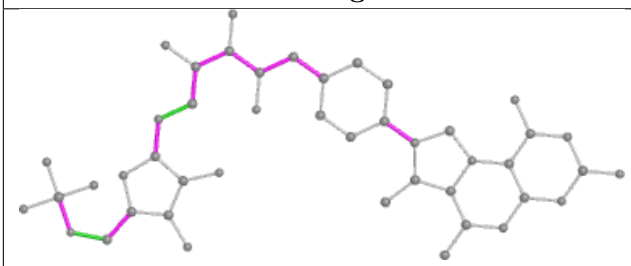
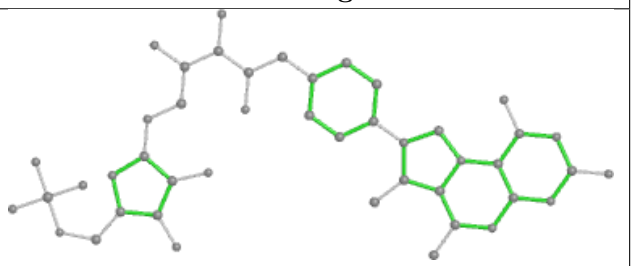


Bond angles

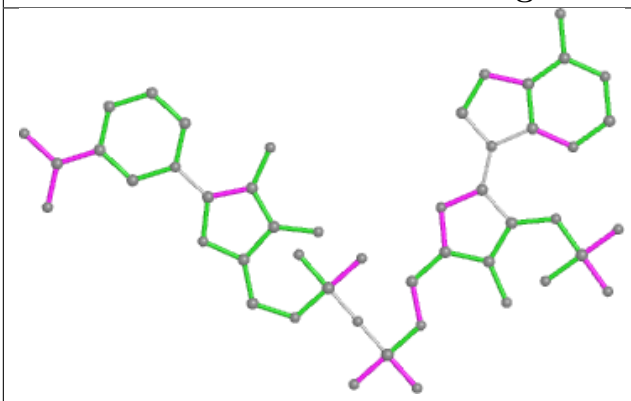


Torsions

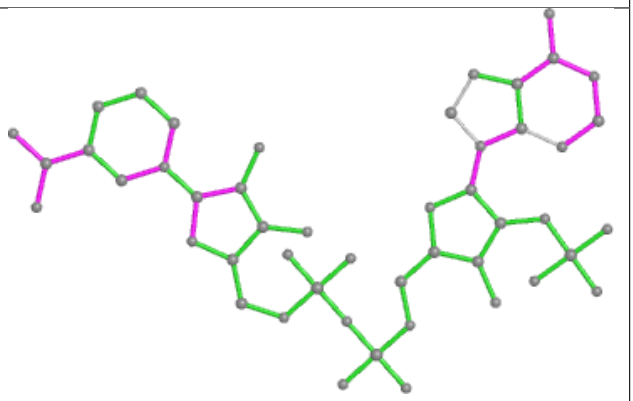


Rings

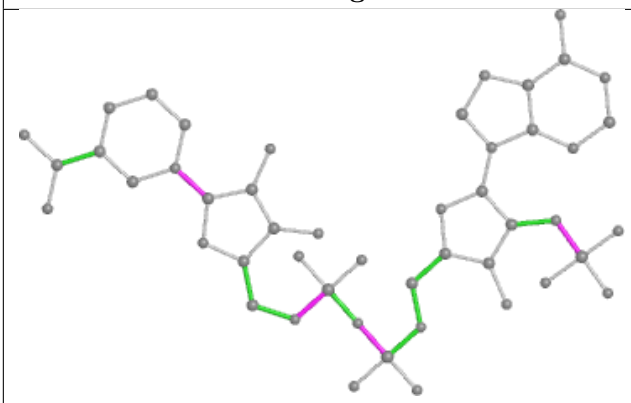
Ligand NAP W 301



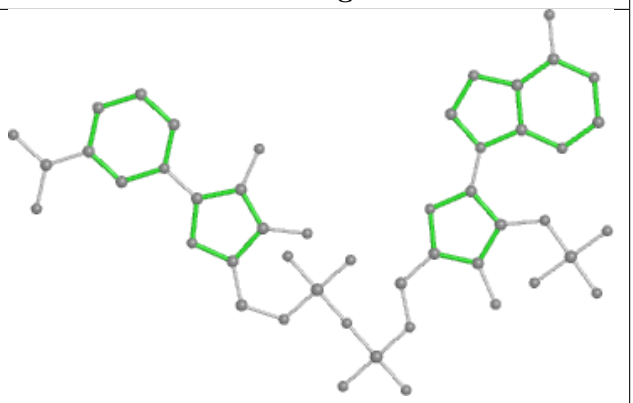
Bond lengths



Bond angles

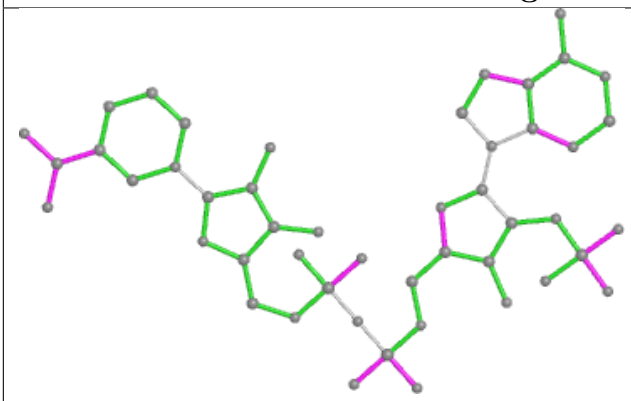


Torsions

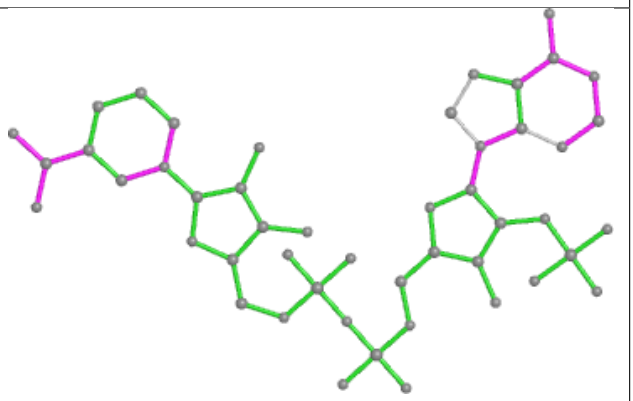


Rings

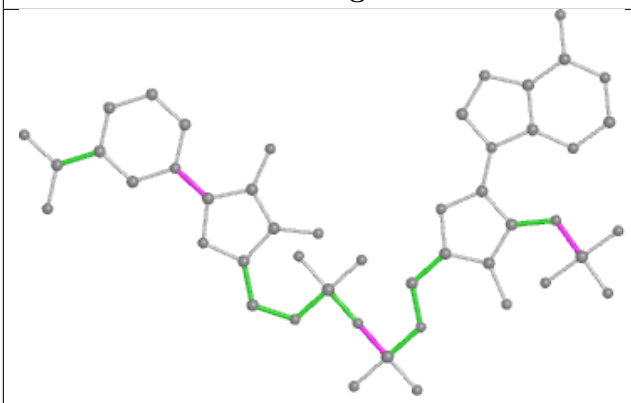
Ligand NAP N 301



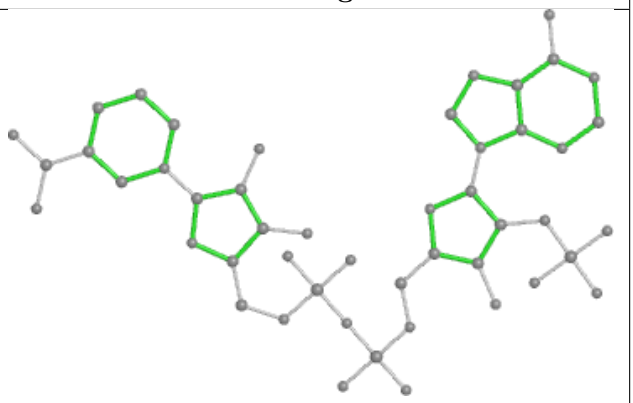
Bond lengths



Bond angles

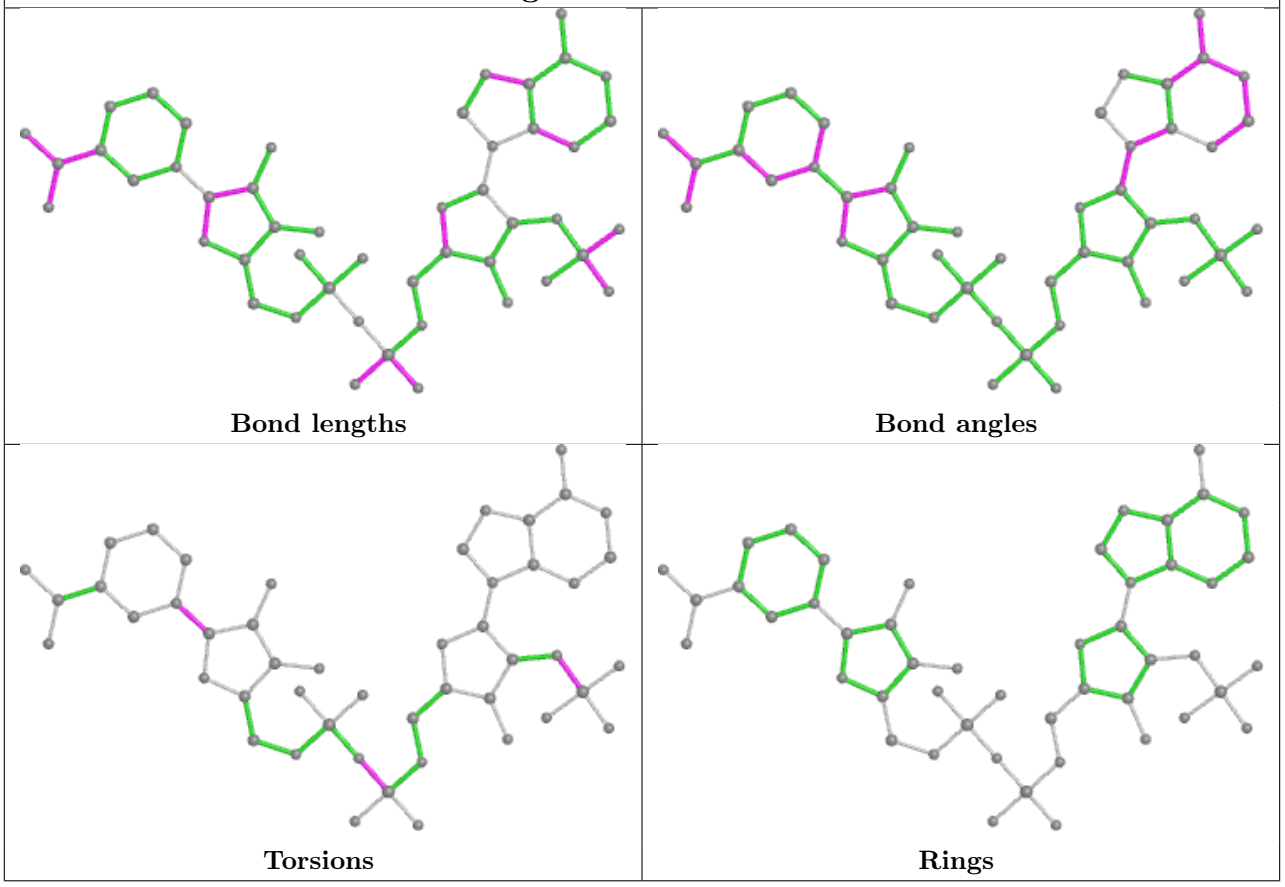


Torsions



Rings

Ligand NAP G 301



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	287/288 (99%)	-0.08	0 100 100	16, 22, 35, 50	0
1	B	287/288 (99%)	-0.07	1 (0%) 94 95	16, 22, 35, 56	0
1	C	287/288 (99%)	-0.02	2 (0%) 87 90	17, 27, 45, 56	0
1	D	287/288 (99%)	0.06	1 (0%) 94 95	16, 26, 41, 57	0
1	E	287/288 (99%)	-0.04	1 (0%) 94 95	16, 22, 35, 49	0
1	F	287/288 (99%)	-0.09	4 (1%) 75 79	16, 23, 36, 48	0
1	G	287/288 (99%)	-0.09	0 100 100	16, 22, 37, 46	0
1	H	287/288 (99%)	-0.16	1 (0%) 94 95	15, 20, 33, 46	0
1	I	287/288 (99%)	-0.01	3 (1%) 82 85	17, 25, 44, 55	0
1	J	287/288 (99%)	-0.18	0 100 100	18, 24, 37, 44	0
1	K	287/288 (99%)	-0.11	0 100 100	17, 23, 37, 53	0
1	L	287/288 (99%)	0.05	3 (1%) 82 85	20, 29, 48, 69	0
1	M	287/288 (99%)	-0.10	1 (0%) 94 95	15, 20, 33, 52	0
1	N	287/288 (99%)	-0.10	1 (0%) 94 95	16, 22, 36, 48	0
1	O	287/288 (99%)	0.04	6 (2%) 63 68	17, 27, 46, 60	0
1	P	287/288 (99%)	0.26	13 (4%) 33 36	19, 29, 45, 59	0
1	Q	287/288 (99%)	0.01	2 (0%) 87 90	16, 23, 38, 56	0
1	R	287/288 (99%)	0.33	13 (4%) 33 36	20, 34, 49, 64	0
1	S	287/288 (99%)	0.32	4 (1%) 75 79	26, 39, 54, 67	0
1	T	287/288 (99%)	0.02	1 (0%) 94 95	20, 27, 39, 55	0
1	U	287/288 (99%)	0.39	13 (4%) 33 36	25, 39, 53, 65	0
1	V	287/288 (99%)	1.14	64 (22%) 0 0	26, 56, 82, 94	0
1	W	287/288 (99%)	0.11	5 (1%) 70 75	21, 28, 41, 59	0
1	X	287/288 (99%)	0.89	40 (13%) 2 2	28, 46, 70, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	6888/6912 (99%)	0.11	179 (2%)	56	61	15, 27, 52, 100	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	241	TYR	7.2
1	X	85	PHE	6.8
1	X	88	PHE	5.6
1	V	231	GLY	5.4
1	V	232	ILE	5.1

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, 95th 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
3	H4M	S	302	45/54	0.44	0.31	39,45,57,57	45
3	H4M	U	302	45/54	0.51	0.36	49,56,58,59	45
3	H4M	W	302	45/54	0.55	0.27	28,37,50,51	45
3	H4M	F	302	45/54	0.56	0.36	20,39,43,47	45
3	H4M	Q	302	45/54	0.59	0.28	41,47,60,62	45
3	H4M	C	302	45/54	0.63	0.29	22,33,46,48	45
3	H4M	V	302	45/54	0.63	0.23	39,44,56,58	45
3	H4M	N	302	45/54	0.63	0.30	46,58,60,61	45
3	H4M	R	302	45/54	0.65	0.32	30,45,60,61	45
3	H4M	D	301	45/54	0.66	0.30	30,41,74,74	0
3	H4M	O	302	45/54	0.68	0.30	28,42,47,49	45
3	H4M	L	302	45/54	0.69	0.31	33,42,48,49	45
3	H4M	X	302	45/54	0.75	0.30	27,61,80,81	45

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	H4M	K	302	45/54	0.76	0.26	20,35,41,44	45
2	NAP	W	301	48/48	0.77	0.38	72,82,92,95	0
3	H4M	I	302	45/54	0.78	0.28	23,38,45,47	45
3	H4M	P	302	45/54	0.80	0.22	21,33,55,57	45
3	H4M	G	302	45/54	0.80	0.21	23,34,60,63	0
3	H4M	J	302	45/54	0.82	0.19	20,32,56,58	0
3	H4M	M	302	45/54	0.82	0.20	21,32,67,69	0
3	H4M	H	302	45/54	0.83	0.25	18,26,39,43	45
3	H4M	B	302	45/54	0.83	0.23	16,24,36,37	45
3	H4M	T	302	45/54	0.84	0.24	43,47,53,54	45
3	H4M	E	302	45/54	0.85	0.20	30,42,46,47	45
3	H4M	A	302	45/54	0.85	0.17	17,26,54,57	0
2	NAP	V	301	48/48	0.88	0.18	43,47,51,52	0
2	NAP	E	301	48/48	0.92	0.18	30,38,46,49	0
2	NAP	S	301	48/48	0.92	0.10	40,48,53,57	0
2	NAP	U	301	48/48	0.93	0.10	42,54,60,60	0
2	NAP	O	301	48/48	0.93	0.11	33,42,53,55	0
2	NAP	L	301	48/48	0.93	0.10	39,42,50,53	0
2	NAP	T	301	48/48	0.94	0.14	28,38,46,46	0
2	NAP	A	301	48/48	0.95	0.09	20,31,36,38	0
2	NAP	G	301	48/48	0.95	0.10	20,27,35,38	0
2	NAP	Q	301	48/48	0.95	0.14	23,29,37,45	0
2	NAP	J	301	48/48	0.95	0.10	22,33,39,41	0
2	NAP	F	301	48/48	0.96	0.10	20,27,33,36	0
2	NAP	P	301	48/48	0.96	0.10	25,28,35,36	0
2	NAP	C	301	48/48	0.96	0.08	23,29,33,39	0
2	NAP	N	301	48/48	0.96	0.09	24,27,36,41	0
2	NAP	D	302	48/48	0.97	0.07	18,24,29,33	0
2	NAP	K	301	48/48	0.97	0.07	18,23,31,38	0
2	NAP	I	301	48/48	0.97	0.08	21,26,33,36	0
2	NAP	M	301	48/48	0.97	0.07	15,19,25,26	0
2	NAP	R	301	48/48	0.97	0.08	24,31,36,41	0
2	NAP	X	301	48/48	0.97	0.10	25,34,49,63	0
4	SO4	H	303	5/5	0.97	0.10	36,45,47,56	0
2	NAP	H	301	48/48	0.98	0.07	16,19,25,32	0
4	SO4	A	303	5/5	0.98	0.08	35,43,45,51	0
4	SO4	D	303	5/5	0.98	0.09	34,38,40,46	0
2	NAP	B	301	48/48	0.98	0.07	18,23,28,37	0
4	SO4	J	303	5/5	0.98	0.09	38,46,55,55	0
4	SO4	M	303	5/5	0.98	0.09	33,35,46,50	0
4	SO4	P	303	5/5	0.98	0.06	40,43,47,53	0
4	SO4	S	303	5/5	0.98	0.09	42,43,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	V	303	5/5	0.98	0.09	45,46,56,60	0

6.5 Other polymers (i)

There are no such residues in this entry.