wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2020 – 03:47 am BST

PDB ID	:	5BP4
Title	:	Modifying region (DH-ER-KR) of a mycocerosic acid synthase-like (MAS-like) PKS
Authors	:	Herbst, D.A.; Jakob, P.R.; Zaehringer, F.; Maier, T.
Deposited on	:	2015-05-27
Resolution	:	3.75 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

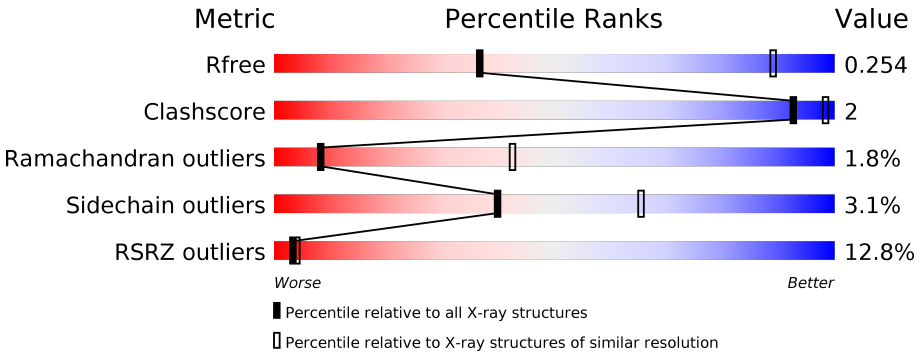
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.75 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	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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 on 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	1140	10% 88% 8%
1	B	1140	5% 89% 7%
1	C	1140	8% 90% 6%
1	D	1140	9% 89% 7%
1	E	1140	21% 89% 6%
1	F	1140	16% 89% 7%

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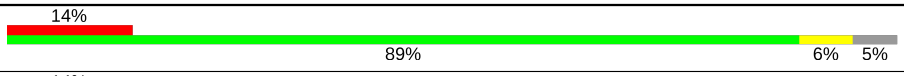
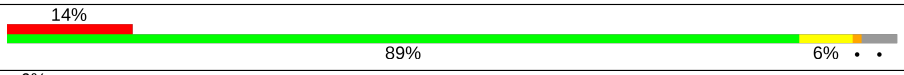
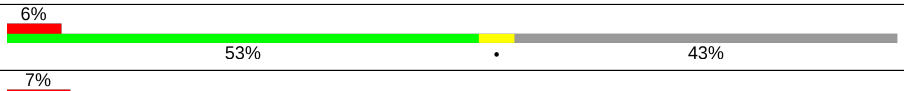
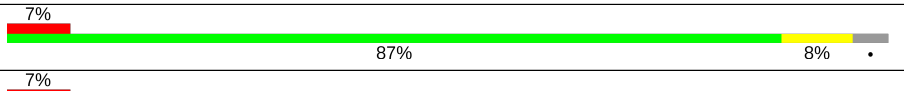
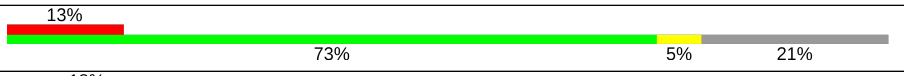
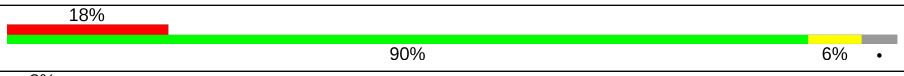
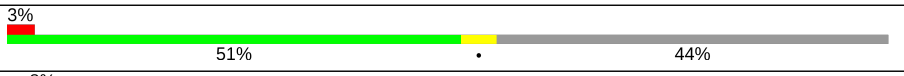
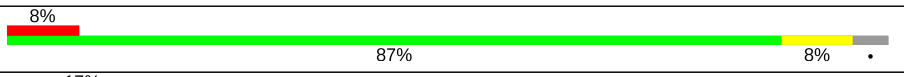
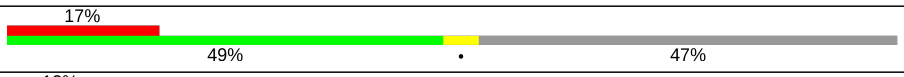
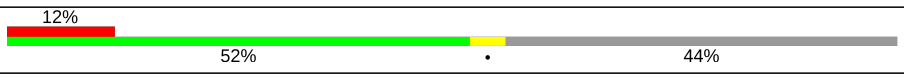
Mol	Chain	Length	Quality of chain
1	G	1140	
1	H	1140	
1	I	1140	
1	J	1140	
1	K	1140	
1	L	1140	
1	M	1140	
1	N	1140	
1	O	1140	
1	P	1140	
1	Q	1140	
1	R	1140	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 262498 atoms, of which 129384 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 Mycocerosic acid synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	B	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	C	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	D	1102	Total	C	H	N	O	S	0	0	0
			16283	5165	8038	1479	1576	25			
1	E	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	F	1093	Total	C	H	N	O	S	0	0	0
			16142	5122	7965	1467	1564	24			
1	G	1088	Total	C	H	N	O	S	0	0	0
			16079	5102	7939	1462	1552	24			
1	H	1097	Total	C	H	N	O	S	0	0	0
			16195	5138	7991	1471	1571	24			
1	I	655	Total	C	H	N	O	S	0	0	0
			9680	3057	4801	872	935	15			
1	J	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	K	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	L	897	Total	C	H	N	O	S	0	0	0
			13209	4199	6535	1183	1272	20			
1	M	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	N	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			
1	O	633	Total	C	H	N	O	S	0	0	0
			9327	2950	4625	839	898	15			
1	P	1089	Total	C	H	N	O	S	0	0	0
			16094	5107	7945	1463	1555	24			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	608	Total	C	H	N	O	S	0	0	0
			8979	2846	4455	804	859	15			
1	R	637	Total	C	H	N	O	S	0	0	0
			9417	2980	4669	844	909	15			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	882	SER	-	expression tag	UNP A0R1E8
A	883	MET	-	expression tag	UNP A0R1E8
A	2021	GLN	-	expression tag	UNP A0R1E8
B	882	SER	-	expression tag	UNP A0R1E8
B	883	MET	-	expression tag	UNP A0R1E8
B	2021	GLN	-	expression tag	UNP A0R1E8
C	882	SER	-	expression tag	UNP A0R1E8
C	883	MET	-	expression tag	UNP A0R1E8
C	2021	GLN	-	expression tag	UNP A0R1E8
D	882	SER	-	expression tag	UNP A0R1E8
D	883	MET	-	expression tag	UNP A0R1E8
D	2021	GLN	-	expression tag	UNP A0R1E8
E	882	SER	-	expression tag	UNP A0R1E8
E	883	MET	-	expression tag	UNP A0R1E8
E	2021	GLN	-	expression tag	UNP A0R1E8
F	882	SER	-	expression tag	UNP A0R1E8
F	883	MET	-	expression tag	UNP A0R1E8
F	2021	GLN	-	expression tag	UNP A0R1E8
G	882	SER	-	expression tag	UNP A0R1E8
G	883	MET	-	expression tag	UNP A0R1E8
G	2021	GLN	-	expression tag	UNP A0R1E8
H	882	SER	-	expression tag	UNP A0R1E8
H	883	MET	-	expression tag	UNP A0R1E8
H	2021	GLN	-	expression tag	UNP A0R1E8
I	882	SER	-	expression tag	UNP A0R1E8
I	883	MET	-	expression tag	UNP A0R1E8
I	2021	GLN	-	expression tag	UNP A0R1E8
J	882	SER	-	expression tag	UNP A0R1E8
J	883	MET	-	expression tag	UNP A0R1E8
J	2021	GLN	-	expression tag	UNP A0R1E8
K	882	SER	-	expression tag	UNP A0R1E8
K	883	MET	-	expression tag	UNP A0R1E8
K	2021	GLN	-	expression tag	UNP A0R1E8
L	882	SER	-	expression tag	UNP A0R1E8

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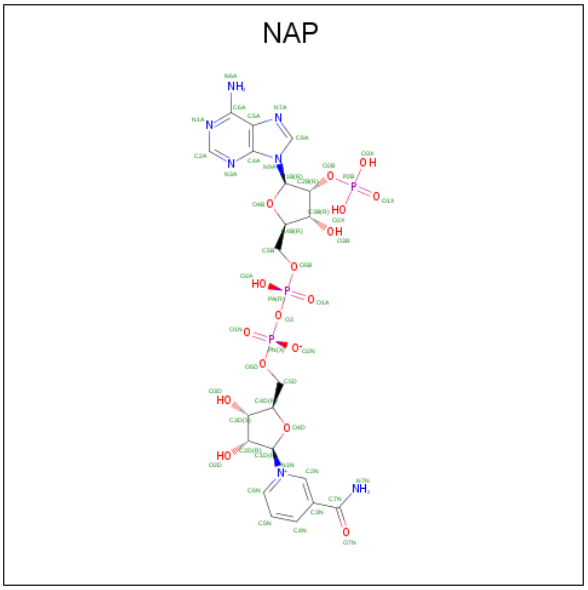
Chain	Residue	Modelled	Actual	Comment	Reference
L	883	MET	-	expression tag	UNP A0R1E8
L	2021	GLN	-	expression tag	UNP A0R1E8
M	882	SER	-	expression tag	UNP A0R1E8
M	883	MET	-	expression tag	UNP A0R1E8
M	2021	GLN	-	expression tag	UNP A0R1E8
N	882	SER	-	expression tag	UNP A0R1E8
N	883	MET	-	expression tag	UNP A0R1E8
N	2021	GLN	-	expression tag	UNP A0R1E8
O	882	SER	-	expression tag	UNP A0R1E8
O	883	MET	-	expression tag	UNP A0R1E8
O	2021	GLN	-	expression tag	UNP A0R1E8
P	882	SER	-	expression tag	UNP A0R1E8
P	883	MET	-	expression tag	UNP A0R1E8
P	2021	GLN	-	expression tag	UNP A0R1E8
Q	882	SER	-	expression tag	UNP A0R1E8
Q	883	MET	-	expression tag	UNP A0R1E8
Q	2021	GLN	-	expression tag	UNP A0R1E8
R	882	SER	-	expression tag	UNP A0R1E8
R	883	MET	-	expression tag	UNP A0R1E8
R	2021	GLN	-	expression tag	UNP A0R1E8

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	B	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	D	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	E	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	F	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	F	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	G	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	G	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	H	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	H	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	I	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	J	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	J	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	K	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	K	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	L	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	M	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

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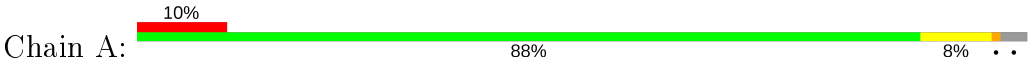
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	M	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	N	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	N	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	O	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	P	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	P	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
2	Q	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
2	R	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

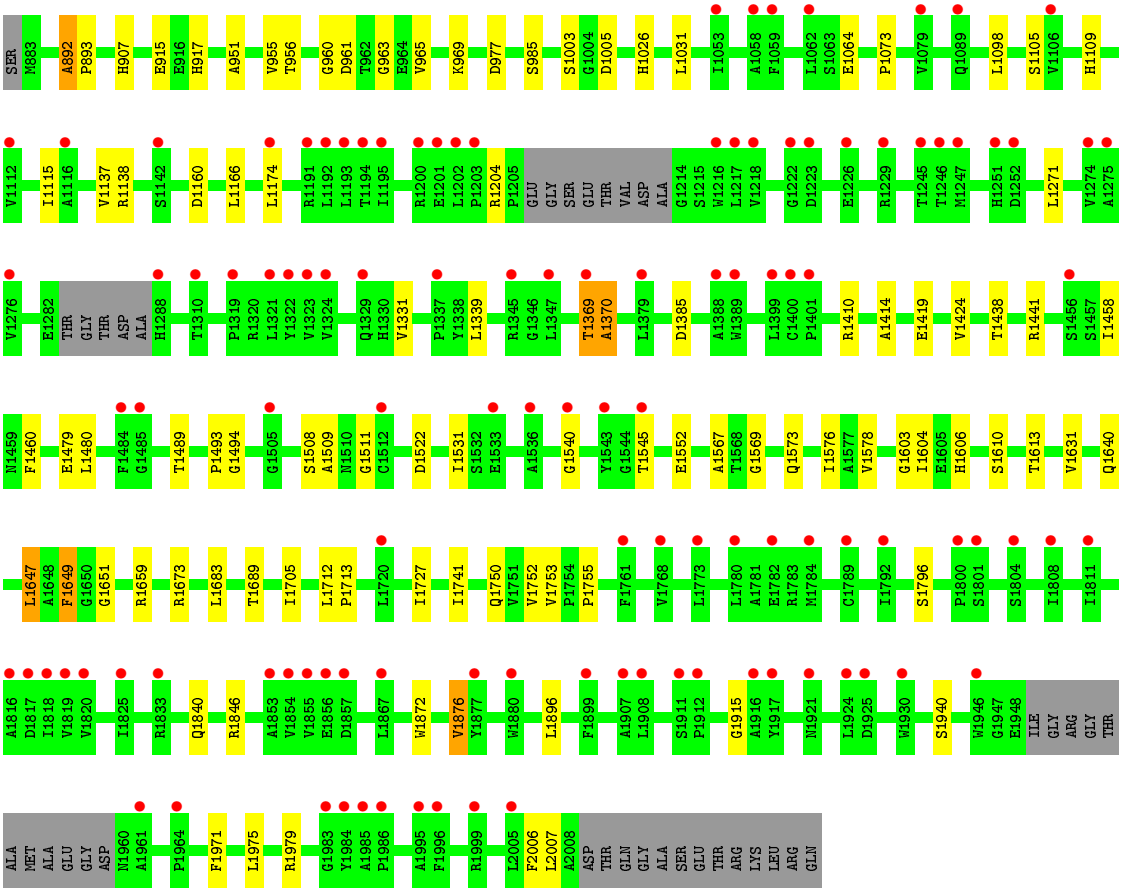
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Mycocerosic acid synthase

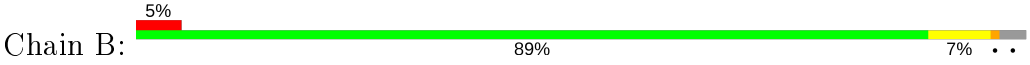
Chain A:

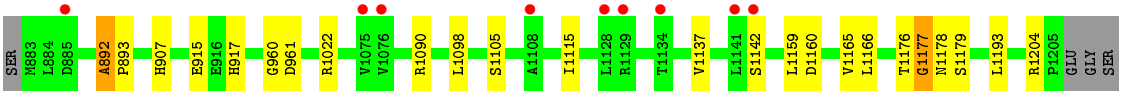


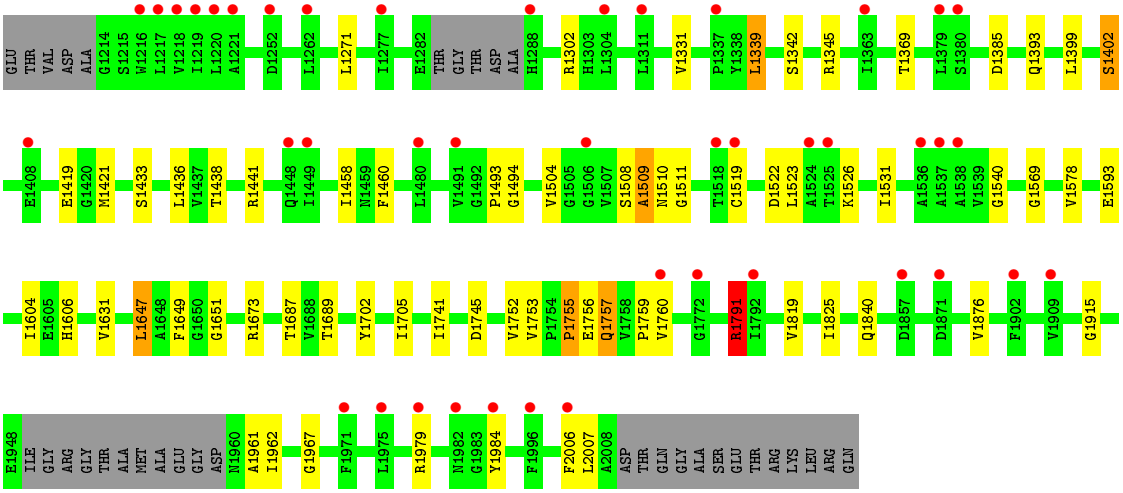


- Molecule 1: Mycocerosic acid synthase

Chain B:

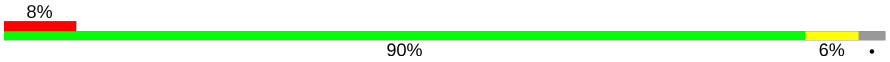


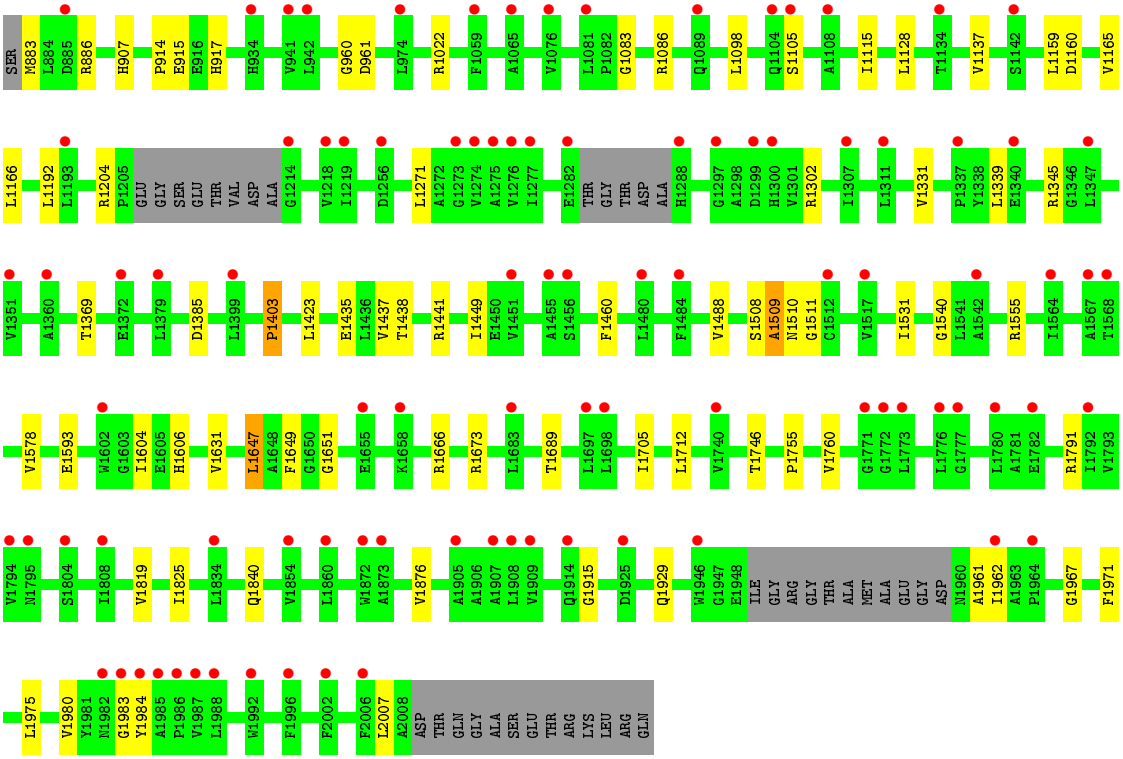




- Molecule 1: Mycocerosic acid synthase

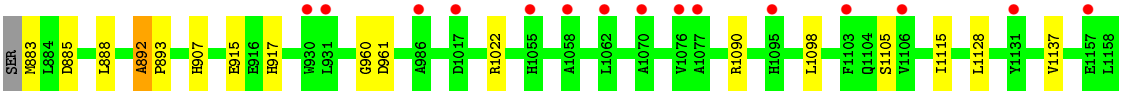
Chain C:

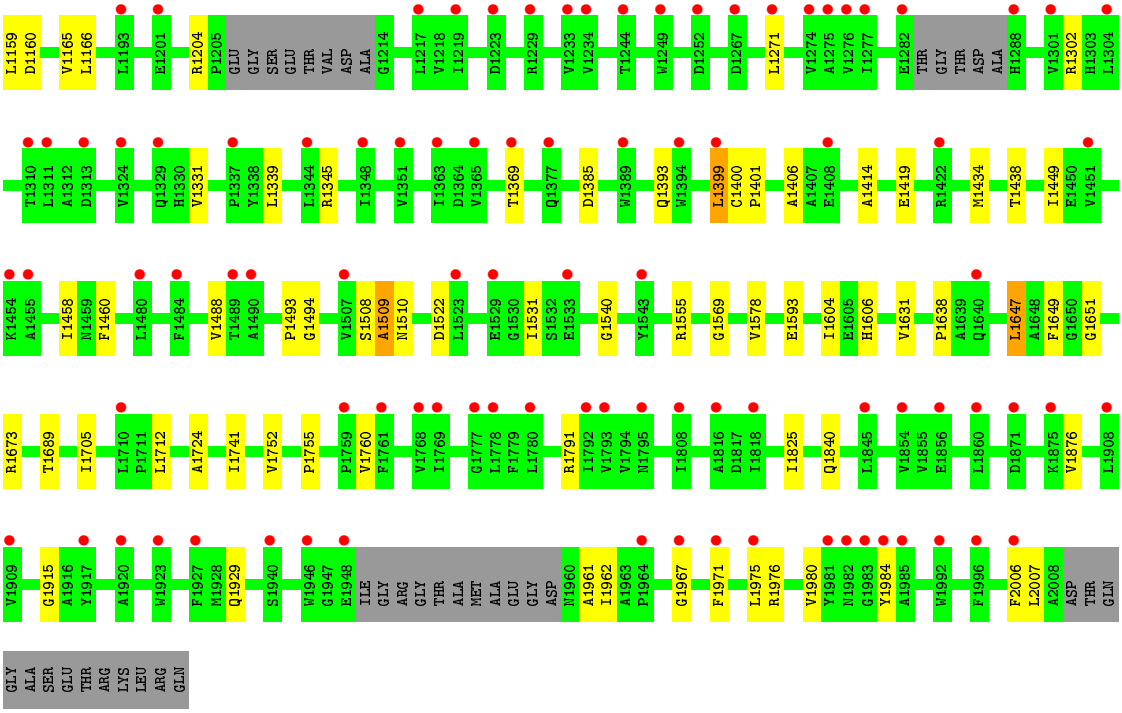




- Molecule 1: Mycocerosic acid synthase

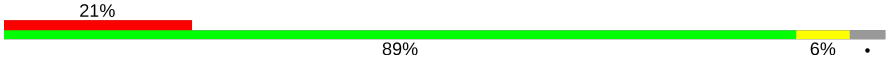
Chain D:

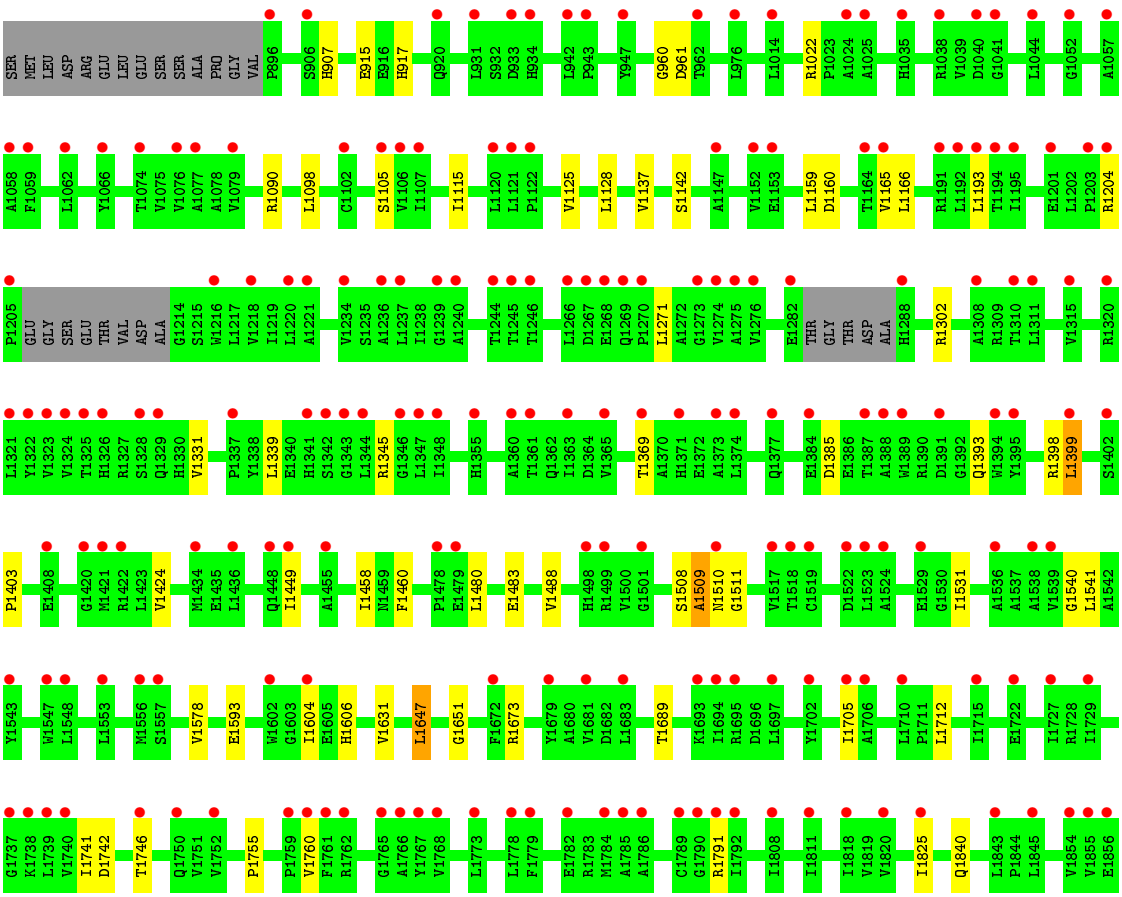


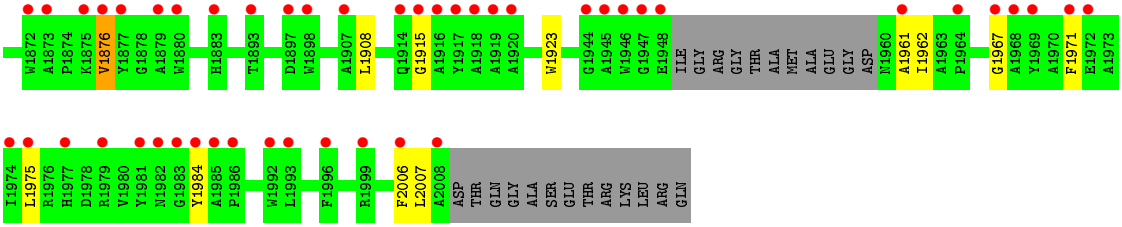


• Molecule 1: Mycocerosic acid synthase

Chain E:

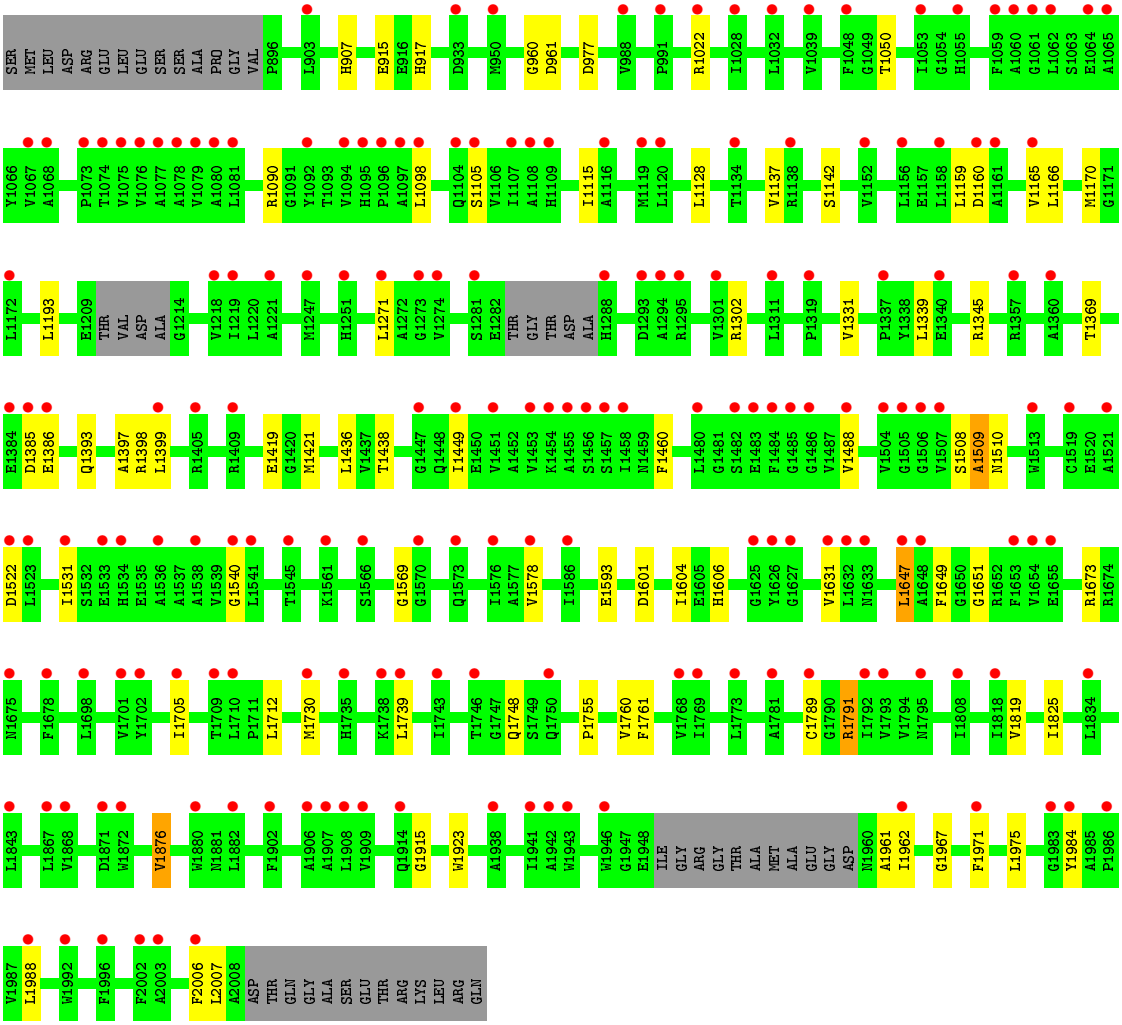






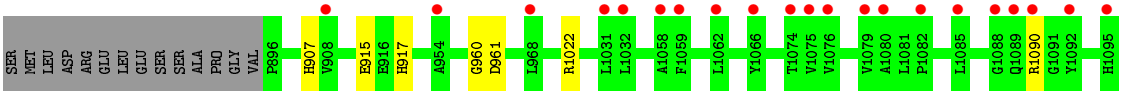
• Molecule 1: Mycocerosic acid synthase

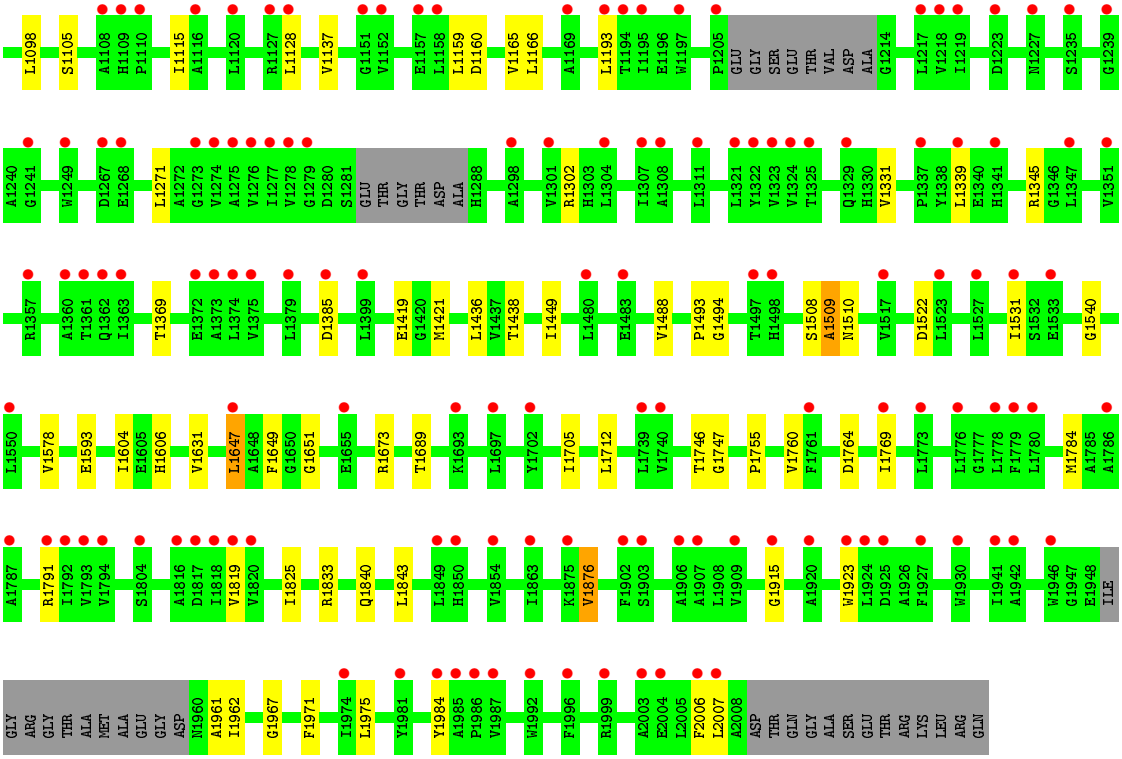
Chain F:



• Molecule 1: Mycocerosic acid synthase

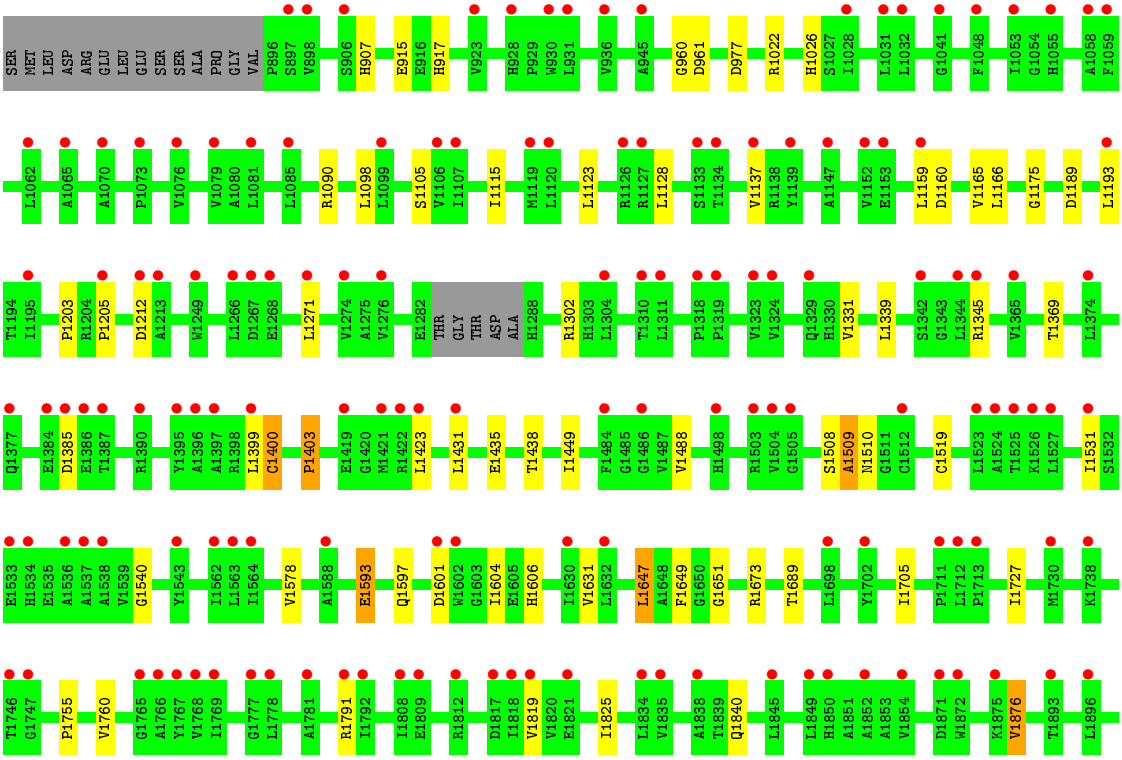
Chain G:

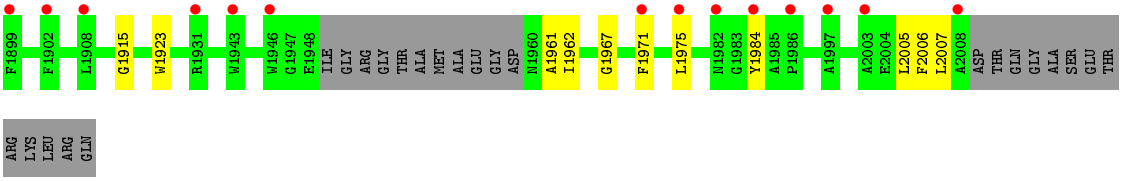




• Molecule 1: Mycocerosic acid synthase

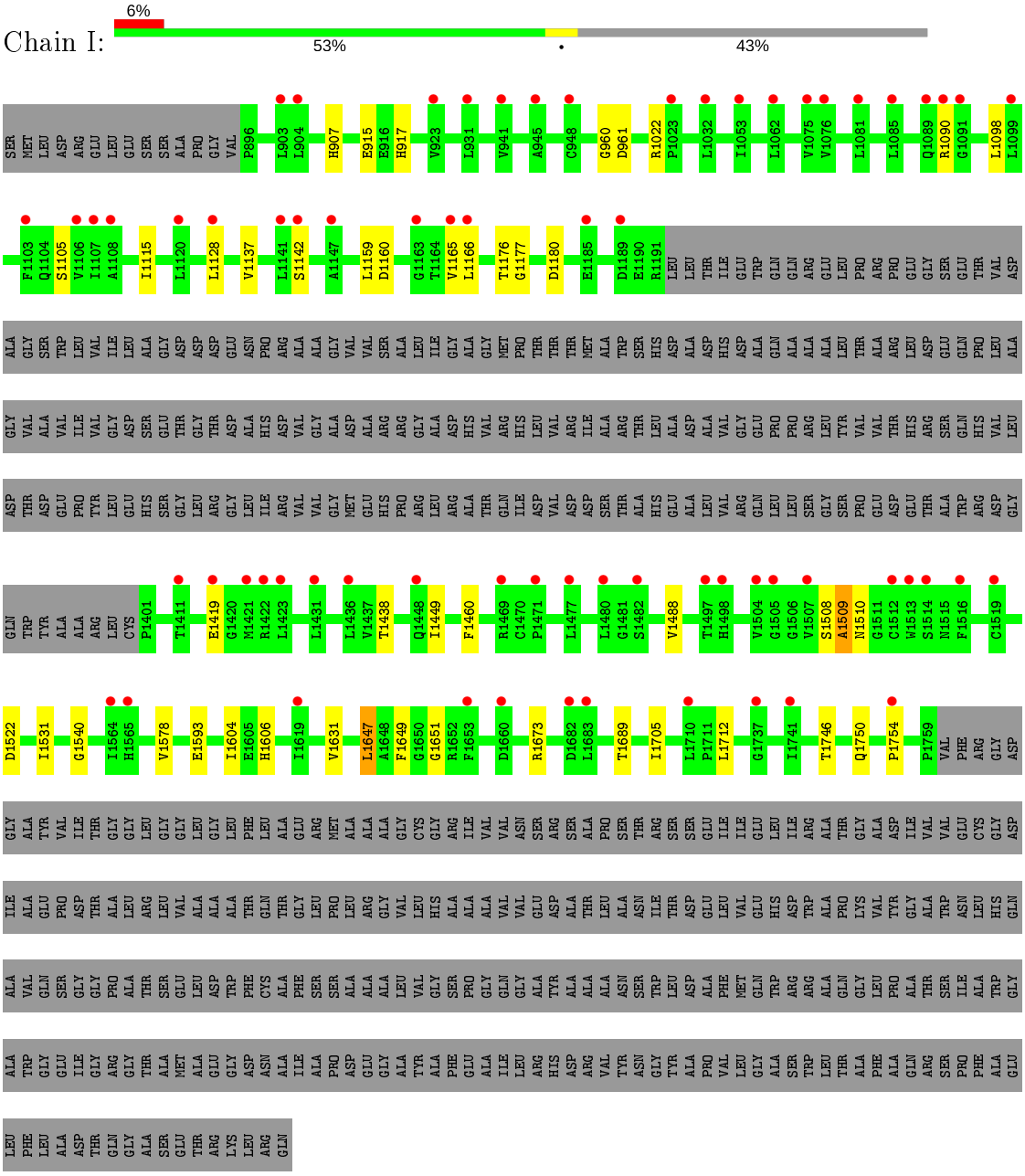
Chain H:





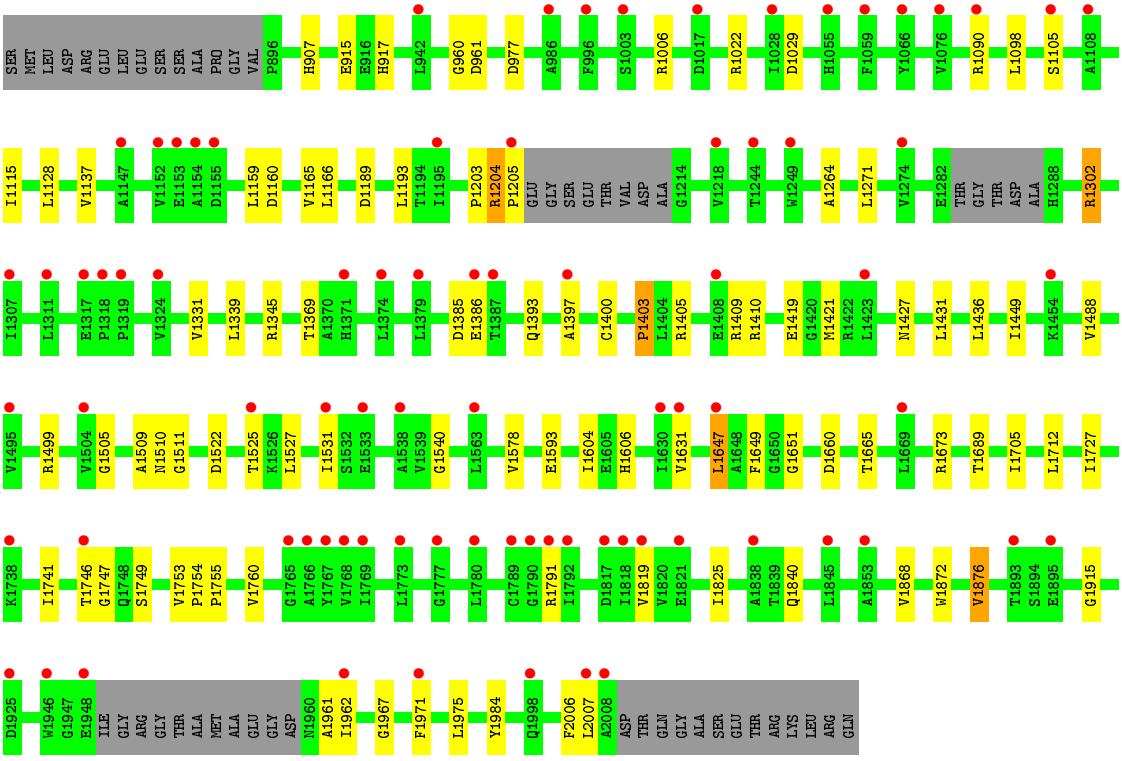
• Molecule 1: Mycocerosic acid synthase

Chain I:



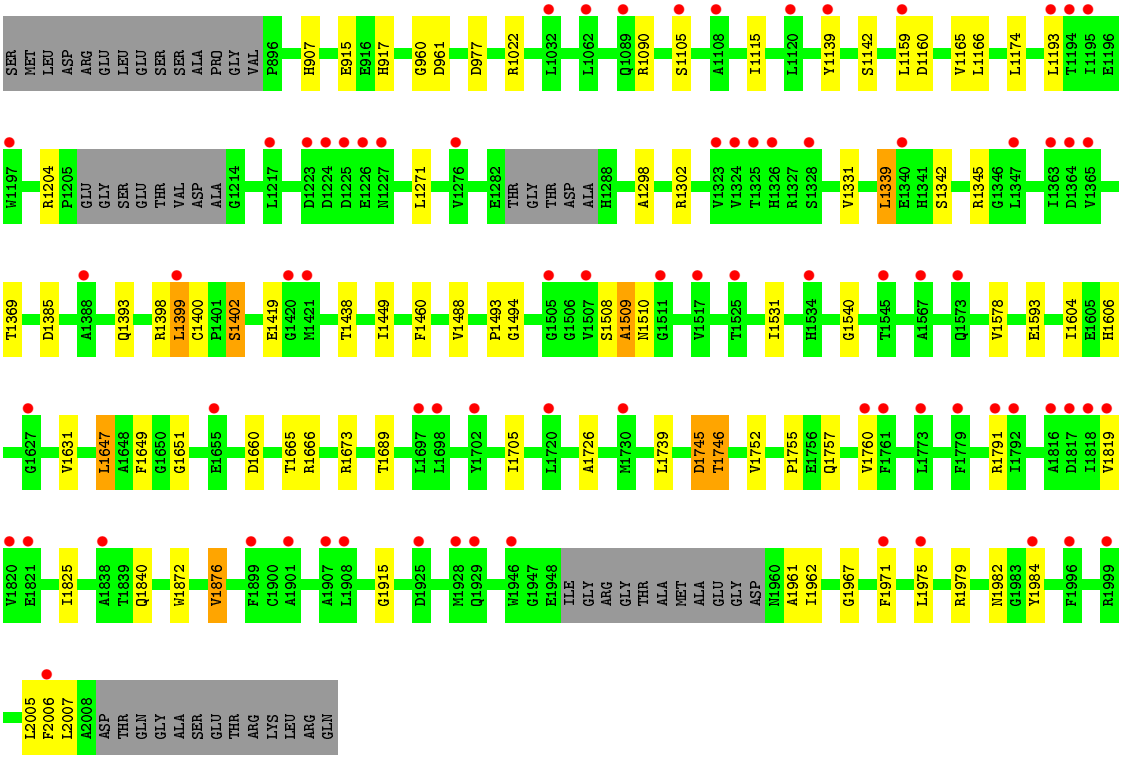
• Molecule 1: Mycocerosic acid synthase

Chain J:



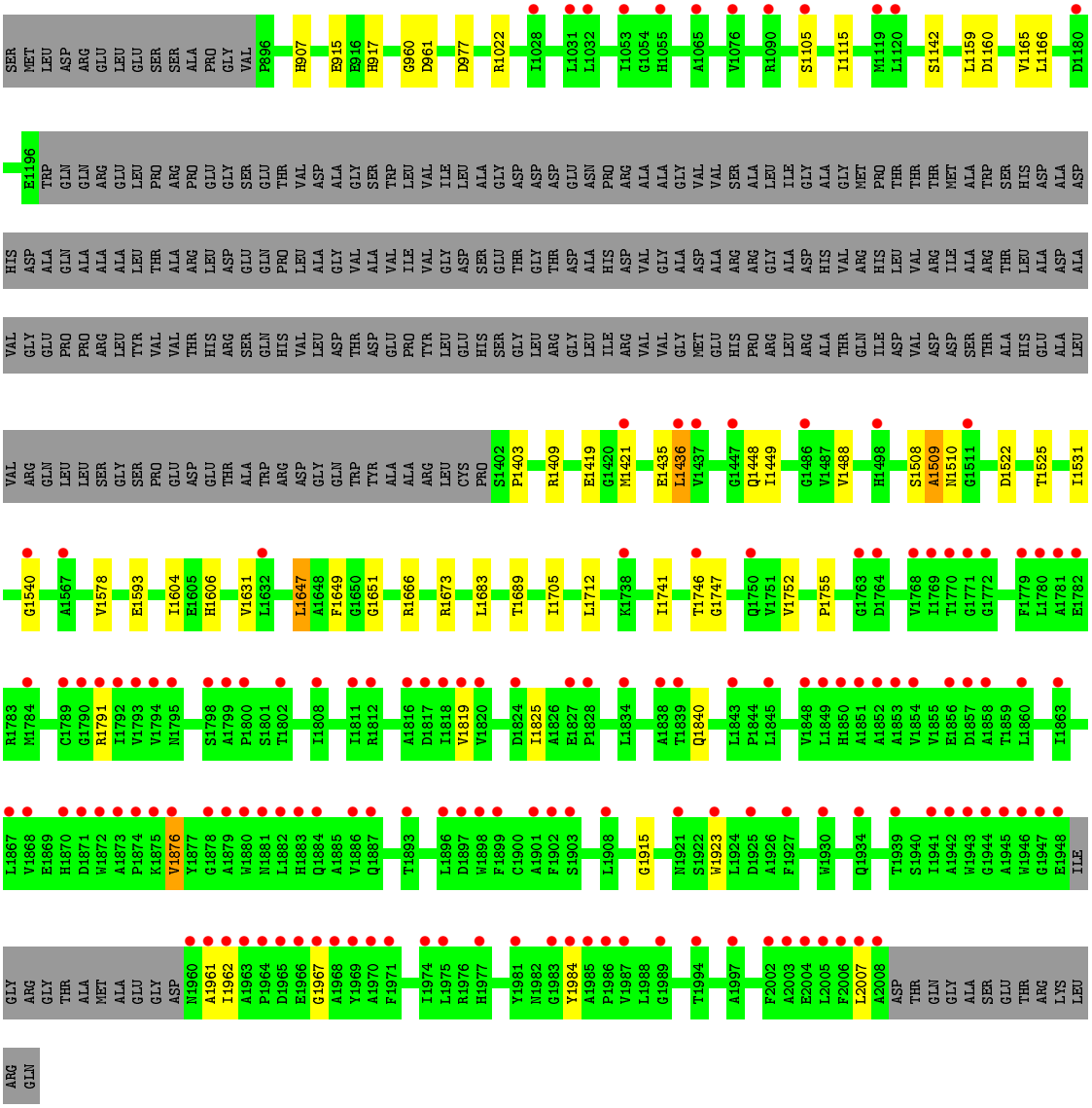
• Molecule 1: Mycocerosic acid synthase

Chain K:



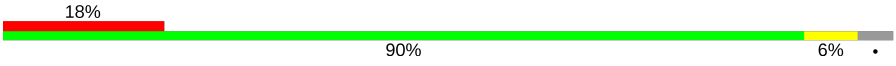
• Molecule 1: Mycocerosic acid synthase

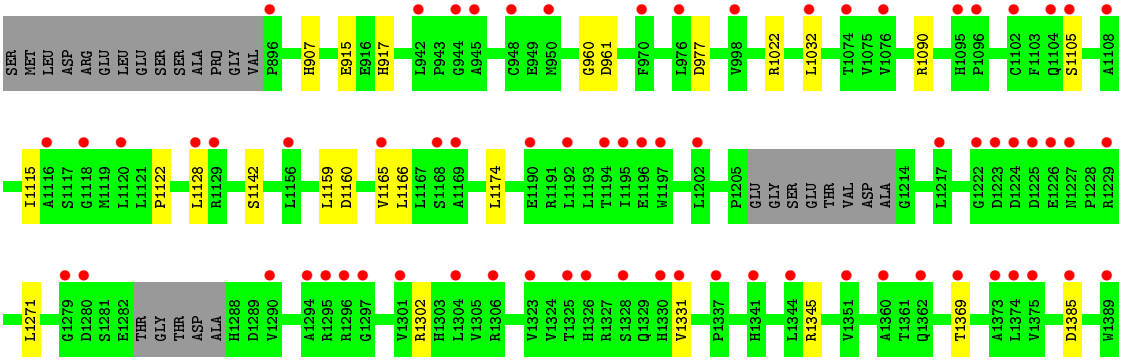
Chain L:

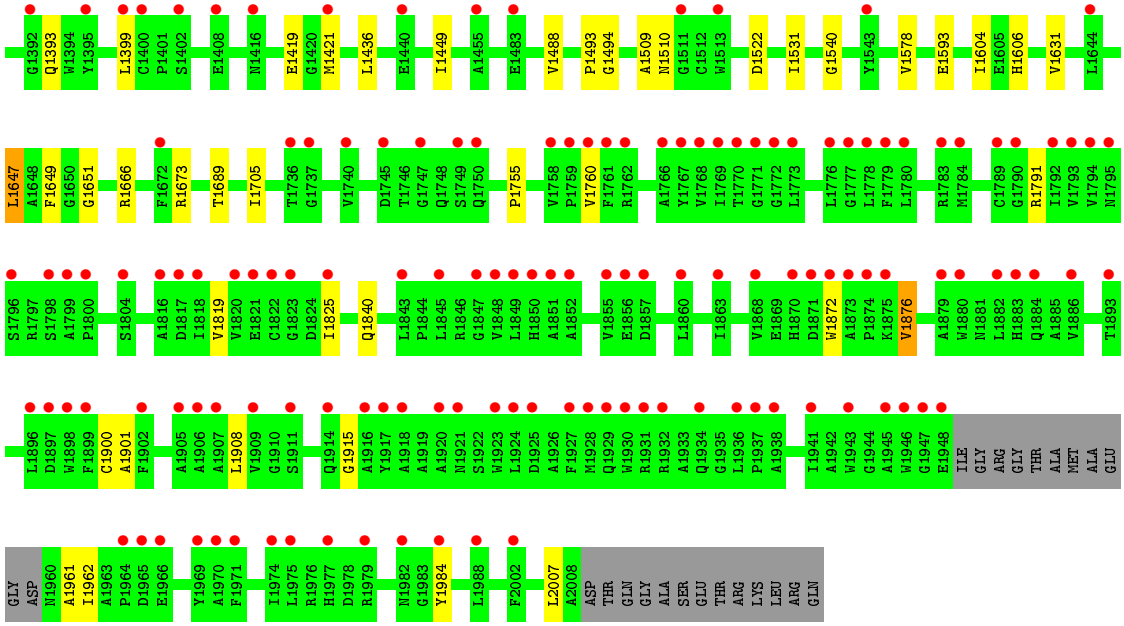


- Molecule 1: Mycocerosic acid synthase

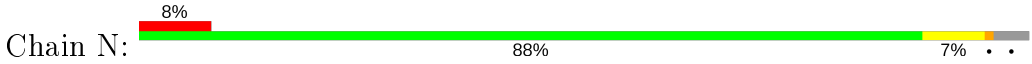
Chain M:

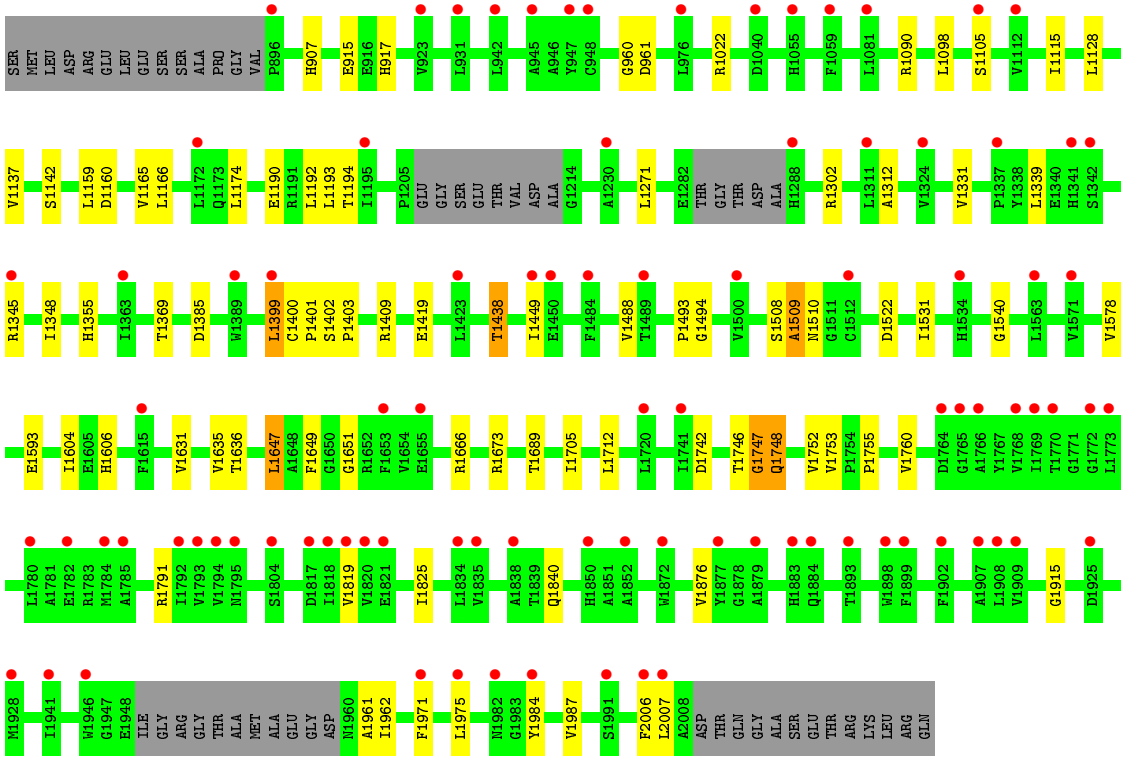




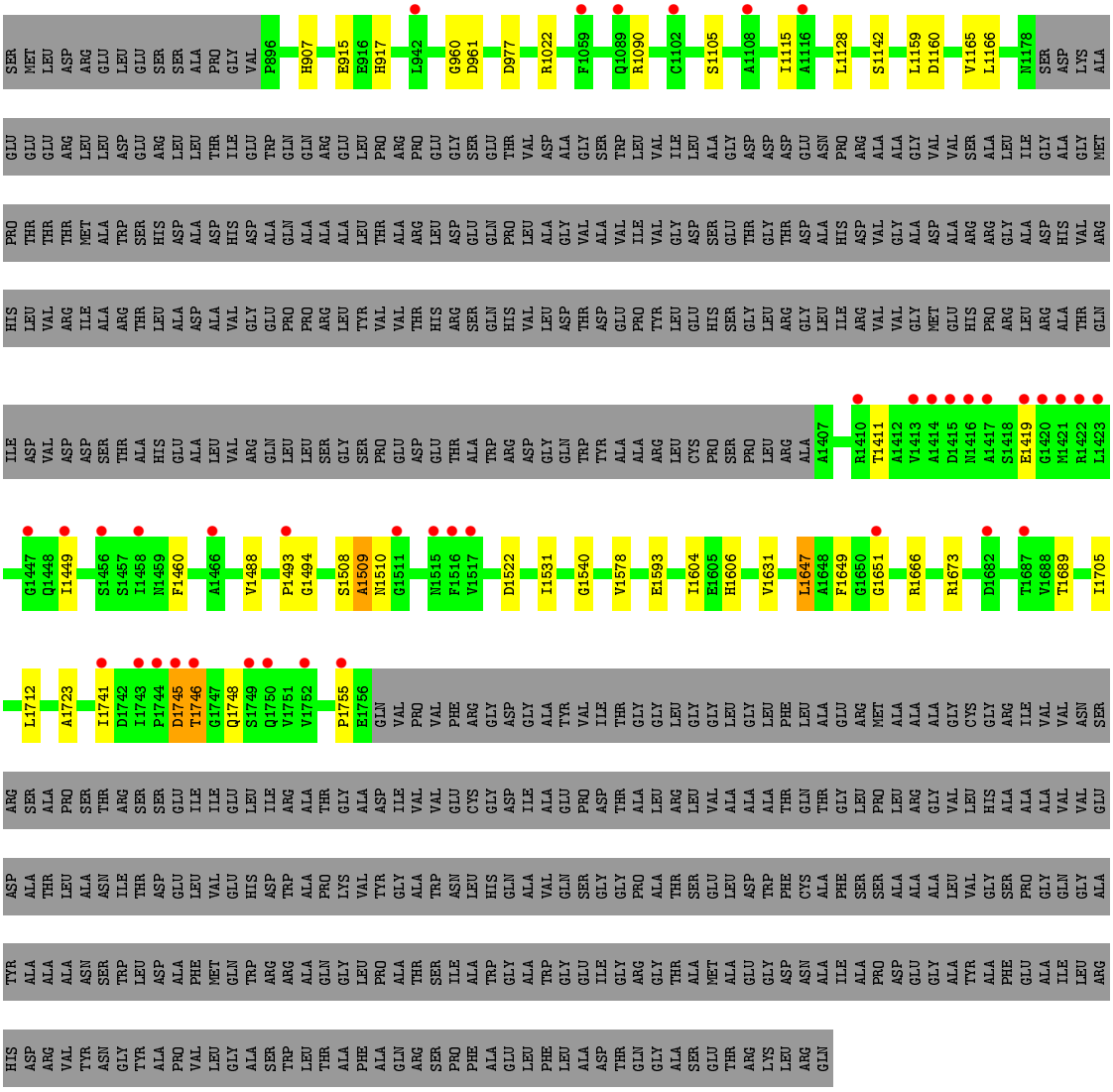


• Molecule 1: Mycocerosic acid synthase



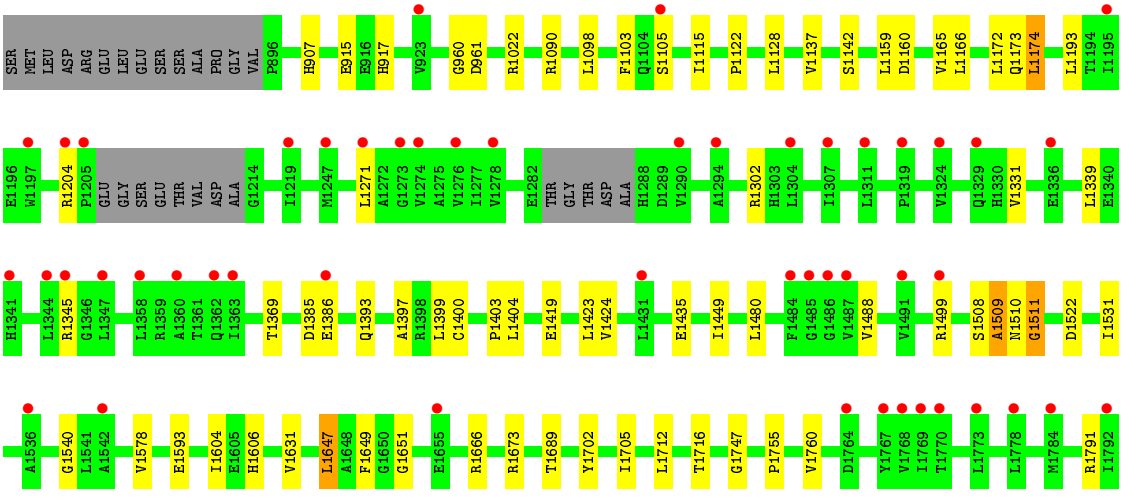


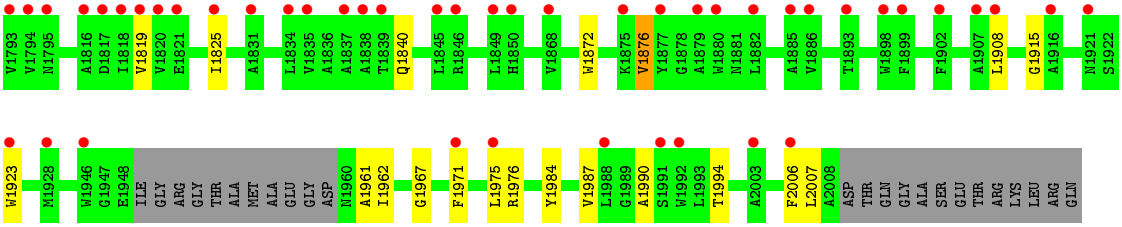
• Molecule 1: Mycocerosic acid synthase



• Molecule 1: Mycocerosic acid synthase

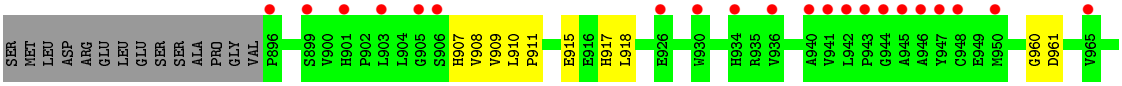
Chain P:

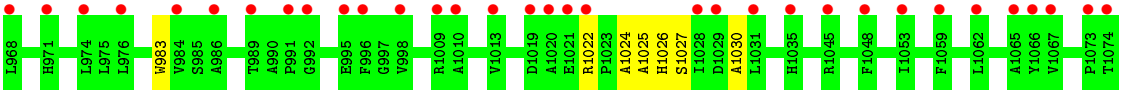


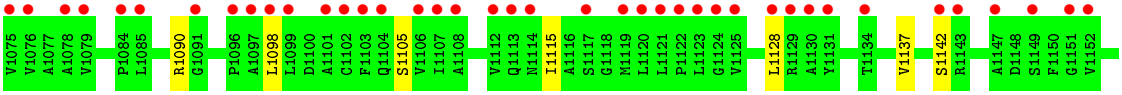


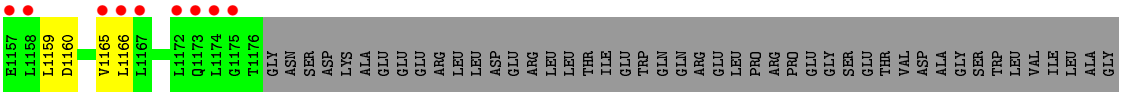
• Molecule 1: Mycocerosic acid synthase

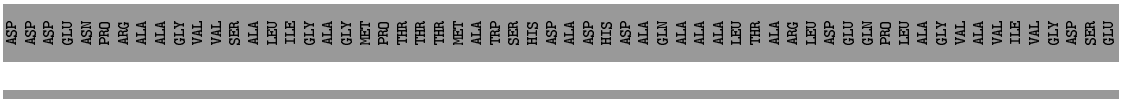
Chain Q:

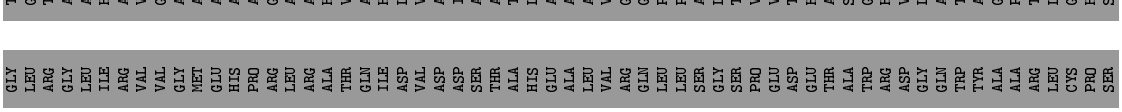


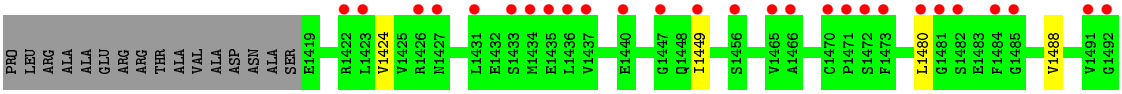


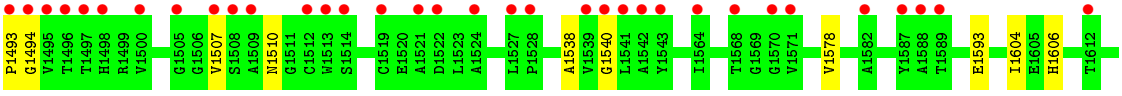


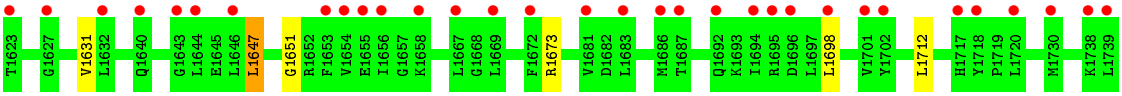


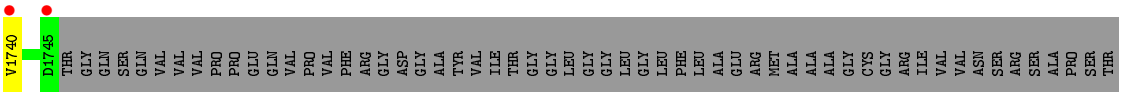


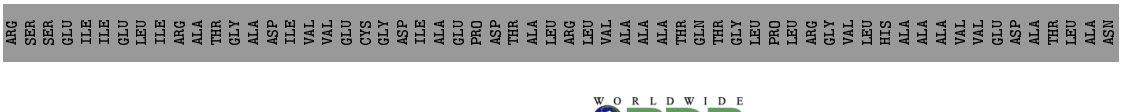












• Molecule 1: Mycocerosic acid synthase

Chain R:

ALA
SER
GLU
THR
ARG
LYS
LEU
ARG
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	151.38Å 190.37Å 270.84Å 95.58° 91.92° 103.65°	Depositor
Resolution (Å)	78.62 – 3.75 78.62 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (78.62-3.75) 99.0 (78.62-3.75)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.78Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.230 , 0.240 0.247 , 0.254	Depositor DCC
R_{free} test set	2985 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	132.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 132.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	262498	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.51	0/8420	0.65	0/11488
1	B	0.45	0/8420	0.62	1/11488 (0.0%)
1	C	0.41	0/8420	0.59	0/11488
1	D	0.41	0/8420	0.59	0/11488
1	E	0.40	0/8323	0.58	0/11356
1	F	0.39	0/8351	0.58	0/11393
1	G	0.42	0/8314	0.59	0/11344
1	H	0.41	0/8379	0.59	0/11434
1	I	0.40	0/4977	0.59	0/6783
1	J	0.42	0/8323	0.59	0/11356
1	K	0.44	0/8323	0.60	0/11356
1	L	0.44	0/6815	0.61	0/9296
1	M	0.40	0/8323	0.58	0/11356
1	N	0.42	0/8323	0.61	0/11356
1	O	0.44	0/4797	0.61	0/6540
1	P	0.43	0/8323	0.60	0/11356
1	Q	0.39	0/4617	0.58	0/6293
1	R	0.40	0/4844	0.60	0/6602
All	All	0.42	0/134712	0.60	1/183773 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1178	ASN	C-N-CA	5.23	134.78	121.70

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	8245	8038	8072	32	0
1	B	8245	8038	8072	33	0
1	C	8245	8038	8072	22	1
1	D	8245	8038	8072	26	0
1	E	8149	7945	7979	23	0
1	F	8177	7965	7999	27	0
1	G	8140	7939	7973	23	0
1	H	8204	7991	8025	35	0
1	I	4879	4801	4822	12	0
1	J	8149	7945	7979	30	1
1	K	8149	7945	7979	30	0
1	L	6674	6535	6560	19	0
1	M	8149	7945	7979	19	0
1	N	8149	7945	7979	24	0
1	O	4702	4625	4646	14	0
1	P	8149	7945	7979	28	0
1	Q	4524	4455	4476	31	0
1	R	4748	4669	4690	23	0
2	A	75	36	36	2	0
2	B	75	36	36	2	0
2	C	79	36	36	1	0
2	D	75	36	36	2	0
2	E	48	25	25	1	0
2	F	75	36	36	2	0
2	G	75	36	36	0	0
2	H	75	36	36	0	0
2	I	48	25	25	1	0
2	J	75	36	36	0	0
2	K	75	36	36	2	0
2	L	48	25	25	1	0
2	M	75	36	36	0	0
2	N	75	36	36	0	0
2	O	48	25	25	1	0
2	P	75	36	36	0	0
2	Q	48	25	25	0	0
2	R	48	25	25	0	0
All	All	133114	129384	129935	406	1

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

The worst 5 of 406 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1348:ILE:CD1	1:N:1348:ILE:CG1	1.80	1.59
1:Q:908:VAL:HG13	1:R:920:GLN:HB2	1.68	0.75
1:N:1193:LEU:HD22	1:N:1399:LEU:HD22	1.70	0.73
1:C:914:PRO:HD3	1:D:1638:PRO:HG3	1.71	0.73
1:Q:909:VAL:O	1:R:983:TRP:NE1	2.21	0.71

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1083:GLY:HA2	1:J:1264:ALA:HB1[1_565]	1.34	0.26

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	1094/1140 (96%)	995 (91%)	79 (7%)	20 (2%)	8 42
1	B	1094/1140 (96%)	1002 (92%)	69 (6%)	23 (2%)	7 40
1	C	1094/1140 (96%)	1002 (92%)	73 (7%)	19 (2%)	9 43
1	D	1094/1140 (96%)	1001 (92%)	72 (7%)	21 (2%)	8 42
1	E	1081/1140 (95%)	993 (92%)	68 (6%)	20 (2%)	8 42
1	F	1085/1140 (95%)	995 (92%)	74 (7%)	16 (2%)	10 45
1	G	1080/1140 (95%)	990 (92%)	72 (7%)	18 (2%)	9 43
1	H	1091/1140 (96%)	996 (91%)	76 (7%)	19 (2%)	9 43
1	I	651/1140 (57%)	601 (92%)	39 (6%)	11 (2%)	9 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	1081/1140 (95%)	991 (92%)	68 (6%)	22 (2%)	7 41
1	K	1081/1140 (95%)	990 (92%)	71 (7%)	20 (2%)	8 42
1	L	891/1140 (78%)	815 (92%)	61 (7%)	15 (2%)	9 43
1	M	1081/1140 (95%)	995 (92%)	71 (7%)	15 (1%)	11 46
1	N	1081/1140 (95%)	982 (91%)	76 (7%)	23 (2%)	7 40
1	O	629/1140 (55%)	580 (92%)	37 (6%)	12 (2%)	8 42
1	P	1081/1140 (95%)	986 (91%)	72 (7%)	23 (2%)	7 40
1	Q	604/1140 (53%)	562 (93%)	35 (6%)	7 (1%)	13 49
1	R	633/1140 (56%)	582 (92%)	39 (6%)	12 (2%)	8 42
All	All	17526/20520 (85%)	16058 (92%)	1152 (7%)	316 (2%)	8 42

5 of 316 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1755	PRO
1	B	892	ALA
1	B	1179	SER
1	C	1755	PRO
1	D	892	ALA

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	836/863 (97%)	802 (96%)	34 (4%)	30 59
1	B	836/863 (97%)	808 (97%)	28 (3%)	38 64
1	C	836/863 (97%)	811 (97%)	25 (3%)	41 66
1	D	836/863 (97%)	809 (97%)	27 (3%)	39 65
1	E	825/863 (96%)	802 (97%)	23 (3%)	43 68
1	F	828/863 (96%)	801 (97%)	27 (3%)	38 64
1	G	824/863 (96%)	802 (97%)	22 (3%)	44 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	831/863 (96%)	809 (97%)	22 (3%)	46 70
1	I	503/863 (58%)	487 (97%)	16 (3%)	39 65
1	J	825/863 (96%)	795 (96%)	30 (4%)	35 63
1	K	825/863 (96%)	800 (97%)	25 (3%)	41 66
1	L	674/863 (78%)	653 (97%)	21 (3%)	40 65
1	M	825/863 (96%)	803 (97%)	22 (3%)	44 69
1	N	825/863 (96%)	795 (96%)	30 (4%)	35 63
1	O	483/863 (56%)	467 (97%)	16 (3%)	38 64
1	P	825/863 (96%)	796 (96%)	29 (4%)	36 63
1	Q	464/863 (54%)	452 (97%)	12 (3%)	46 70
1	R	490/863 (57%)	478 (98%)	12 (2%)	49 71
All	All	13391/15534 (86%)	12970 (97%)	421 (3%)	40 65

5 of 421 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1128	LEU
1	J	1393	GLN
1	P	1712	LEU
1	H	1400	CYS
1	I	1438	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	1597	GLN
1	J	1459	ASN
1	P	1633	ASN
1	H	1633	ASN
1	D	1459	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	J	3001	-	45,52,52	0.85	2 (4%)	56,80,80	0.98	4 (7%)
2	NAP	B	3002	-	25,29,52	0.85	0	31,45,80	1.36	3 (9%)
2	NAP	D	3001	-	45,52,52	0.93	2 (4%)	56,80,80	1.11	2 (3%)
2	NAP	F	3001	-	45,52,52	1.15	3 (6%)	56,80,80	1.02	4 (7%)
2	NAP	Q	3001	-	45,52,52	0.98	2 (4%)	56,80,80	0.86	3 (5%)
2	NAP	B	3001	-	45,52,52	0.96	3 (6%)	56,80,80	0.99	3 (5%)
2	NAP	H	3001	-	45,52,52	0.80	1 (2%)	56,80,80	0.85	2 (3%)
2	NAP	C	3001	-	45,52,52	0.84	2 (4%)	56,80,80	0.93	3 (5%)
2	NAP	G	3002	-	25,29,52	0.71	0	31,45,80	1.24	3 (9%)
2	NAP	M	3001	-	45,52,52	0.97	3 (6%)	56,80,80	0.86	2 (3%)
2	NAP	L	3001	-	45,52,52	0.95	2 (4%)	56,80,80	0.87	2 (3%)
2	NAP	P	3002	-	25,29,52	0.78	0	31,45,80	1.29	5 (16%)
2	NAP	N	3001	-	45,52,52	0.98	2 (4%)	56,80,80	0.93	3 (5%)
2	NAP	G	3001	-	45,52,52	0.91	1 (2%)	56,80,80	0.84	2 (3%)
2	NAP	E	3001	-	45,52,52	0.95	3 (6%)	56,80,80	0.79	1 (1%)
2	NAP	A	3001	-	45,52,52	1.04	1 (2%)	56,80,80	1.05	3 (5%)
2	NAP	O	3001	-	45,52,52	1.01	3 (6%)	56,80,80	0.87	1 (1%)
2	NAP	C	3002	-	27,33,52	0.78	0	35,52,80	1.06	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	K	3001	-	45,52,52	1.52	3 (6%)	56,80,80	1.03	4 (7%)
2	NAP	I	3001	-	45,52,52	0.89	1 (2%)	56,80,80	0.92	3 (5%)
2	NAP	A	3002	-	25,29,52	0.74	0	31,45,80	1.14	2 (6%)
2	NAP	M	3002	-	25,29,52	0.94	1 (4%)	31,45,80	1.14	3 (9%)
2	NAP	P	3001	-	45,52,52	0.94	2 (4%)	56,80,80	1.07	3 (5%)
2	NAP	D	3002	-	25,29,52	0.77	0	31,45,80	1.26	5 (16%)
2	NAP	R	3001	-	45,52,52	0.76	1 (2%)	56,80,80	0.91	2 (3%)
2	NAP	F	3002	-	25,29,52	0.76	0	31,45,80	1.24	4 (12%)
2	NAP	N	3002	-	25,29,52	0.91	1 (4%)	31,45,80	1.43	3 (9%)
2	NAP	K	3002	-	25,29,52	0.68	0	31,45,80	1.31	5 (16%)
2	NAP	H	3002	-	25,29,52	0.77	0	31,45,80	1.21	6 (19%)
2	NAP	J	3002	-	25,29,52	0.82	0	31,45,80	1.20	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	J	3001	-	-	4/31/67/67	0/5/5/5
2	NAP	B	3002	-	-	5/11/31/67	0/3/3/5
2	NAP	D	3001	-	-	10/31/67/67	0/5/5/5
2	NAP	F	3001	-	-	11/31/67/67	0/5/5/5
2	NAP	Q	3001	-	-	6/31/67/67	0/5/5/5
2	NAP	B	3001	-	-	9/31/67/67	0/5/5/5
2	NAP	H	3001	-	-	8/31/67/67	0/5/5/5
2	NAP	C	3001	-	-	8/31/67/67	0/5/5/5
2	NAP	G	3002	-	-	4/11/31/67	0/3/3/5
2	NAP	M	3001	-	-	8/31/67/67	0/5/5/5
2	NAP	L	3001	-	-	7/31/67/67	0/5/5/5
2	NAP	P	3002	-	-	5/11/31/67	0/3/3/5
2	NAP	N	3001	-	-	8/31/67/67	0/5/5/5
2	NAP	G	3001	-	-	7/31/67/67	0/5/5/5
2	NAP	E	3001	-	-	10/31/67/67	0/5/5/5
2	NAP	A	3001	-	-	12/31/67/67	0/5/5/5
2	NAP	O	3001	-	-	11/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	3002	-	-	5/17/37/67	0/3/3/5
2	NAP	K	3001	-	-	12/31/67/67	0/5/5/5
2	NAP	I	3001	-	-	11/31/67/67	0/5/5/5
2	NAP	A	3002	-	-	4/11/31/67	0/3/3/5
2	NAP	M	3002	-	-	4/11/31/67	0/3/3/5
2	NAP	P	3001	-	-	5/31/67/67	0/5/5/5
2	NAP	D	3002	-	-	6/11/31/67	0/3/3/5
2	NAP	R	3001	-	-	10/31/67/67	0/5/5/5
2	NAP	F	3002	-	-	6/11/31/67	0/3/3/5
2	NAP	N	3002	-	-	5/11/31/67	0/3/3/5
2	NAP	K	3002	-	-	5/11/31/67	0/3/3/5
2	NAP	H	3002	-	-	5/11/31/67	0/3/3/5
2	NAP	J	3002	-	-	5/11/31/67	0/3/3/5

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	3001	NAP	C2N-N1N	8.07	1.44	1.35
2	F	3001	NAP	C2N-N1N	5.28	1.41	1.35
2	Q	3001	NAP	C2N-N1N	4.89	1.40	1.35
2	A	3001	NAP	C2N-N1N	4.69	1.40	1.35
2	G	3001	NAP	C2N-N1N	4.58	1.40	1.35

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	3001	NAP	O4D-C1D-C2D	-5.01	99.60	106.93
2	A	3001	NAP	O4D-C1D-C2D	-4.39	100.51	106.93
2	P	3001	NAP	O4D-C1D-C2D	-4.37	100.54	106.93
2	N	3002	NAP	O2B-P2B-O1X	-4.34	92.64	109.39
2	R	3001	NAP	O4D-C1D-C2D	-4.27	100.68	106.93

There are no chirality outliers.

5 of 216 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	3001	NAP	C2B-O2B-P2B-O1X
2	J	3001	NAP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
2	B	3002	NAP	C5B-O5B-PA-O1A
2	B	3002	NAP	C5B-O5B-PA-O2A
2	B	3002	NAP	C5B-O5B-PA-O3

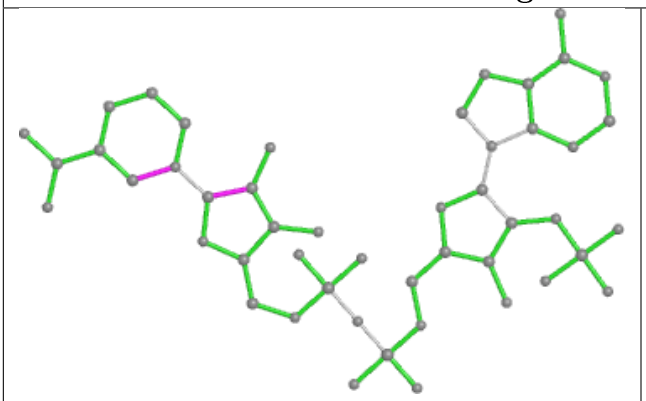
There are no ring outliers.

10 monomers are involved in 15 short contacts:

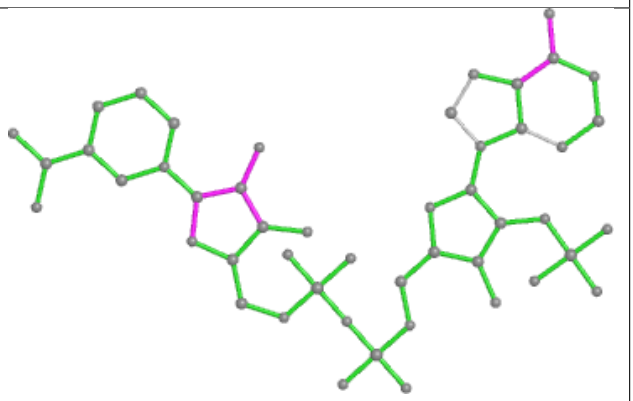
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3001	NAP	2	0
2	F	3001	NAP	2	0
2	B	3001	NAP	2	0
2	C	3001	NAP	1	0
2	L	3001	NAP	1	0
2	E	3001	NAP	1	0
2	A	3001	NAP	2	0
2	O	3001	NAP	1	0
2	K	3001	NAP	2	0
2	I	3001	NAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

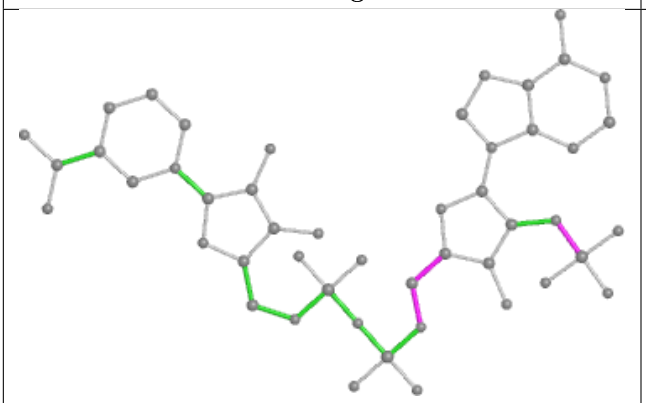
Ligand NAP J 3001



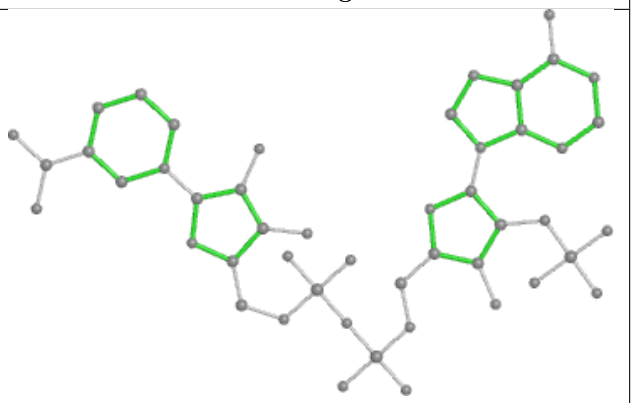
Bond lengths



Bond angles

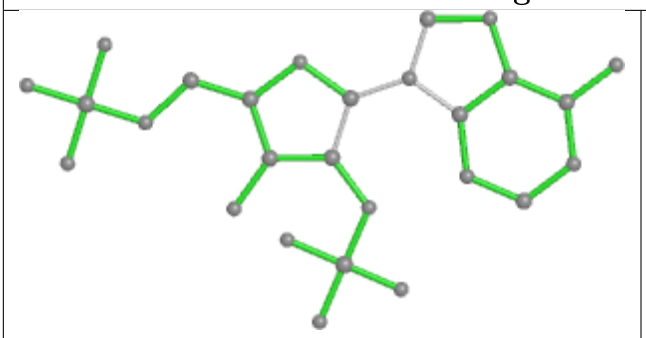


Torsions

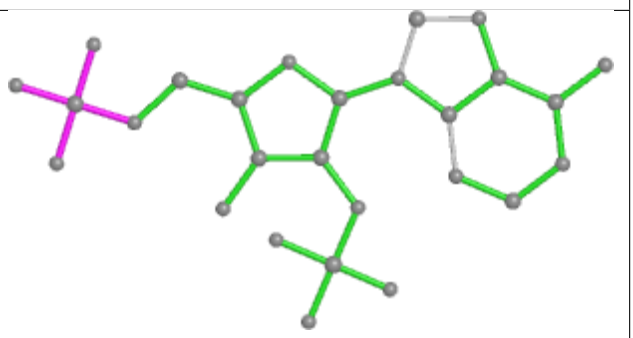


Rings

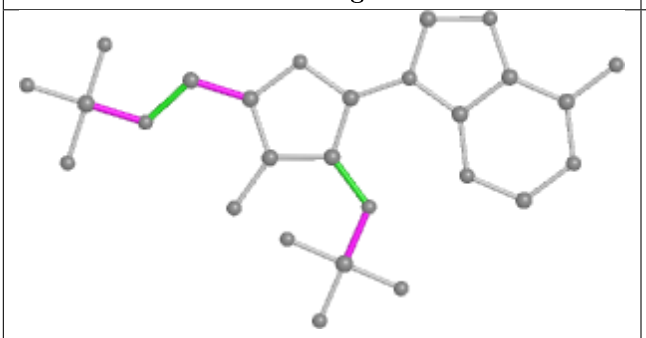
Ligand NAP B 3002



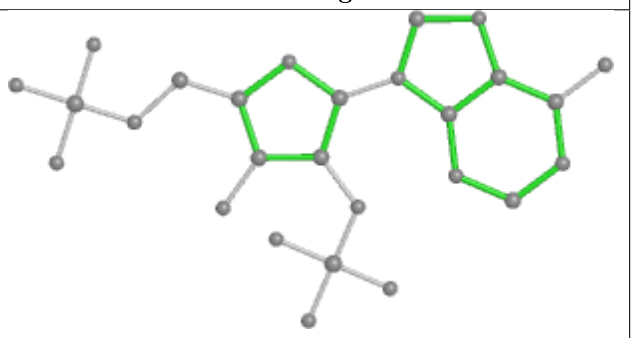
Bond lengths



Bond angles

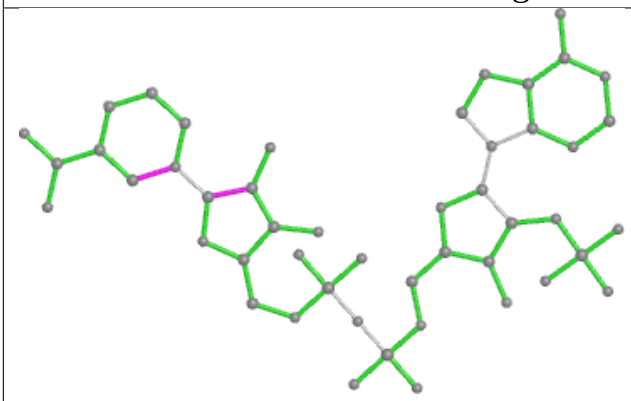


Torsions

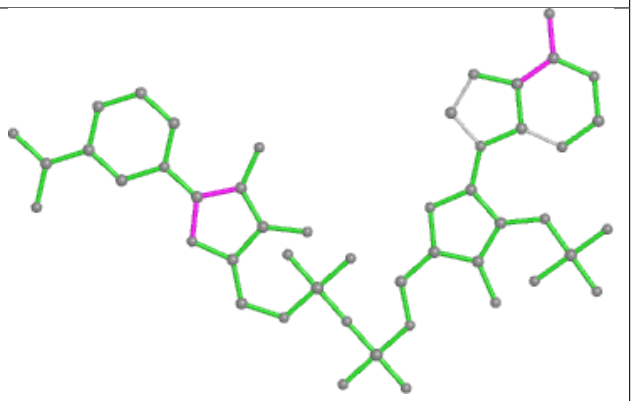


Rings

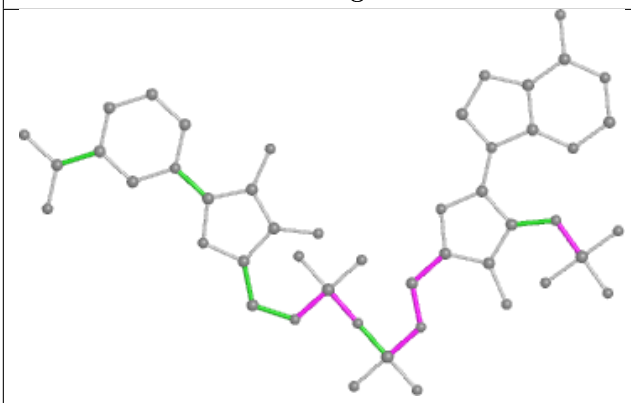
Ligand NAP D 3001



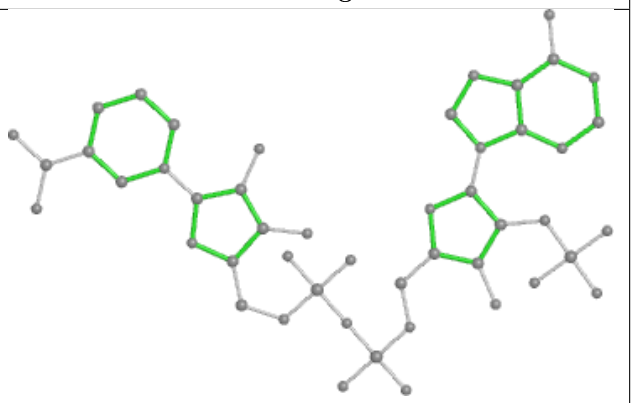
Bond lengths



Bond angles

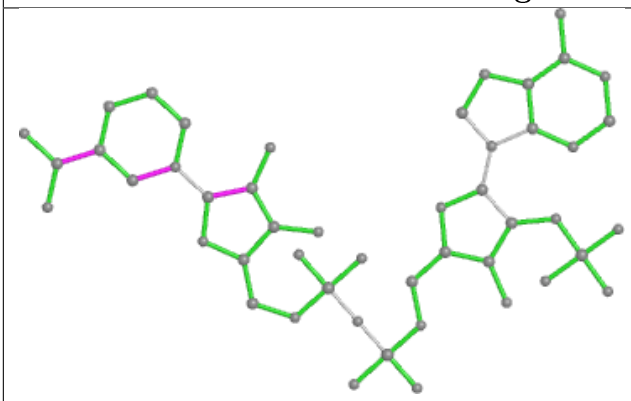


Torsions

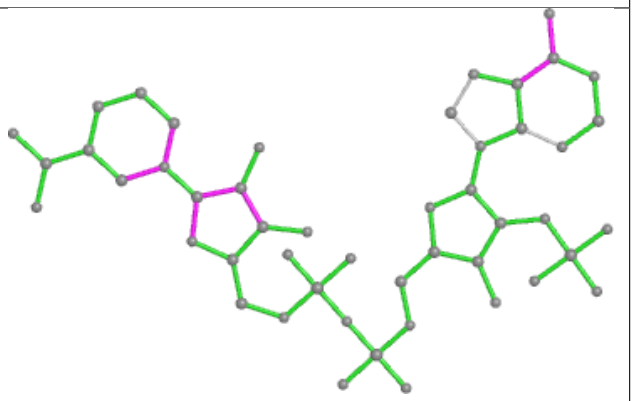


Rings

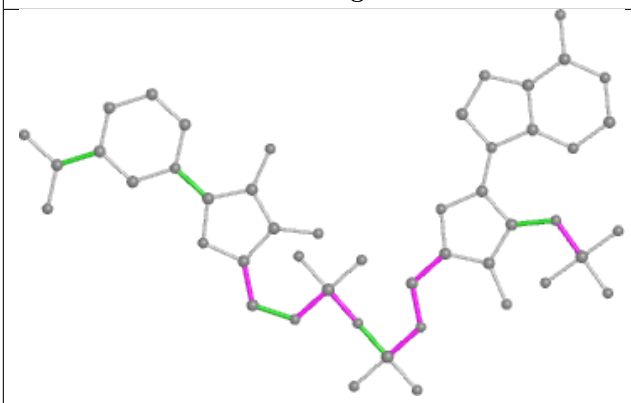
Ligand NAP F 3001



Bond lengths



Bond angles



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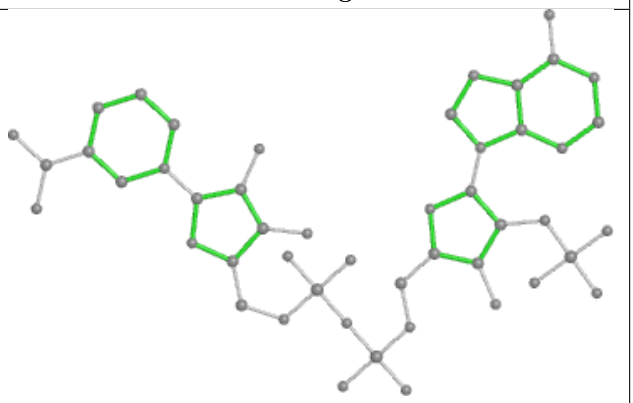
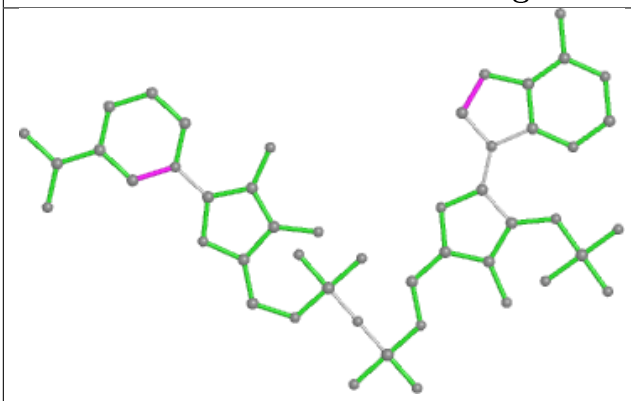
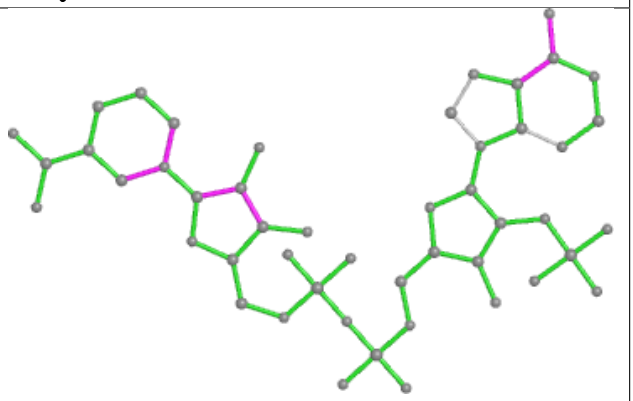


Rings

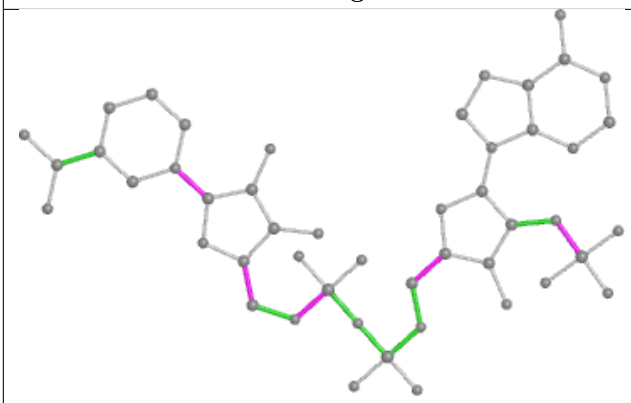
Ligand NAP Q 3001



Bond lengths



Bond angles



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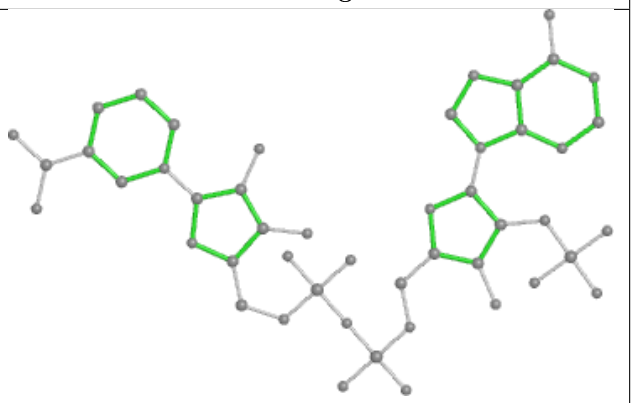
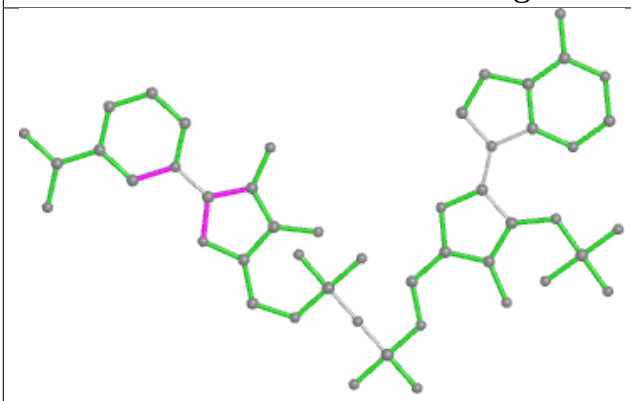
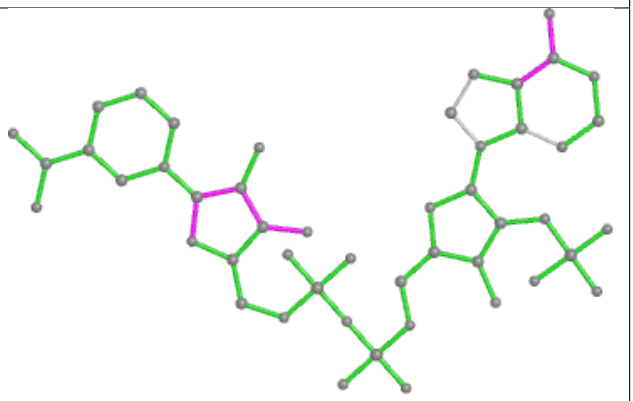


Rings

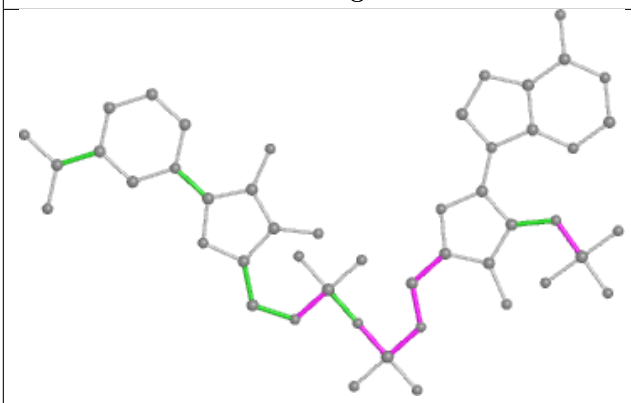
Ligand NAP B 3001



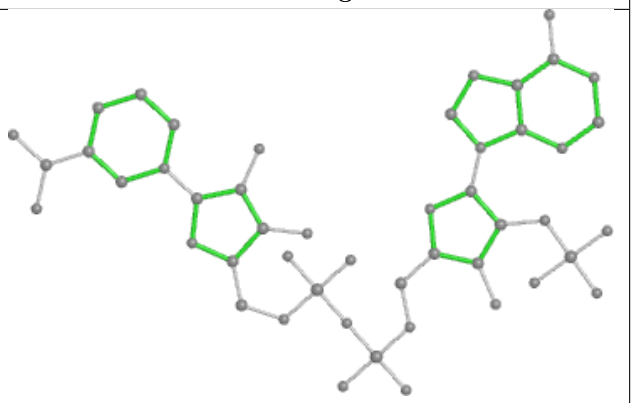
Bond lengths



Bond angles

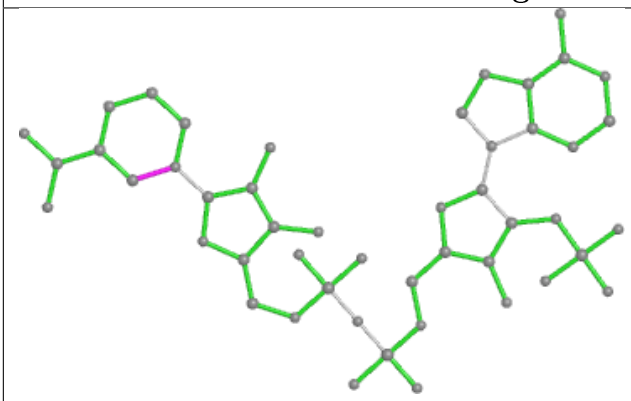


Torsions

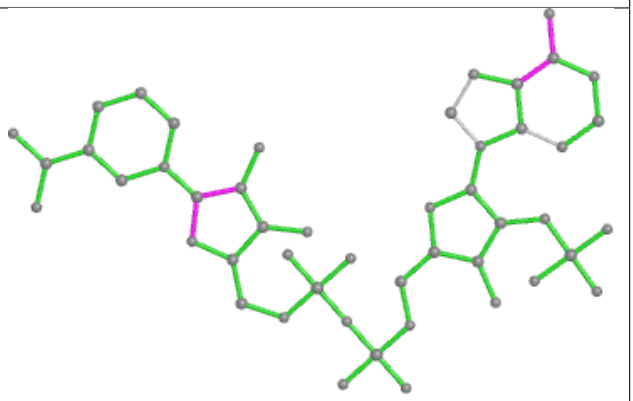


Rings

Ligand NAP H 3001



Bond lengths



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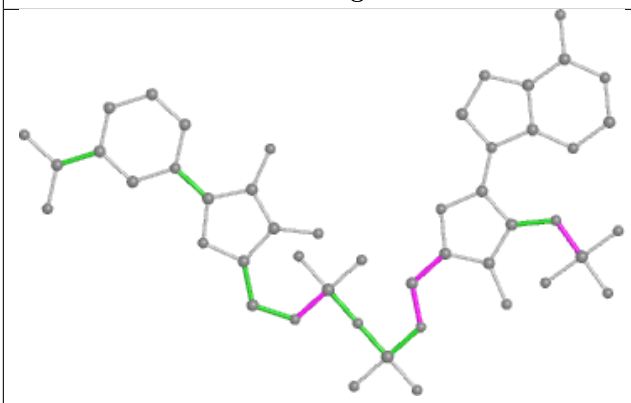

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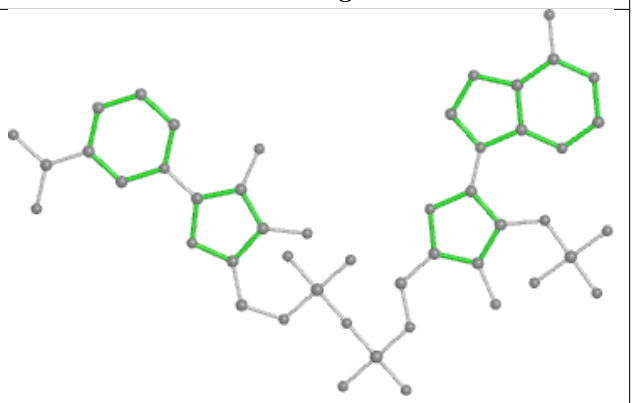
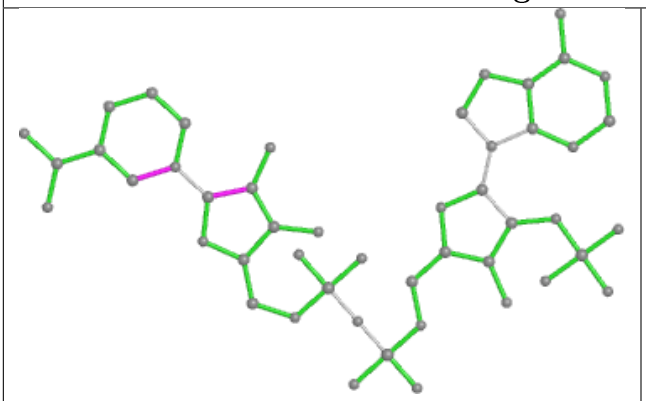
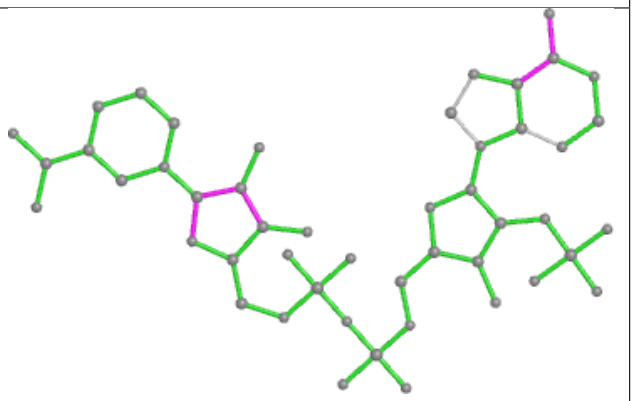


Rings

Ligand NAP C 3001



Bond lengths



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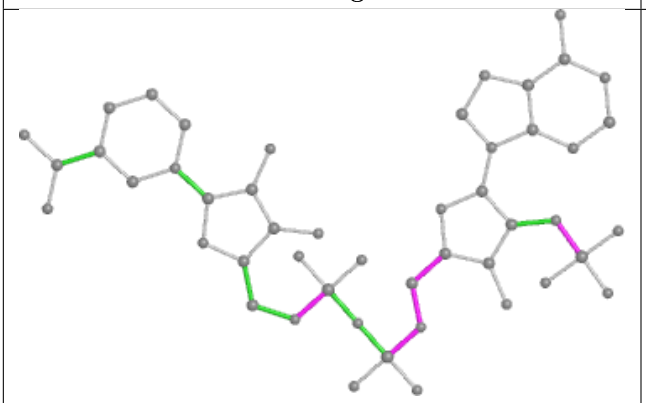
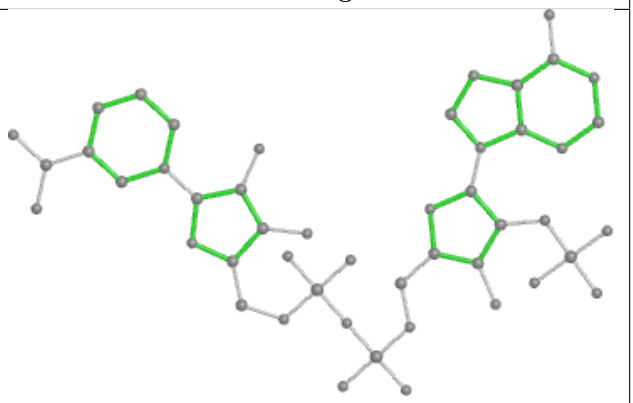
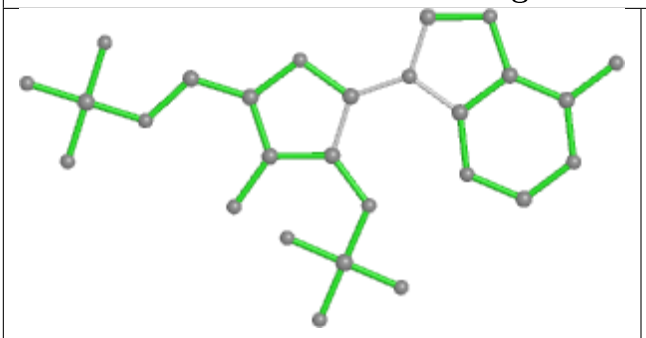


Torsions

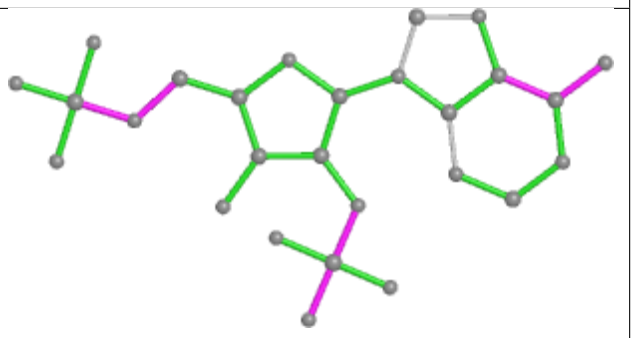


Rings

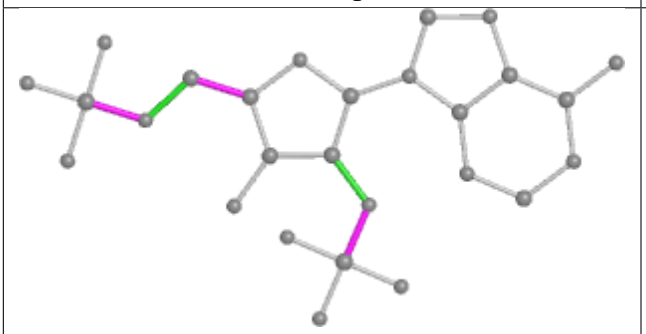
Ligand NAP G 3002



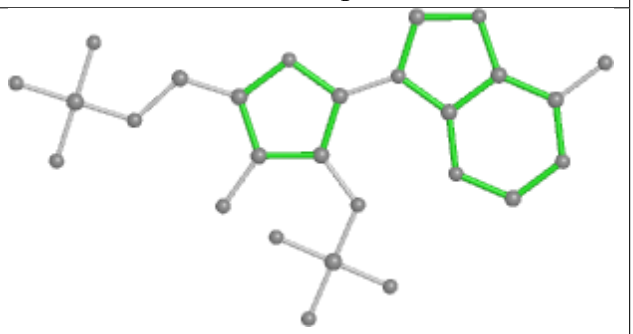
Bond lengths



Bond angles

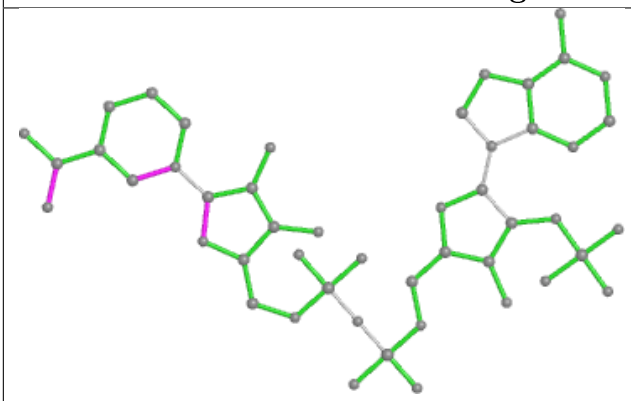


Torsions



Rings

Ligand NAP M 3001



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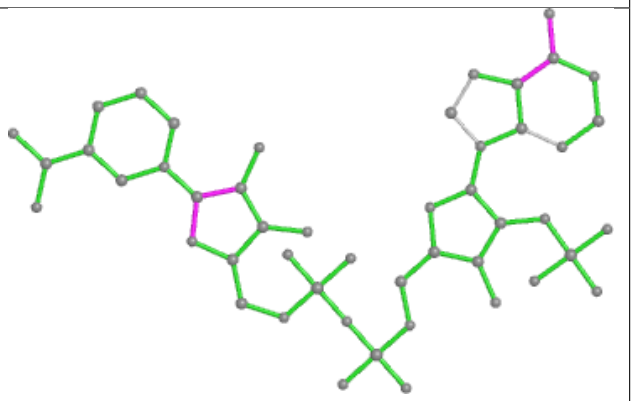
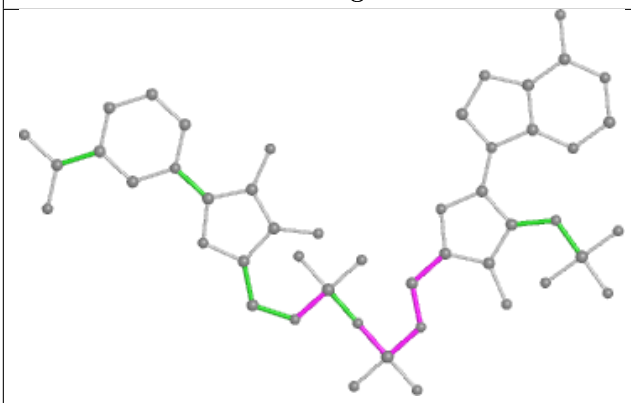


Bond angles



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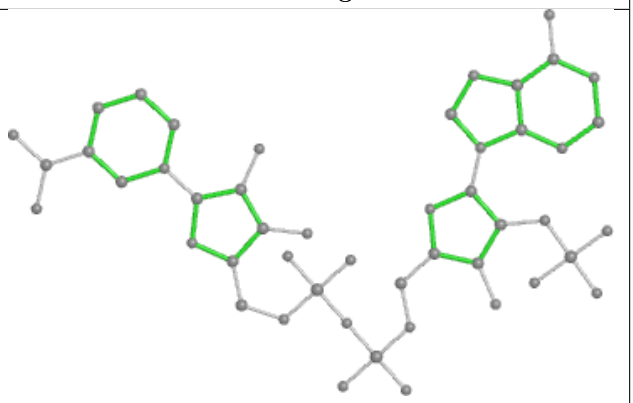
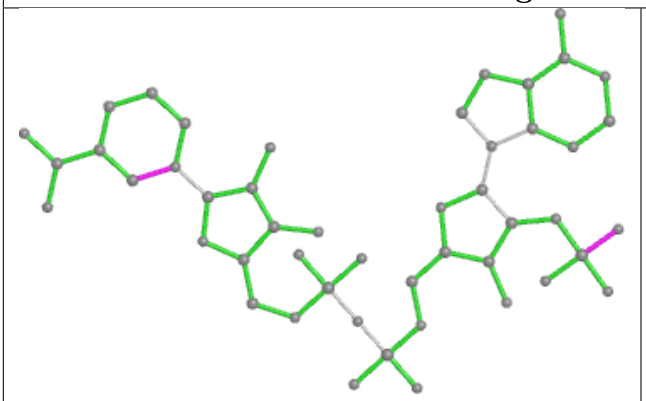


Rings

Ligand NAP L 3001



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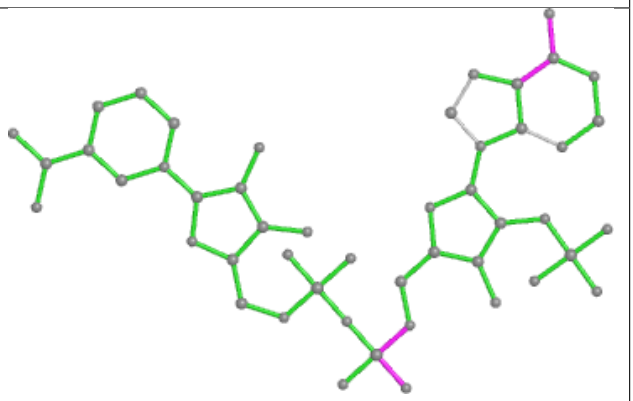

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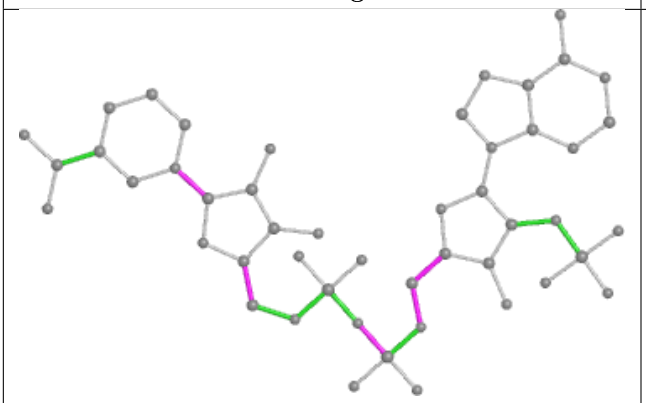

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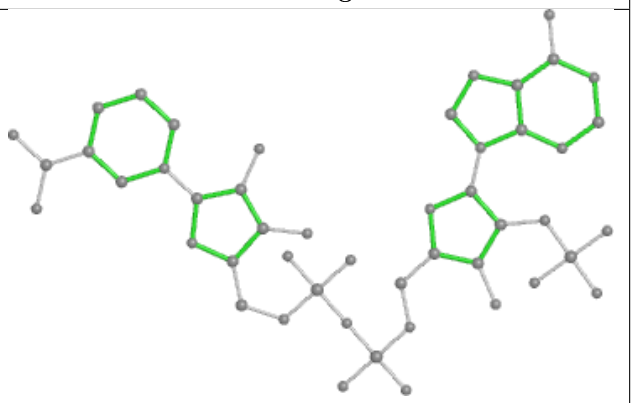
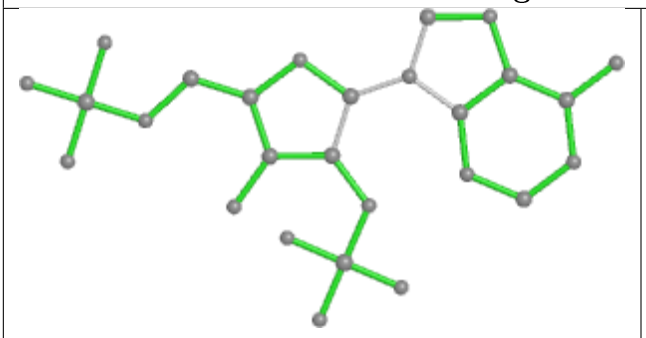


Rings

Ligand NAP P 3002



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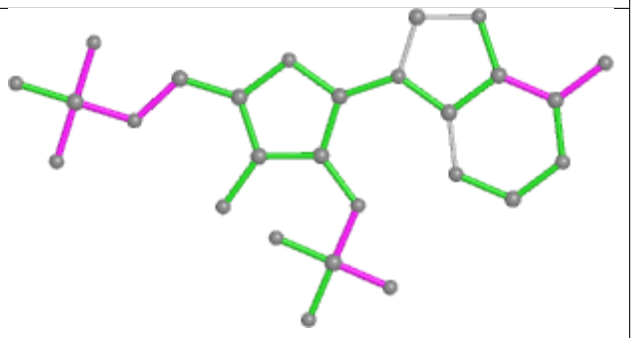

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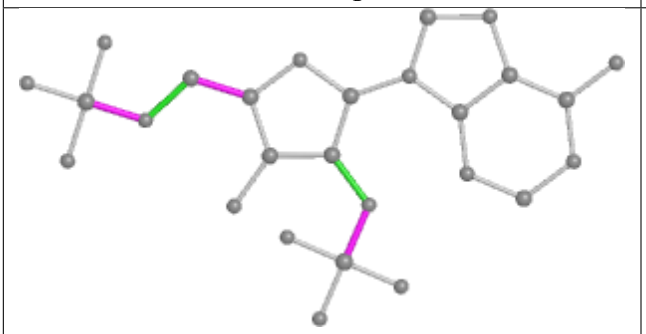

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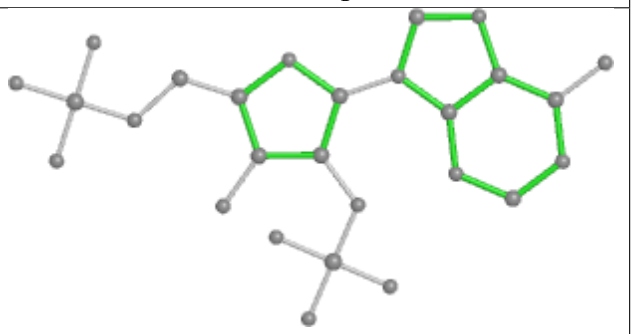
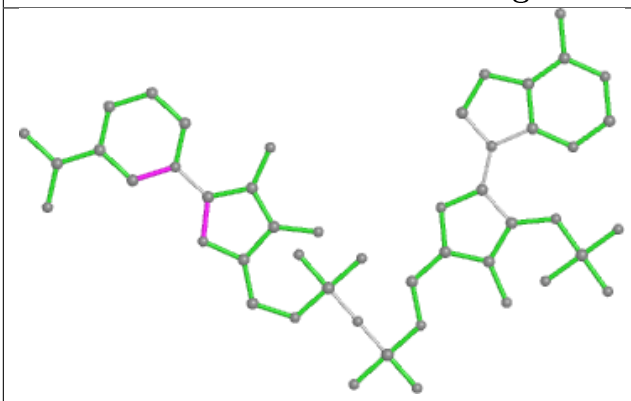


Rings

Ligand NAP N 3001



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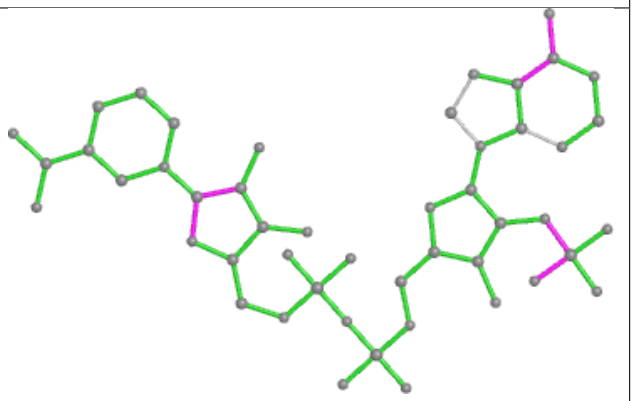
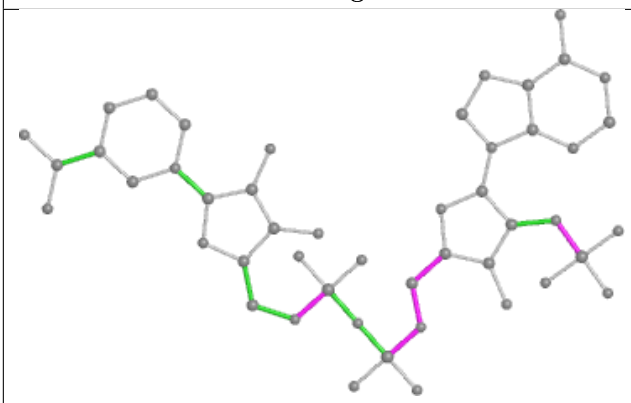


Bond angles



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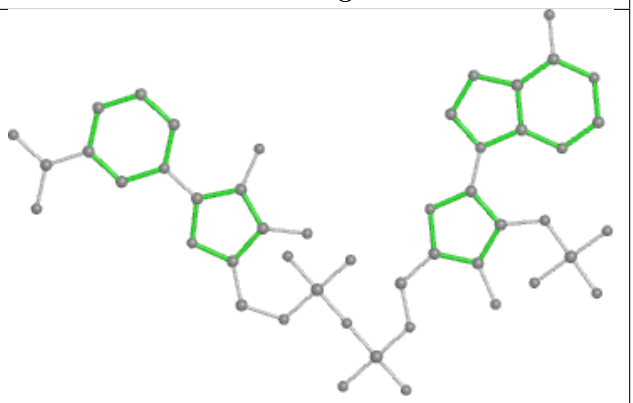
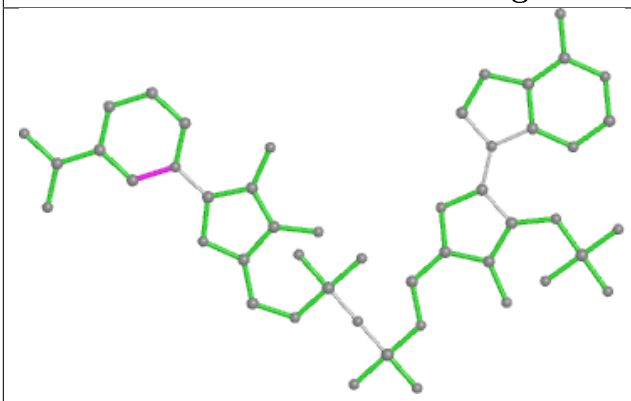


Rings

Ligand NAP G 3001



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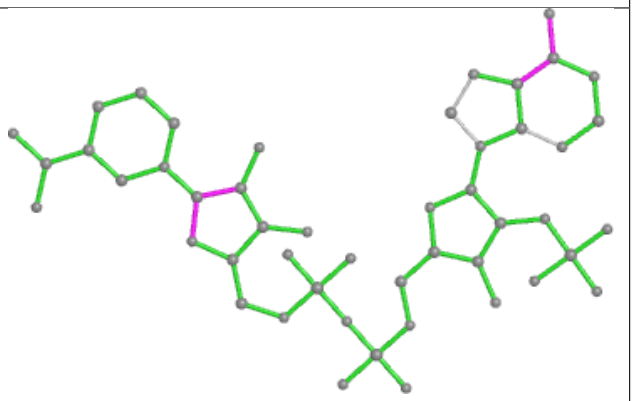
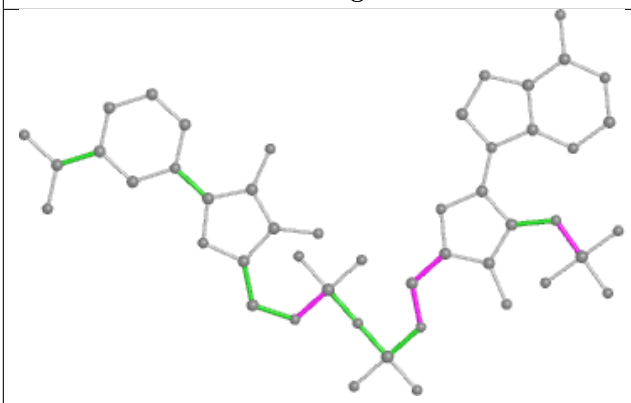


Bond angles



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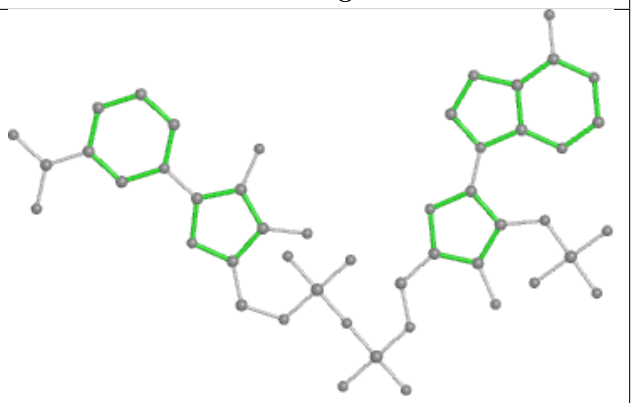
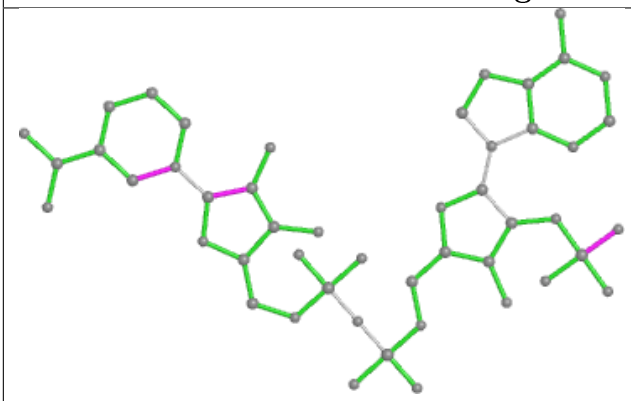


Rings

Ligand NAP E 3001



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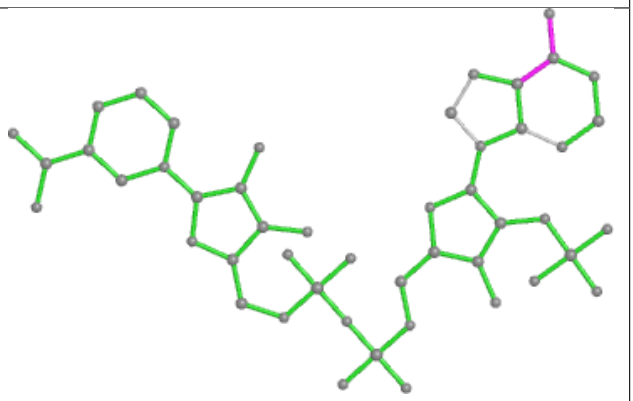
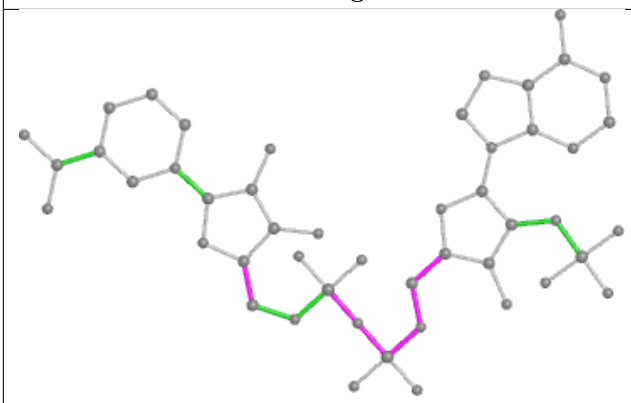


Bond angles



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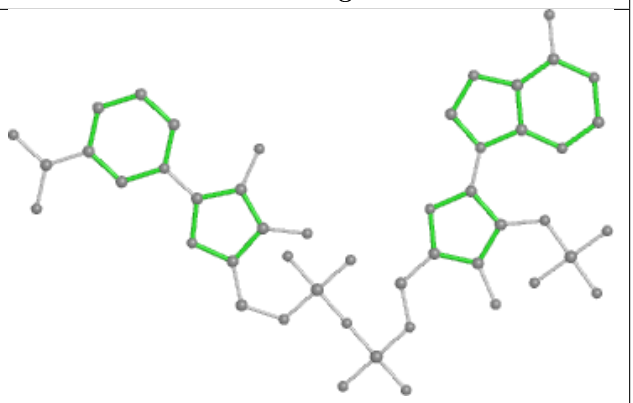
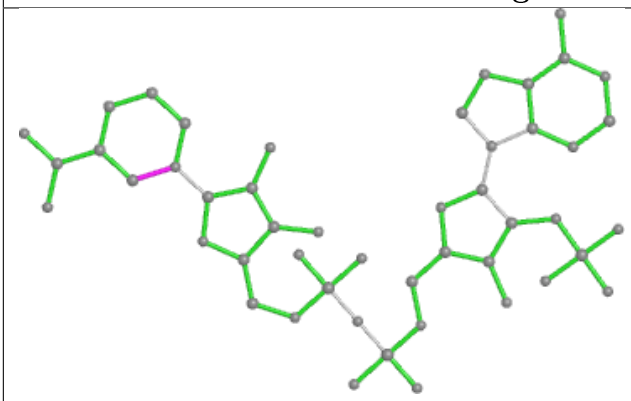


Rings

Ligand NAP A 3001



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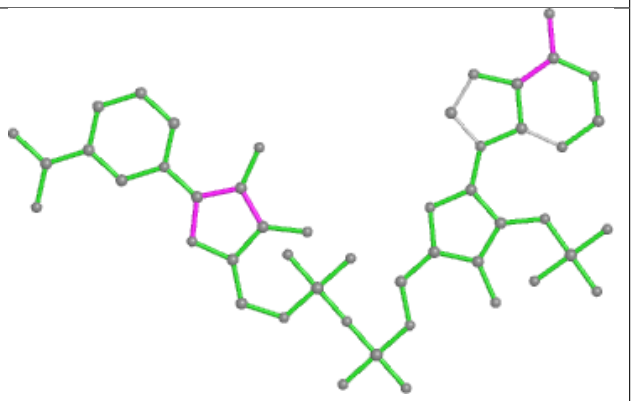
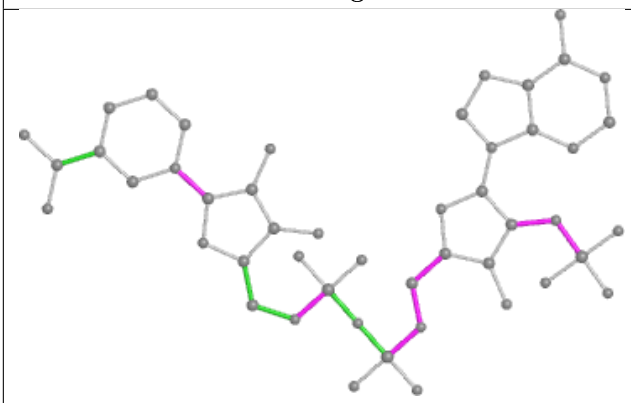


Bond angles



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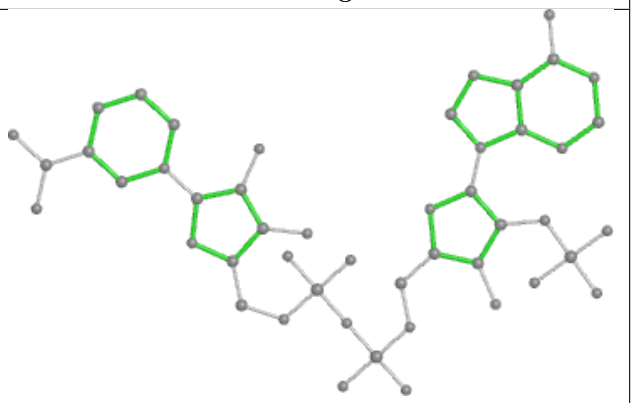
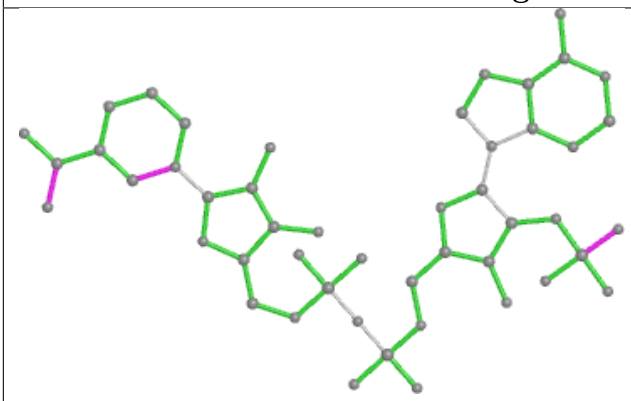


Rings

Ligand NAP O 3001



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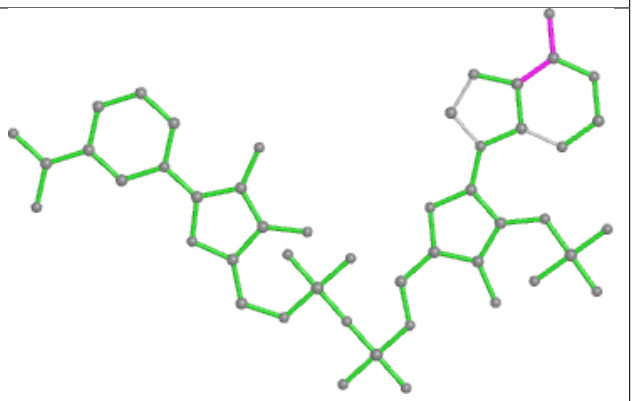
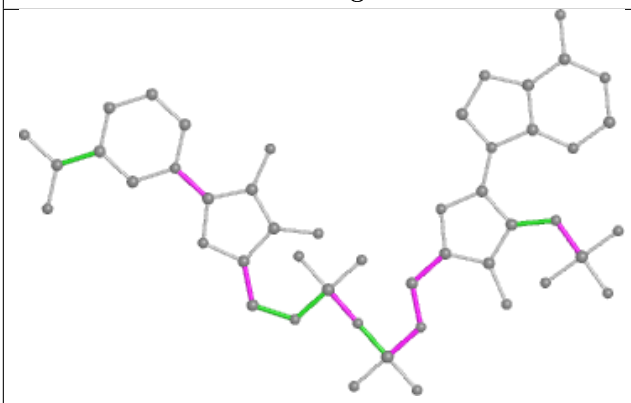


Bond angles



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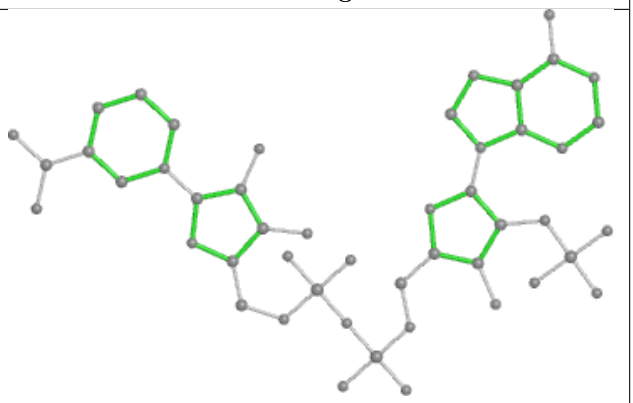
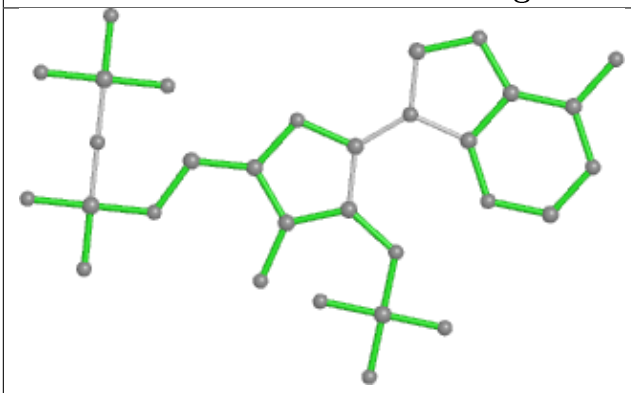


Rings

Ligand NAP C 3002



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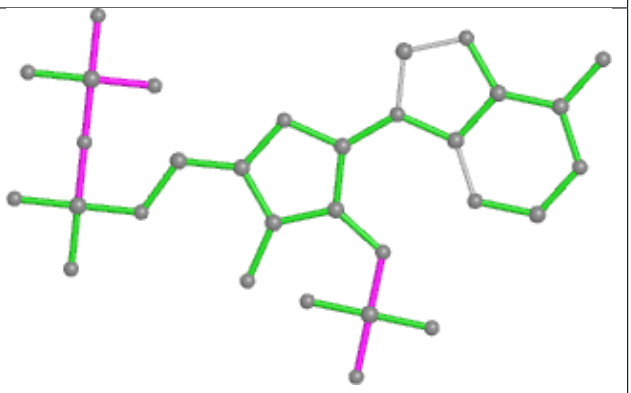
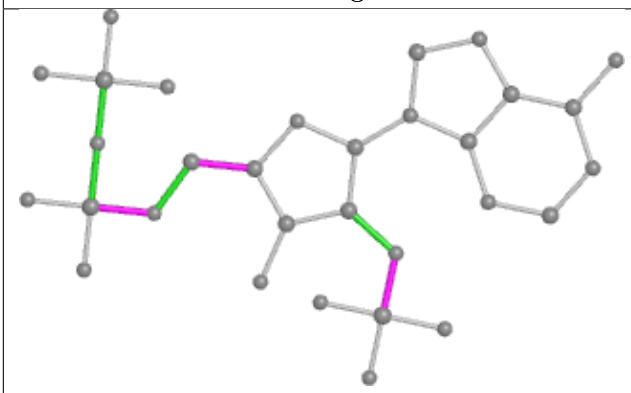
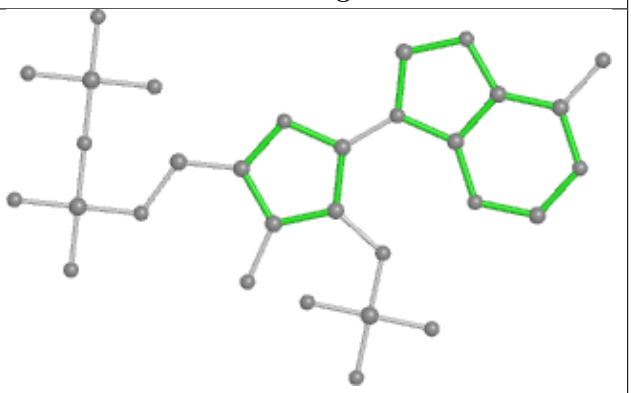


Bond angles

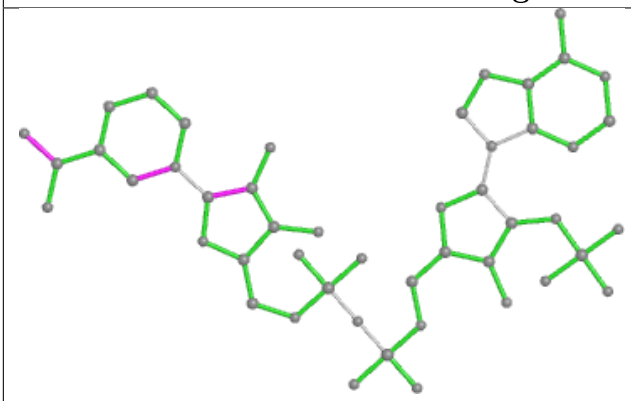


Torsions



Rings

Ligand NAP K 3001



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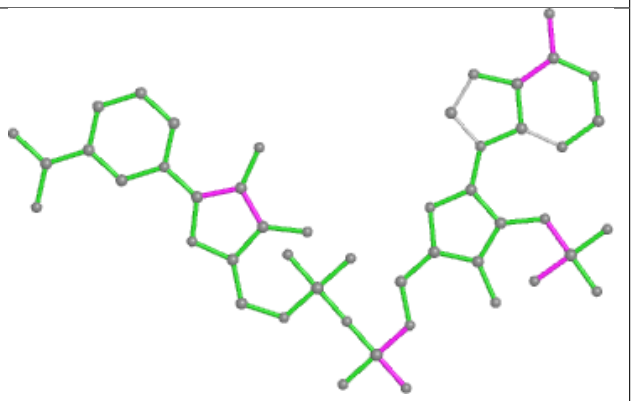
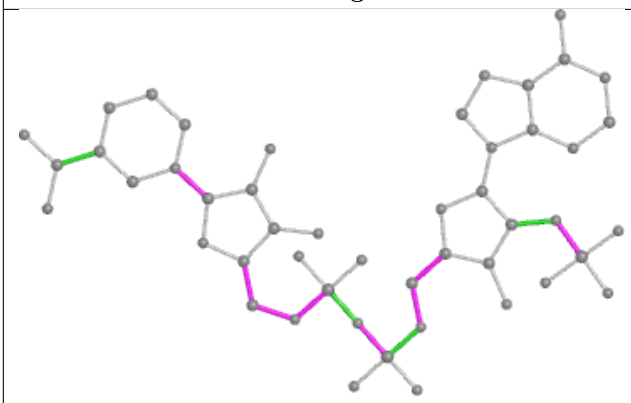


Bond angles



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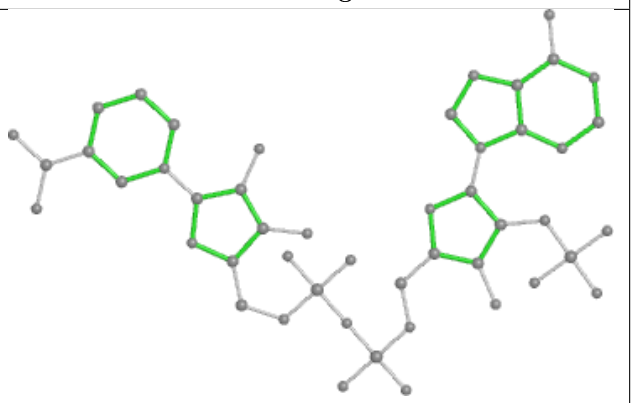
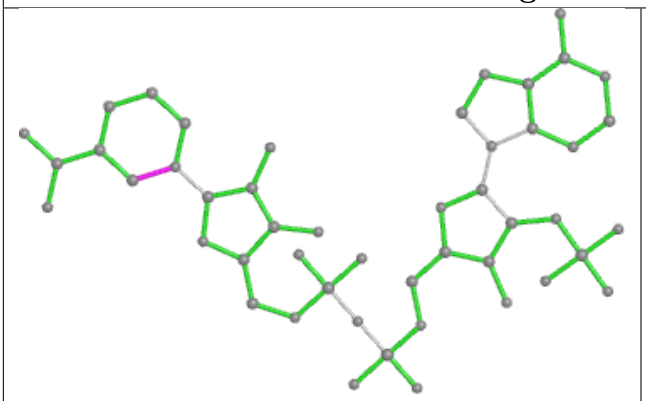


Rings

Ligand NAP I 3001



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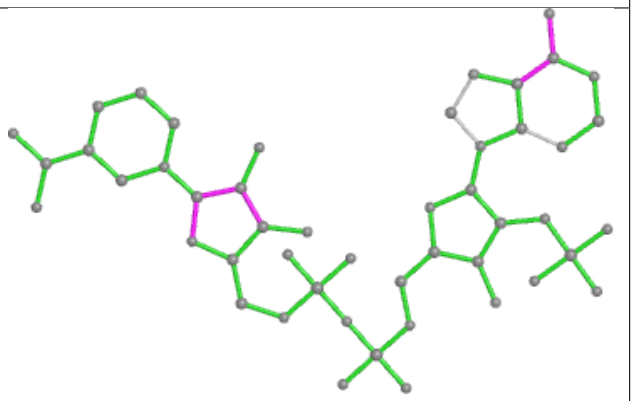
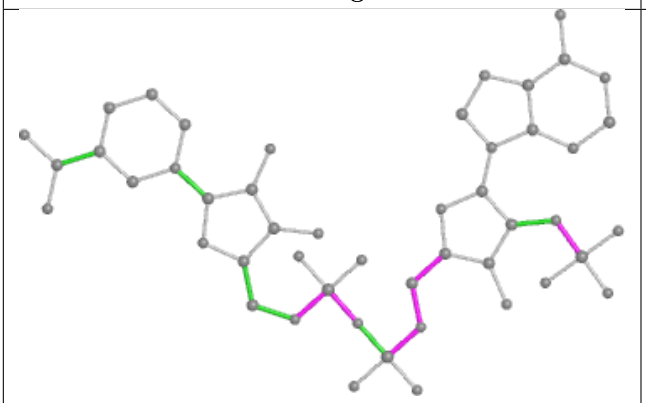


Bond angles



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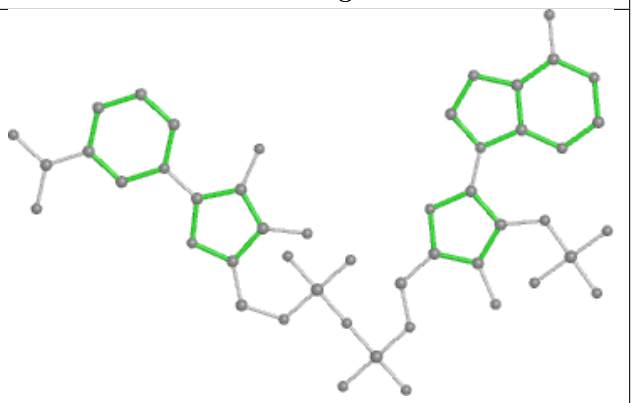
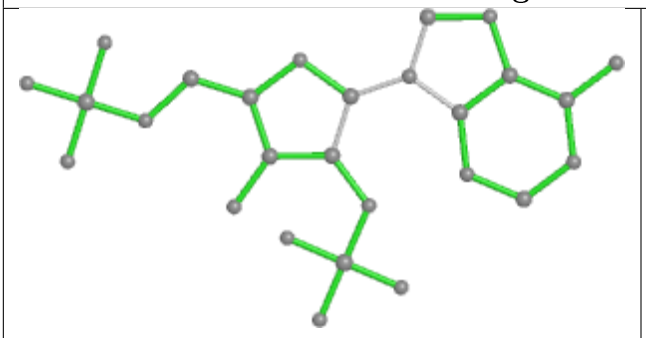


Rings

Ligand NAP A 3002



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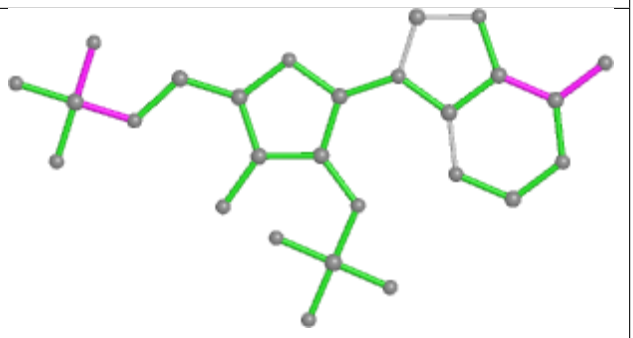
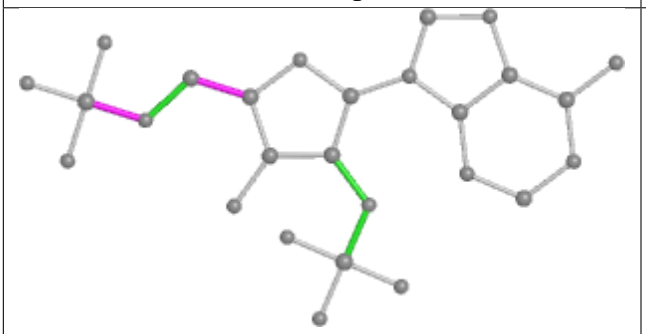
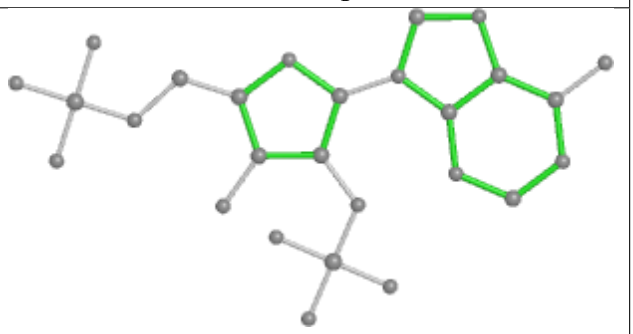


Bond angles

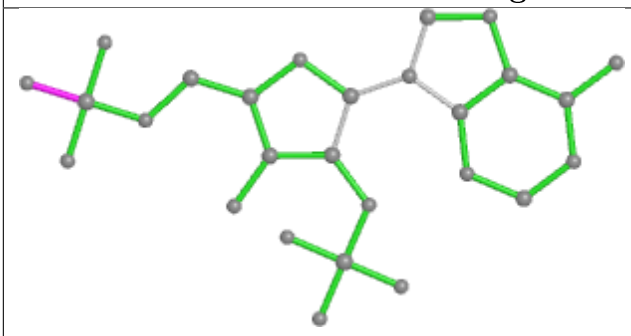


Torsions



Rings

Ligand NAP M 3002



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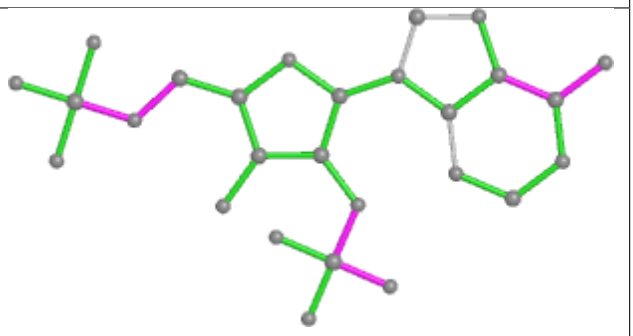
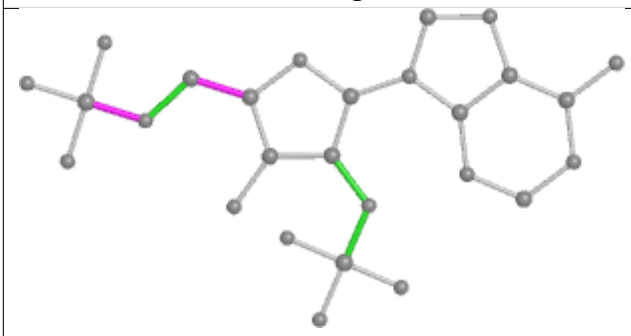
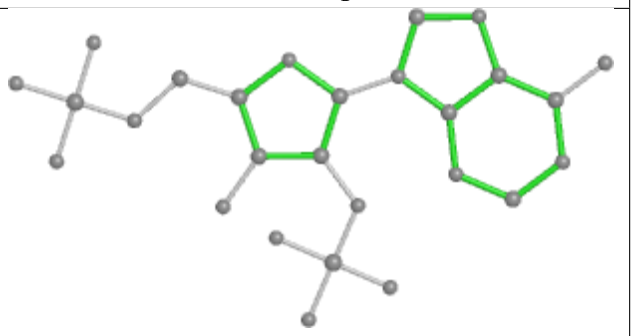


Bond angles

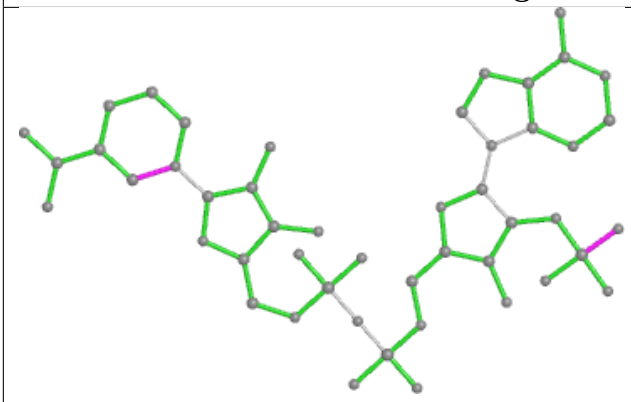


Torsions



Rings

Ligand NAP P 3001



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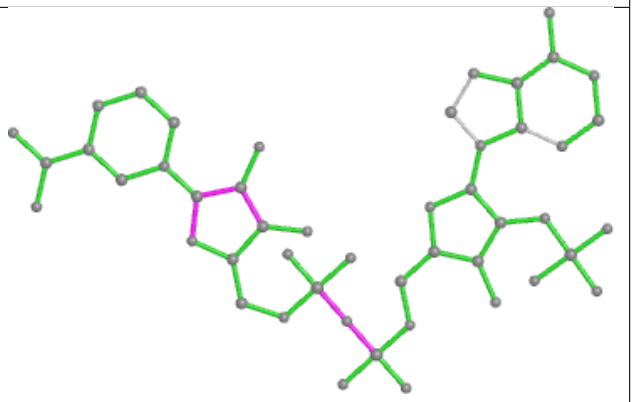
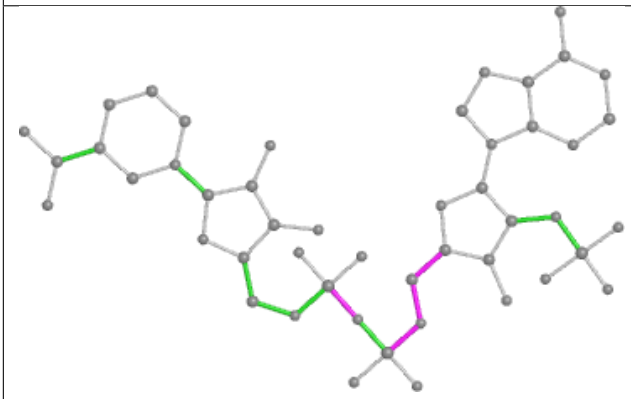
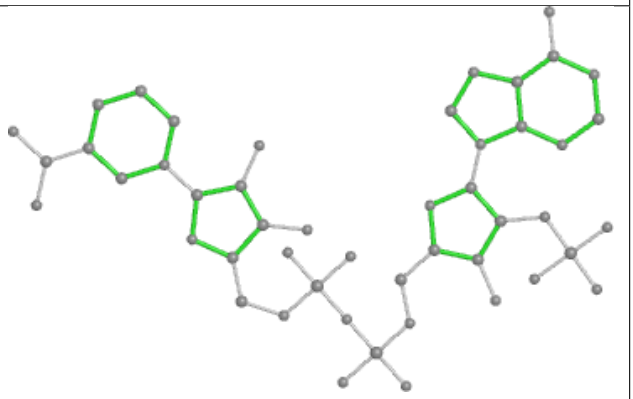


Bond angles

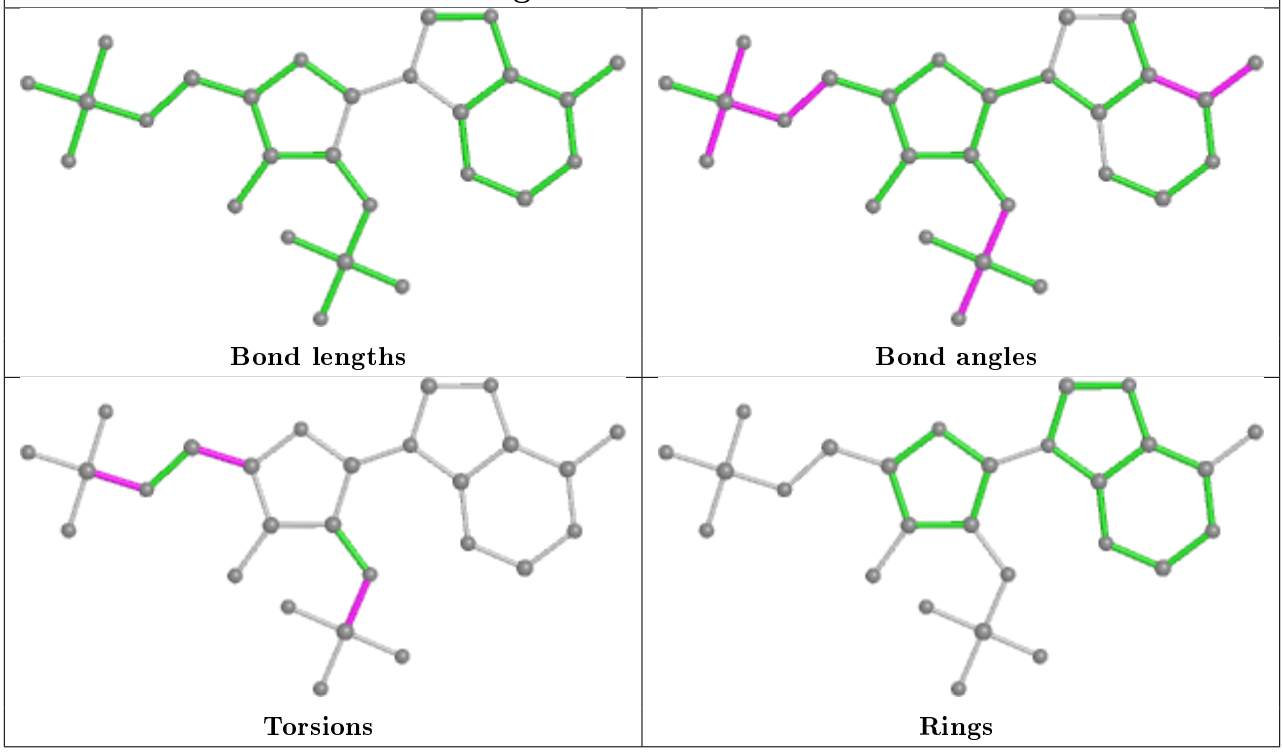


Torsions

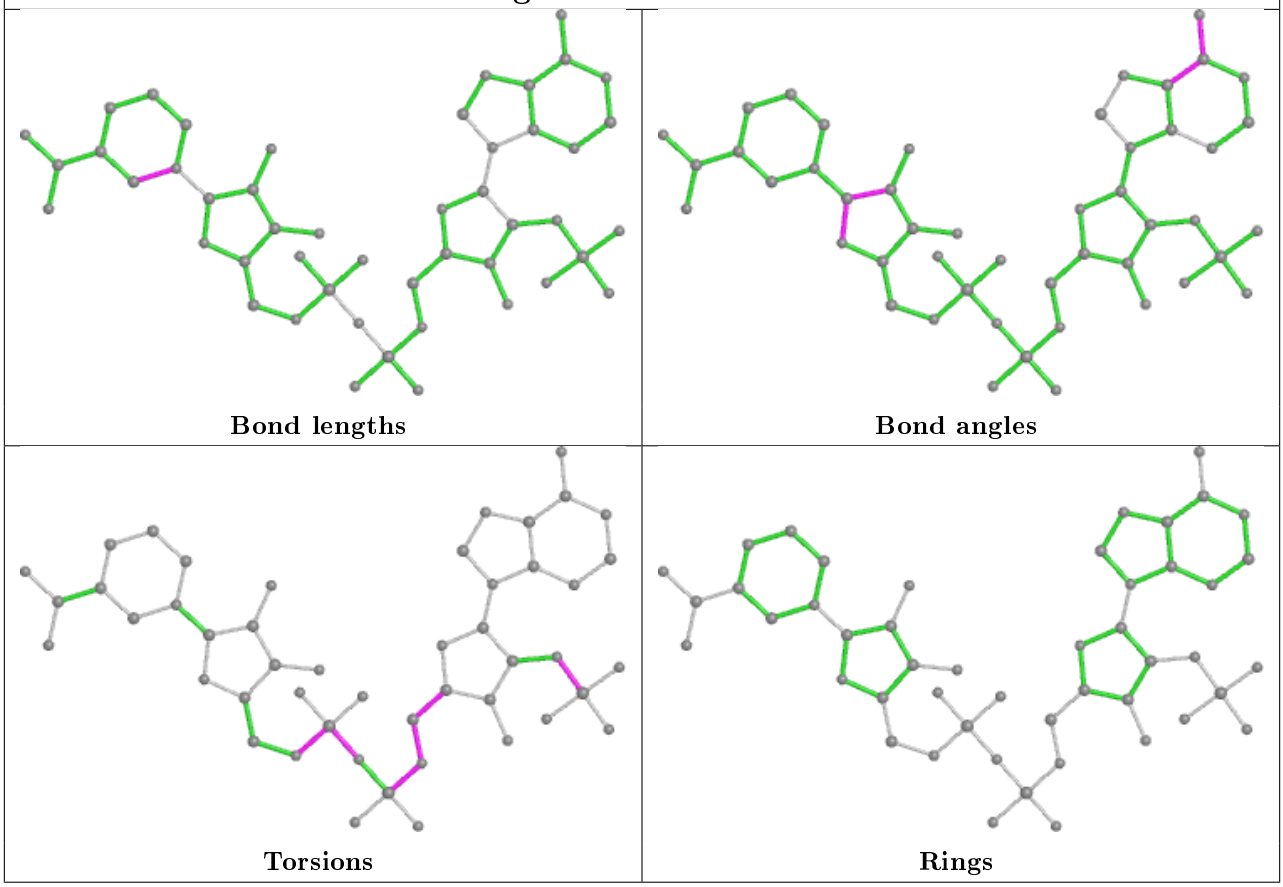


Rings

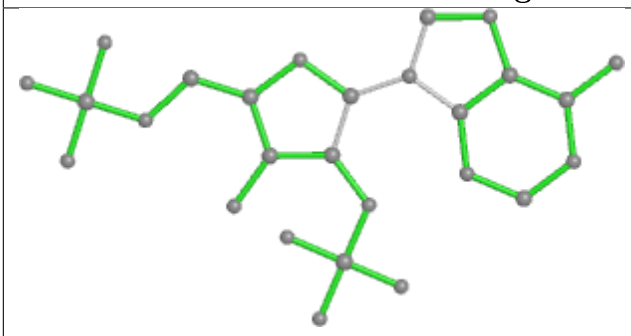
Ligand NAP D 3002



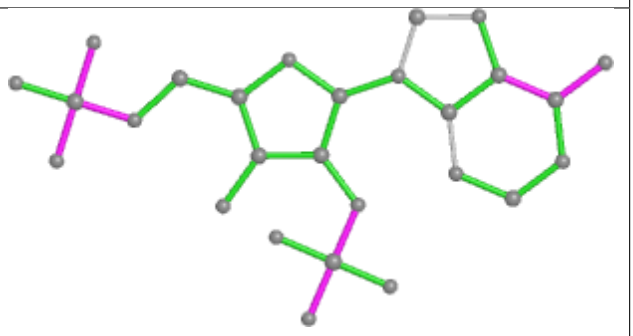
Ligand NAP R 3001



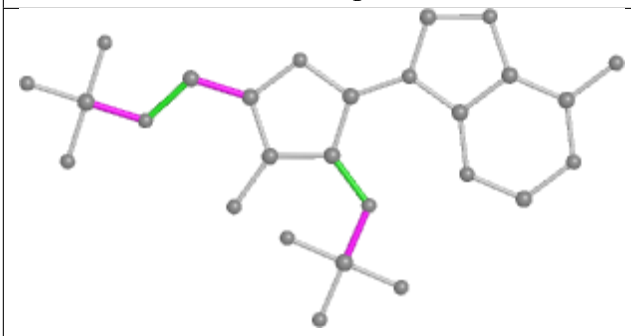
Ligand NAP F 3002



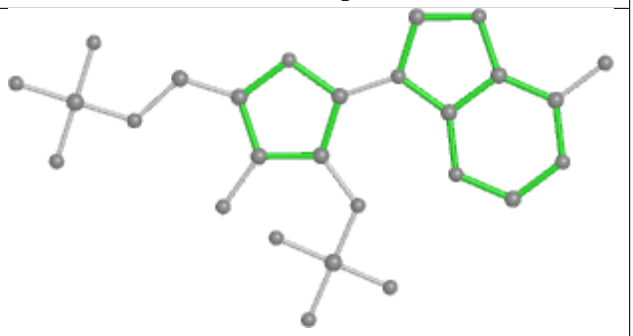
Bond lengths



Bond angles

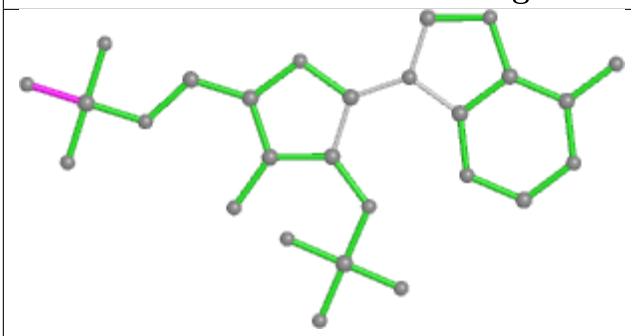


Torsions

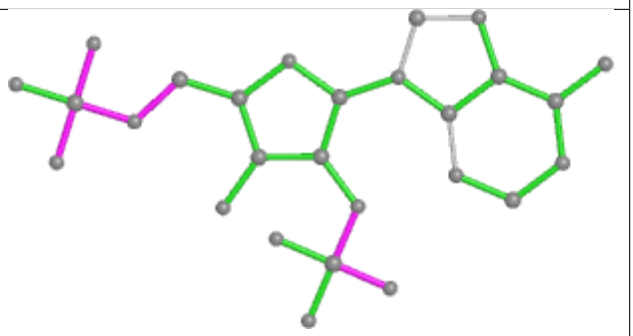


Rings

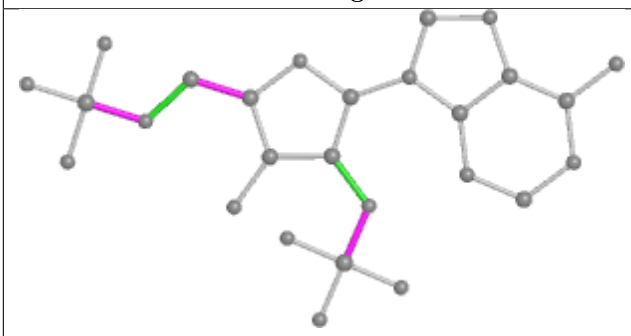
Ligand NAP N 3002



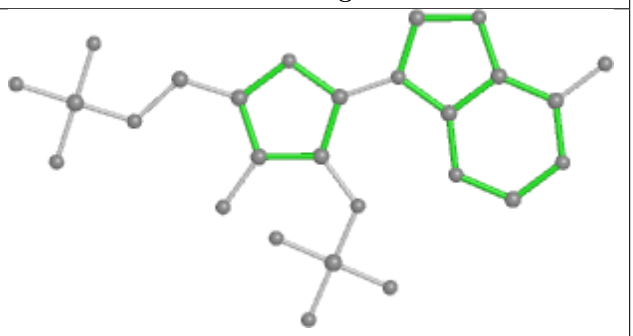
Bond lengths



Bond angles

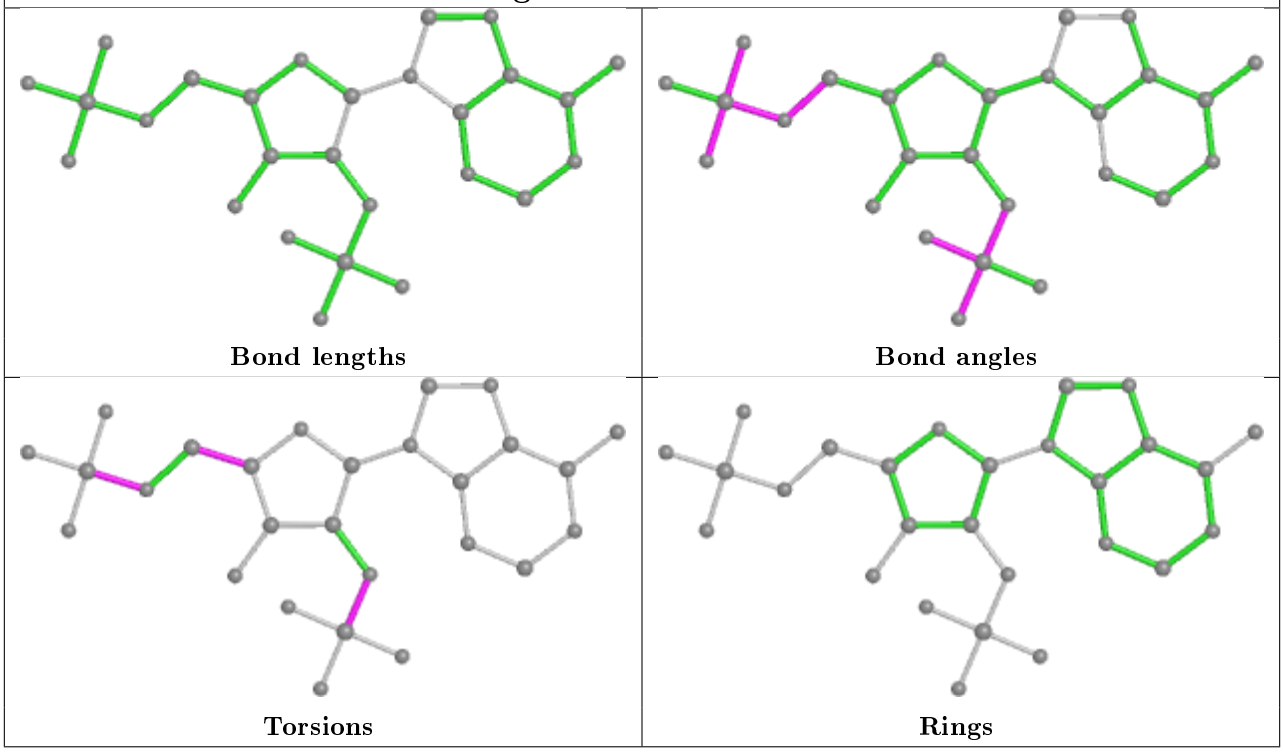


Torsions

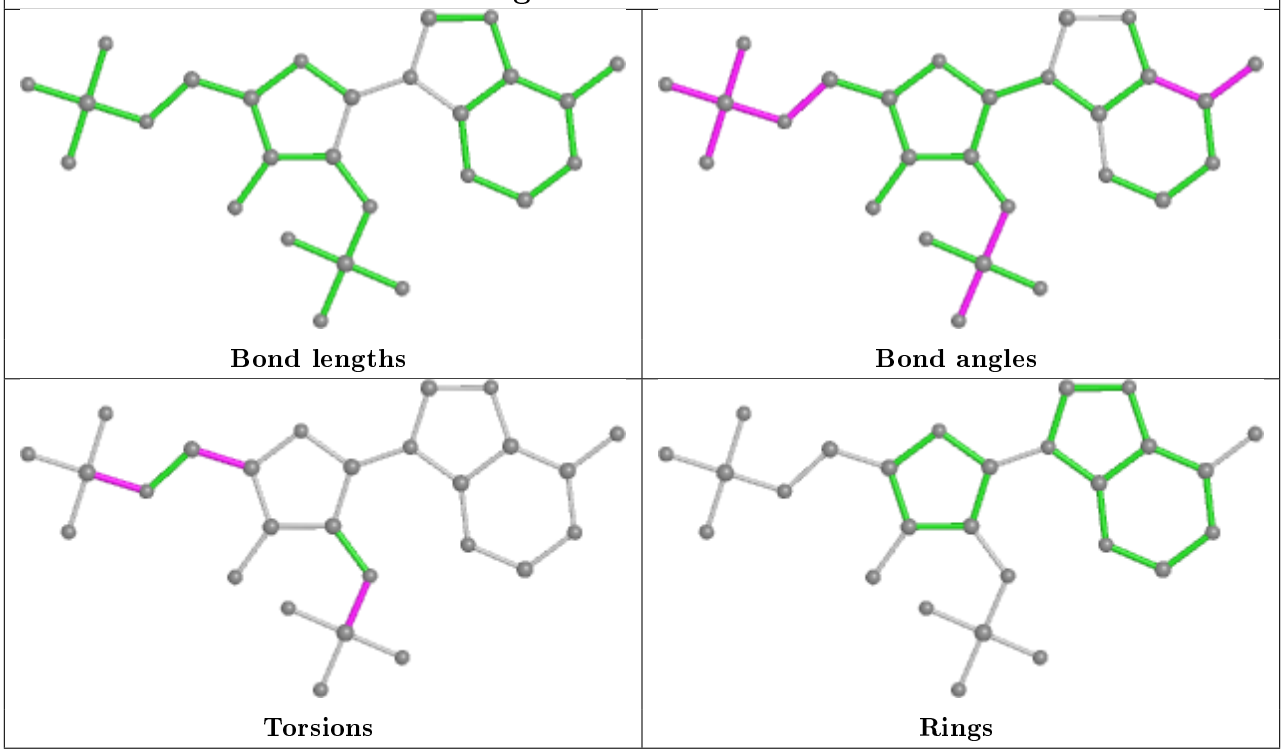


Rings

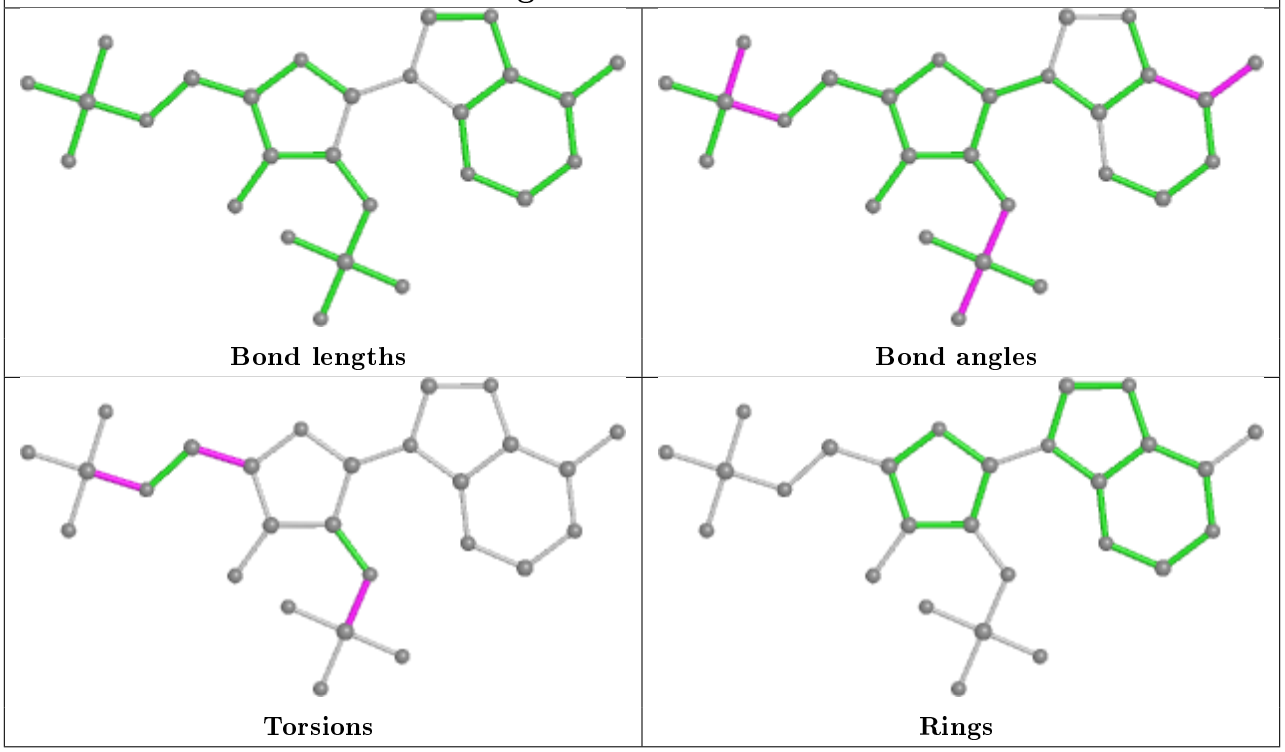
Ligand NAP K 3002



Ligand NAP H 3002



Ligand NAP J 3002



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	1102/1140 (96%)	0.77	114 (10%) 6 6	84, 166, 265, 278	0
1	B	1102/1140 (96%)	0.61	52 (4%) 31 28	85, 136, 221, 240	0
1	C	1102/1140 (96%)	0.66	95 (8%) 10 9	89, 162, 233, 261	0
1	D	1102/1140 (96%)	0.70	108 (9%) 7 6	92, 173, 262, 282	0
1	E	1089/1140 (95%)	1.14	245 (22%) 0 0	127, 204, 264, 278	0
1	F	1093/1140 (95%)	0.97	184 (16%) 1 1	125, 193, 236, 259	0
1	G	1088/1140 (95%)	0.82	154 (14%) 2 3	108, 174, 224, 261	0
1	H	1097/1140 (96%)	0.85	161 (14%) 2 2	113, 180, 220, 255	0
1	I	655/1140 (57%)	0.80	67 (10%) 6 6	96, 167, 220, 254	0
1	J	1089/1140 (95%)	0.68	81 (7%) 14 12	95, 166, 213, 252	0
1	K	1089/1140 (95%)	0.68	76 (6%) 16 13	85, 138, 187, 226	0
1	L	897/1140 (78%)	1.13	149 (16%) 1 1	81, 145, 244, 264	0
1	M	1089/1140 (95%)	1.06	208 (19%) 1 1	111, 175, 239, 265	0
1	N	1089/1140 (95%)	0.66	92 (8%) 11 10	107, 157, 205, 254	0
1	O	633/1140 (55%)	0.69	39 (6%) 20 17	84, 131, 183, 222	0
1	P	1089/1140 (95%)	0.72	96 (8%) 10 8	85, 150, 211, 247	0
1	Q	608/1140 (53%)	1.75	198 (32%) 0 0	180, 229, 263, 279	0
1	R	637/1140 (55%)	1.10	139 (21%) 0 0	158, 210, 247, 266	0
All	All	17650/20520 (86%)	0.85	2258 (12%) 3 4	81, 170, 243, 282	0

The worst 5 of 2258 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	1074	THR	18.0
1	L	1871	ASP	17.2
1	Q	1073	PRO	13.5

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Mol	Chain	Res	Type	RSRZ
1	Q	943	PRO	13.2
1	Q	942	LEU	12.6

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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	M	3002	27/48	0.54	0.28	233,235,240,240	0
2	NAP	N	3002	27/48	0.59	0.26	156,165,181,182	0
2	NAP	A	3002	27/48	0.61	0.26	229,235,241,242	0
2	NAP	Q	3001	48/48	0.61	0.40	222,225,232,235	0
2	NAP	P	3002	27/48	0.61	0.21	191,203,209,210	0
2	NAP	H	3002	27/48	0.64	0.30	179,187,190,190	0
2	NAP	F	3002	27/48	0.67	0.28	164,168,171,171	0
2	NAP	D	3002	27/48	0.68	0.28	193,197,199,199	0
2	NAP	J	3002	27/48	0.69	0.30	166,169,175,176	0
2	NAP	G	3002	27/48	0.70	0.20	195,201,205,205	0
2	NAP	C	3002	31/48	0.73	0.27	141,162,203,205	0
2	NAP	K	3002	27/48	0.75	0.31	135,151,159,161	0
2	NAP	R	3001	48/48	0.77	0.23	210,221,233,234	0
2	NAP	B	3002	27/48	0.78	0.29	120,134,148,148	0
2	NAP	E	3001	48/48	0.82	0.35	181,193,197,198	0
2	NAP	H	3001	48/48	0.85	0.32	129,146,170,171	0
2	NAP	F	3001	48/48	0.85	0.33	165,176,183,184	0
2	NAP	I	3001	48/48	0.87	0.33	133,144,150,151	0
2	NAP	M	3001	48/48	0.89	0.36	132,144,158,161	0
2	NAP	N	3001	48/48	0.89	0.32	141,152,175,175	0
2	NAP	G	3001	48/48	0.90	0.31	117,132,158,158	0

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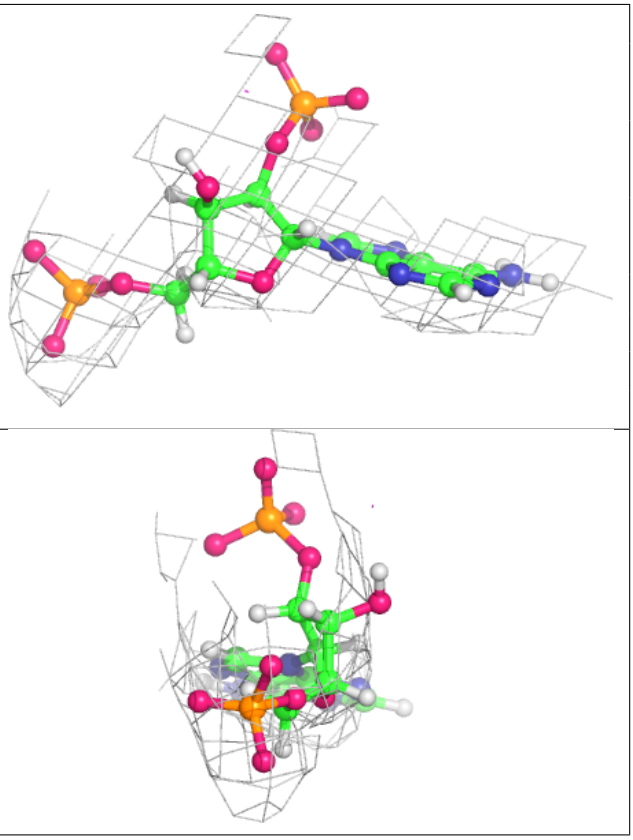
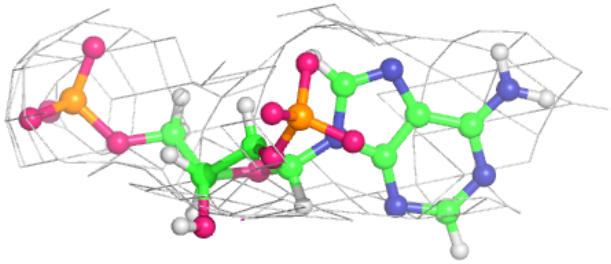
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	D	3001	48/48	0.91	0.31	114,124,138,139	0
2	NAP	C	3001	48/48	0.91	0.33	110,132,150,153	0
2	NAP	L	3001	48/48	0.91	0.37	110,118,130,134	0
2	NAP	O	3001	48/48	0.92	0.35	101,113,135,138	0
2	NAP	B	3001	48/48	0.92	0.34	103,111,127,129	0
2	NAP	J	3001	48/48	0.92	0.30	115,126,149,153	0
2	NAP	A	3001	48/48	0.92	0.35	104,124,136,137	0
2	NAP	P	3001	48/48	0.93	0.33	106,124,132,136	0
2	NAP	K	3001	48/48	0.94	0.34	109,123,141,145	0

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

Electron density around NAP M 3002:

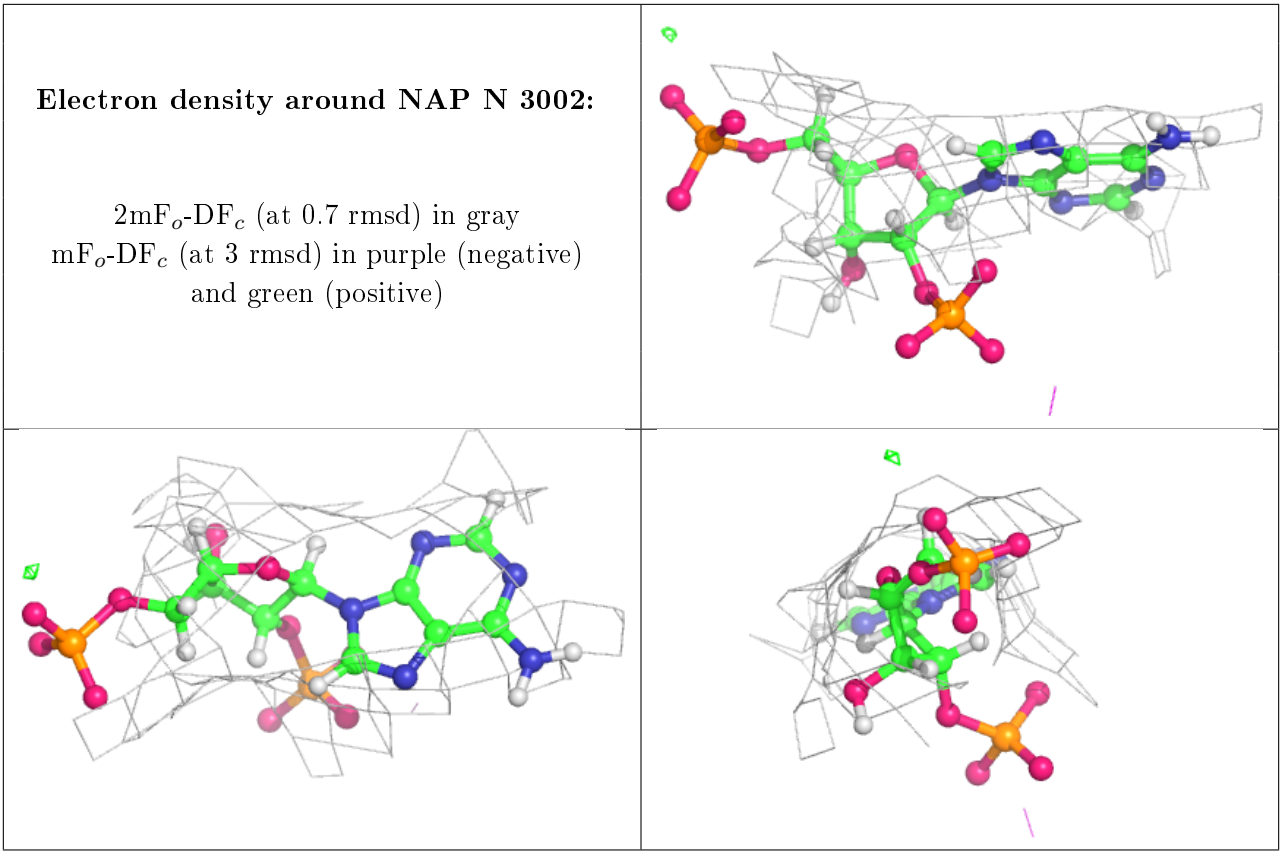
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





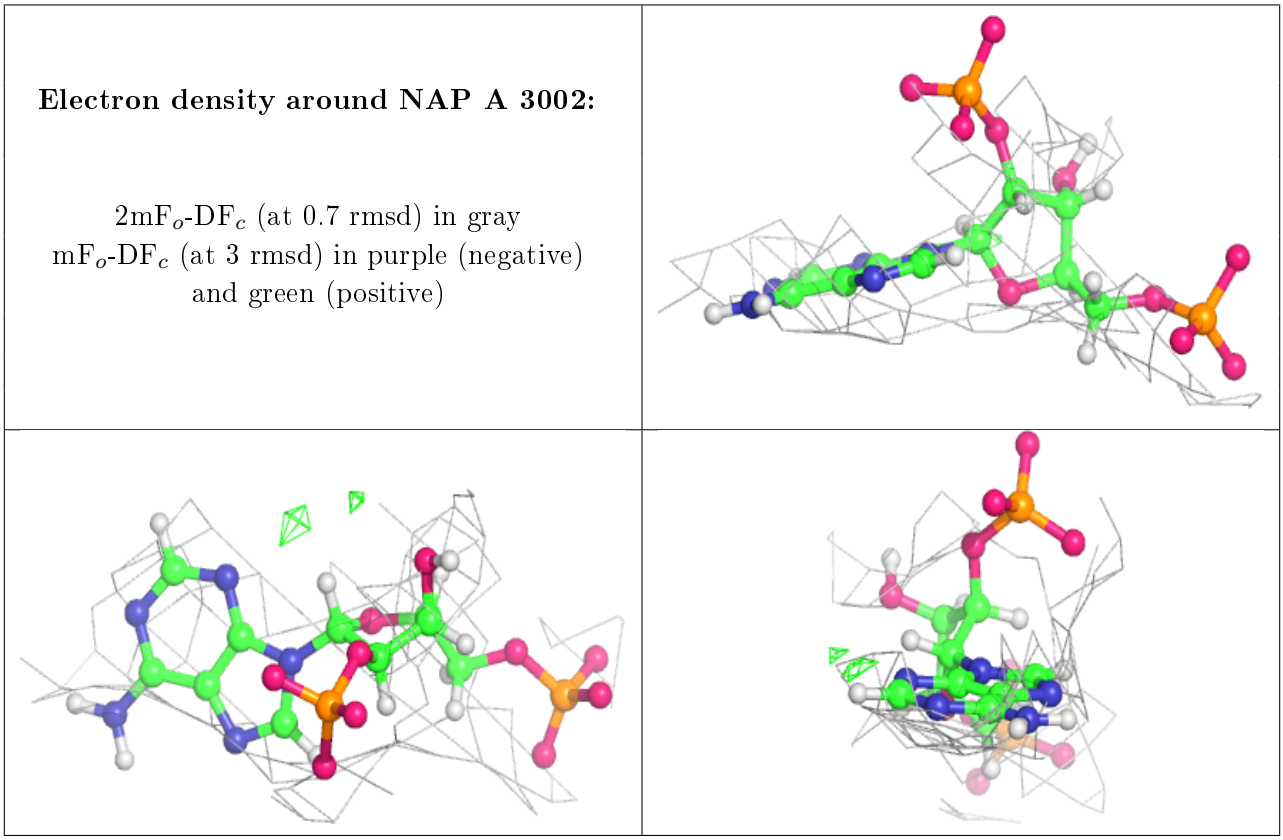
Electron density around NAP N 3002:

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



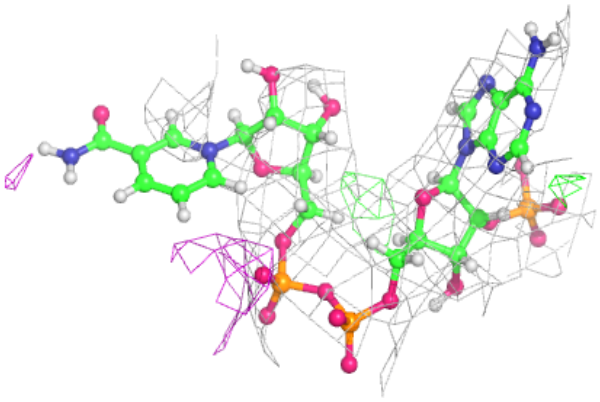
Electron density around NAP A 3002:

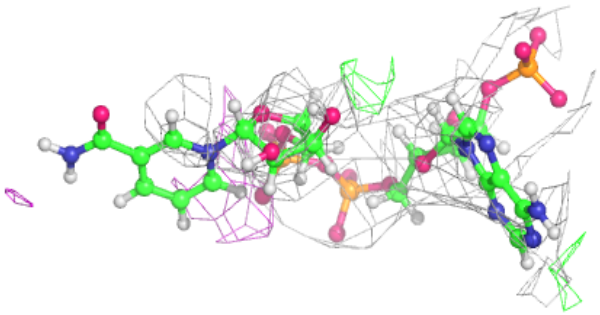
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

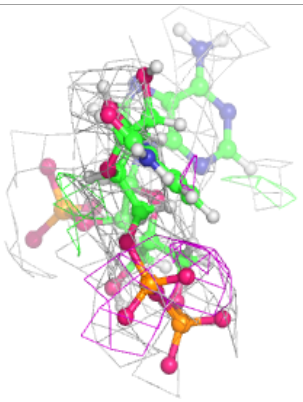


Electron density around NAP Q 3001:

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







Electron density around NAP P 3002:

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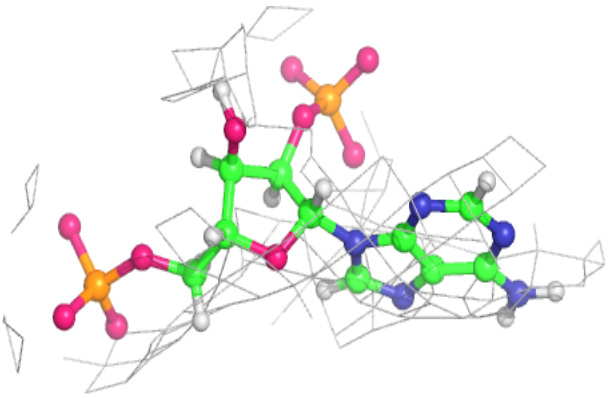
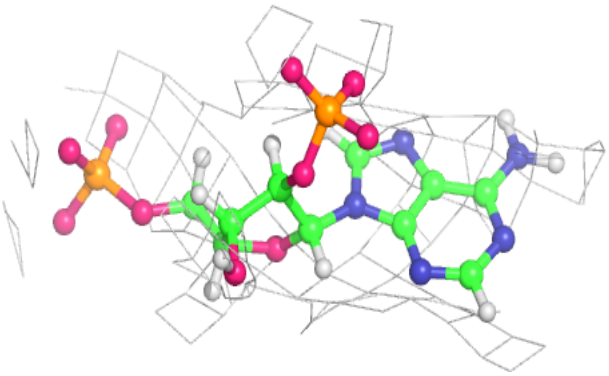
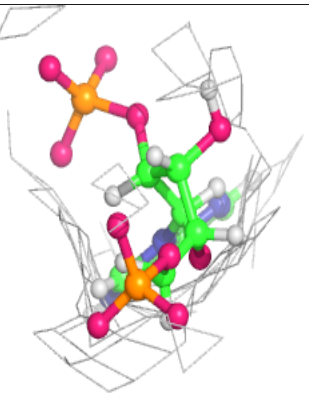
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

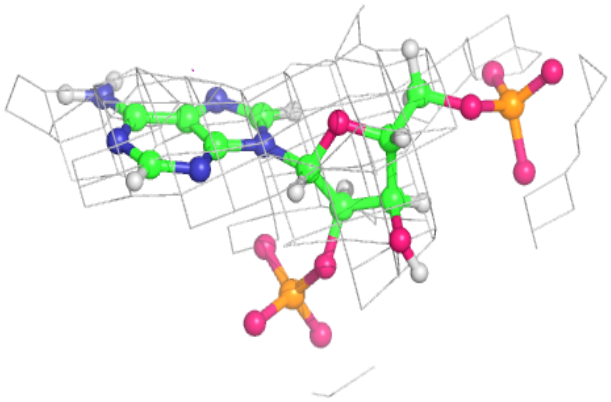


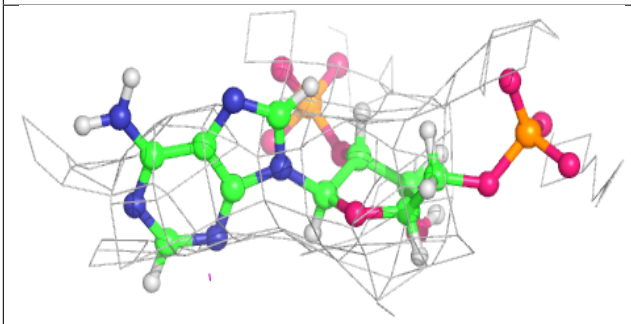


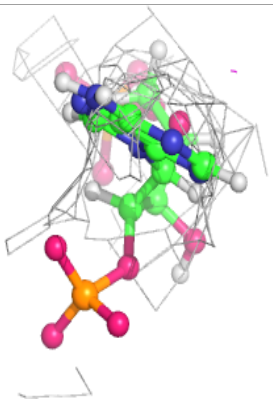


Electron density around NAP H 3002:

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

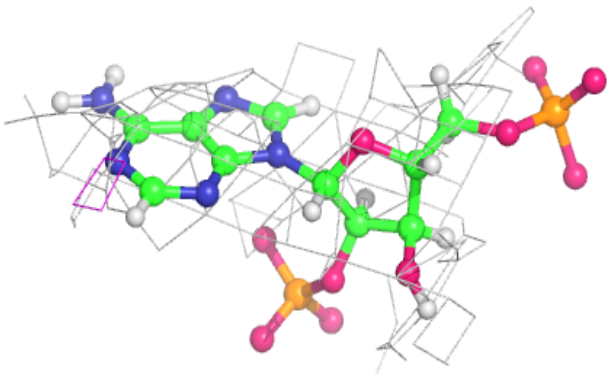


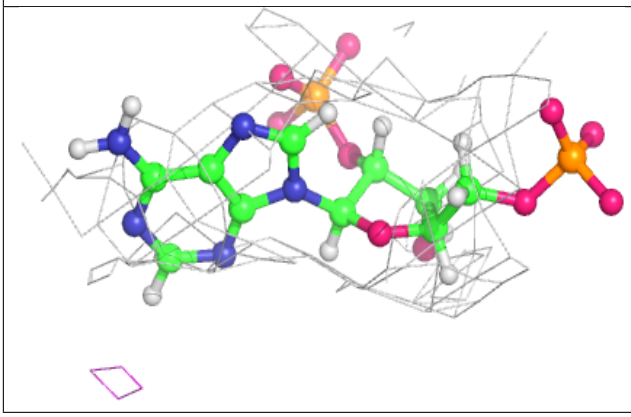


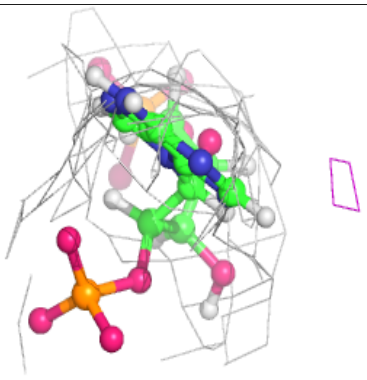


Electron density around NAP F 3002:

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

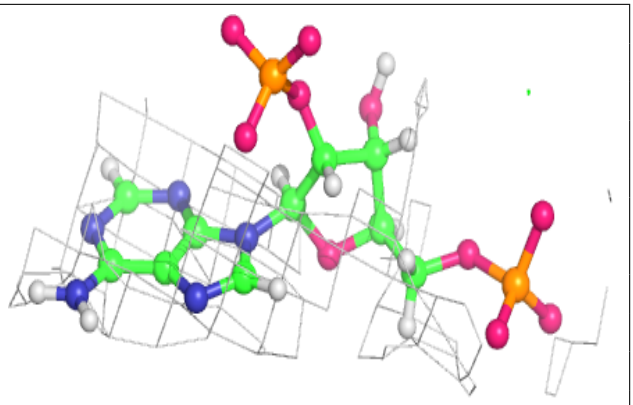


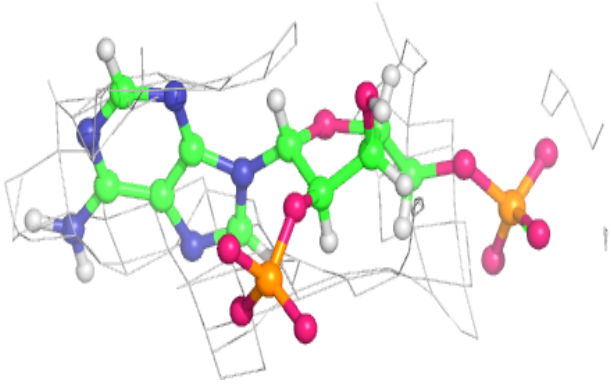


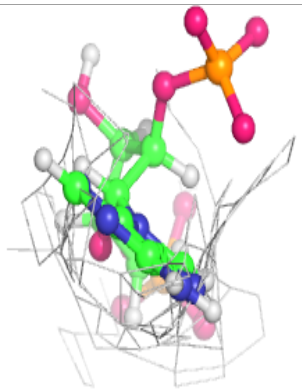


Electron density around NAP D 3002:

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

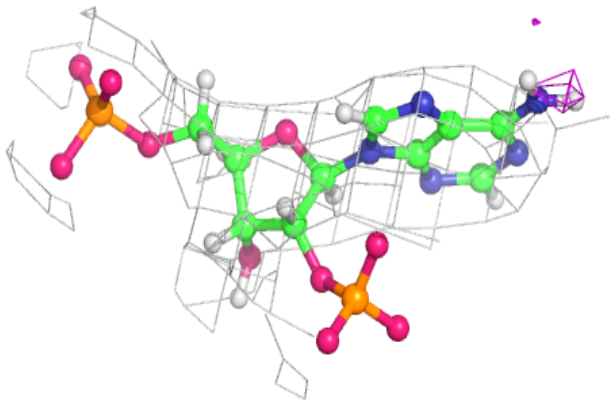


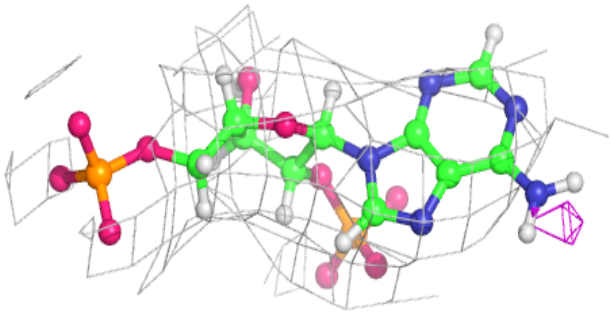


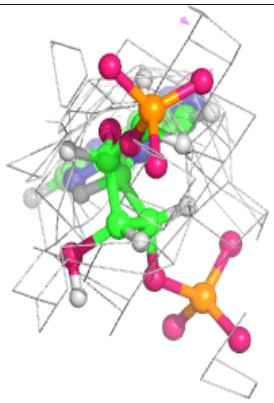


Electron density around NAP J 3002:

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

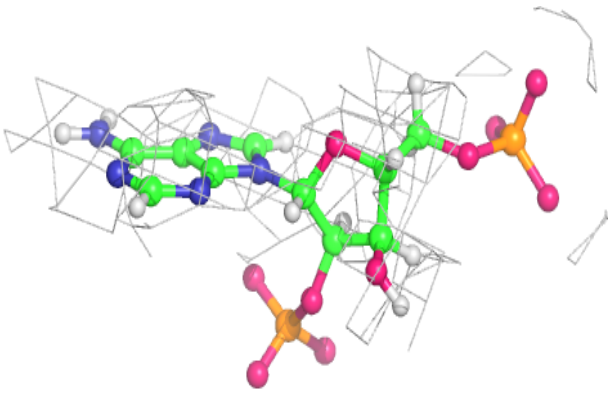


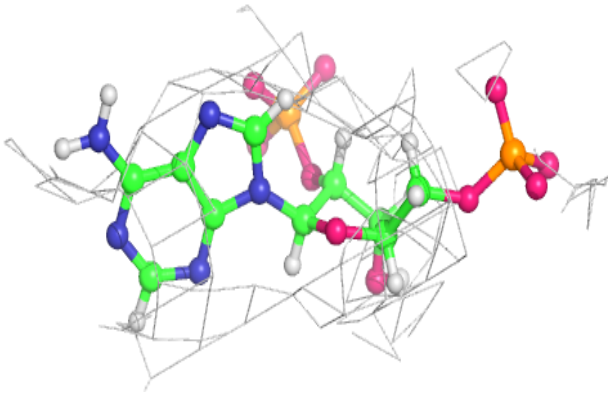


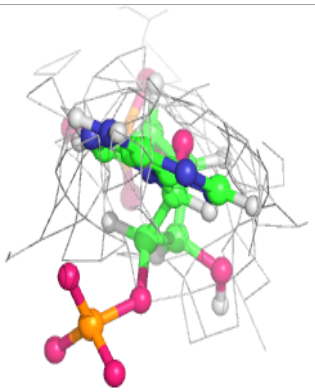


Electron density around NAP G 3002:

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

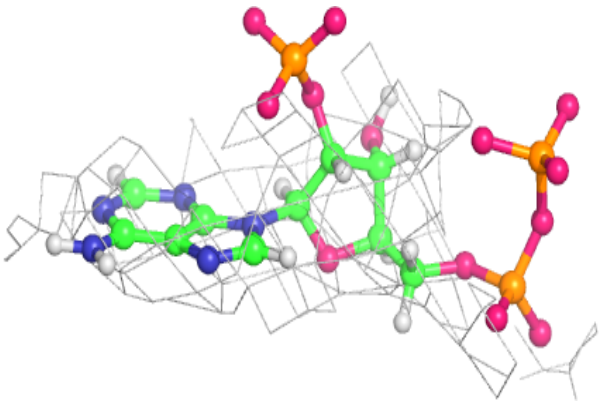


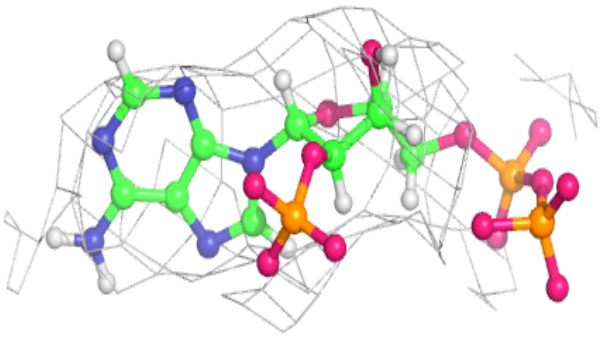


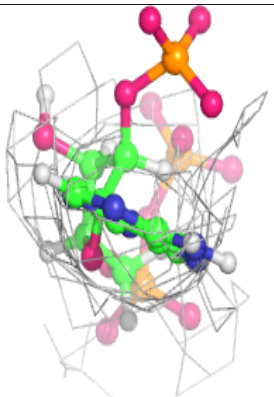


Electron density around NAP C 3002:

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

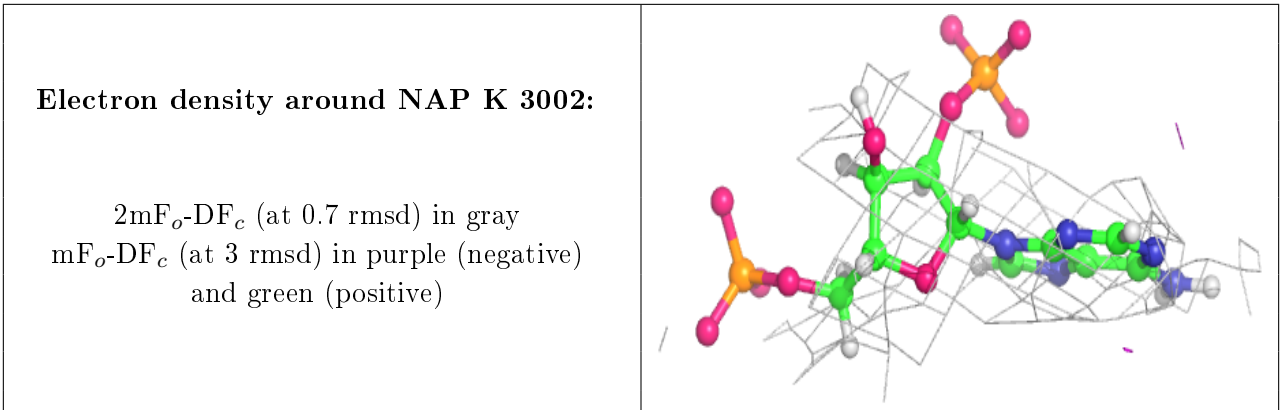


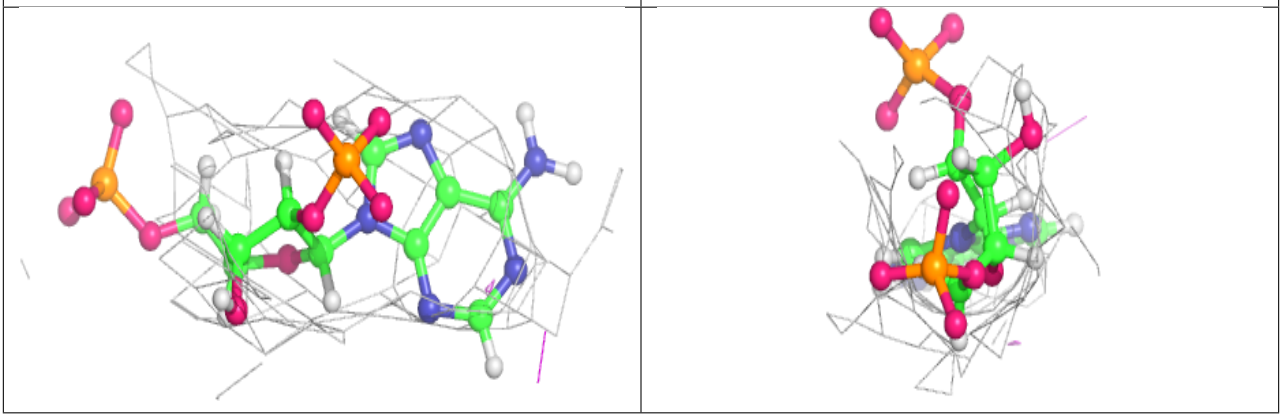




Electron density around NAP K 3002:

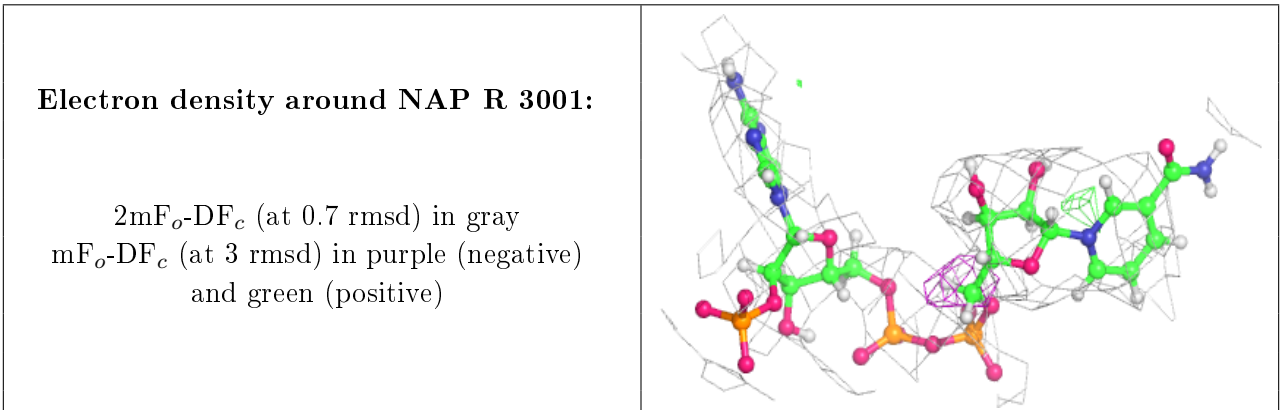
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

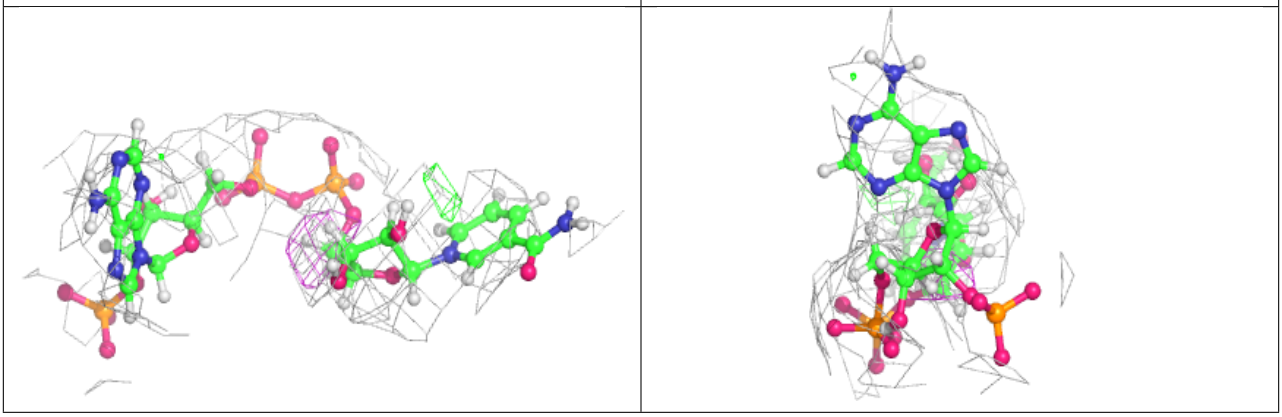




Electron density around NAP R 3001:

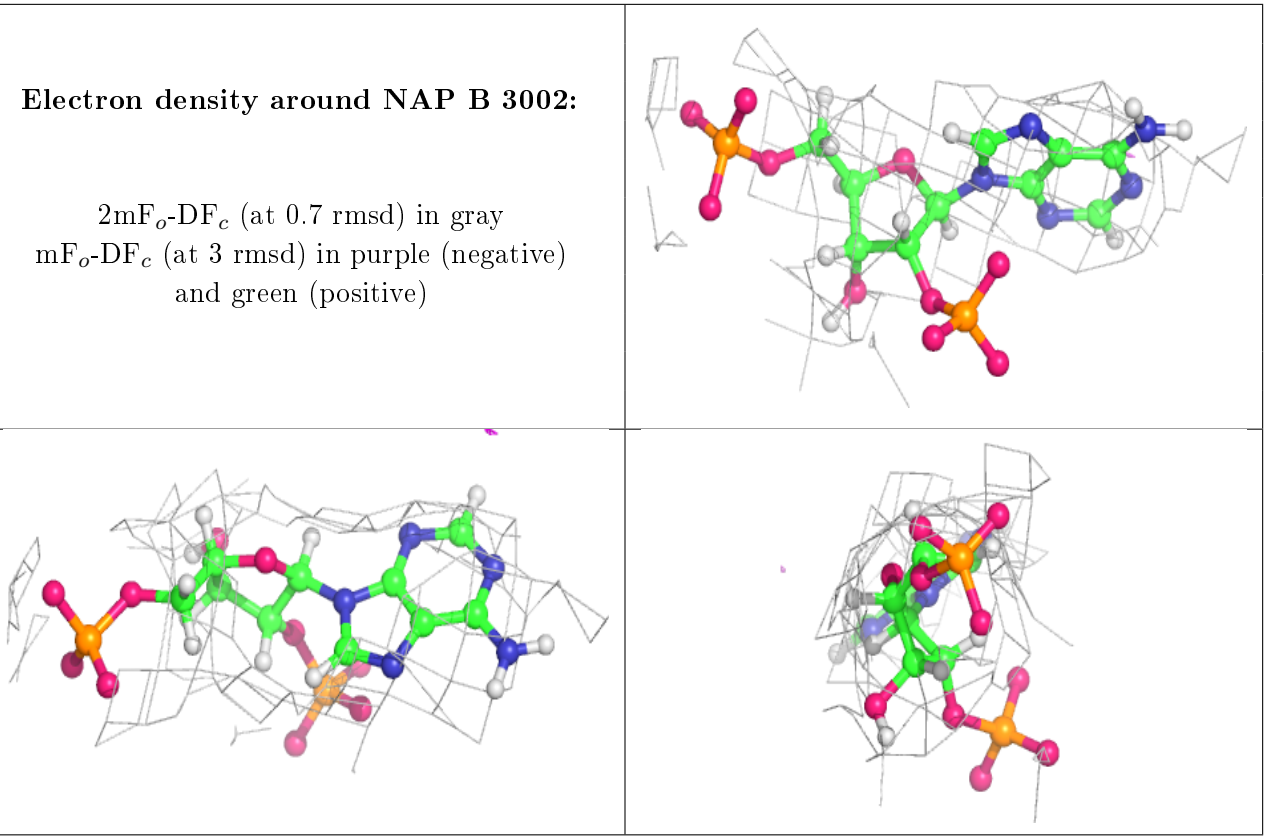
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





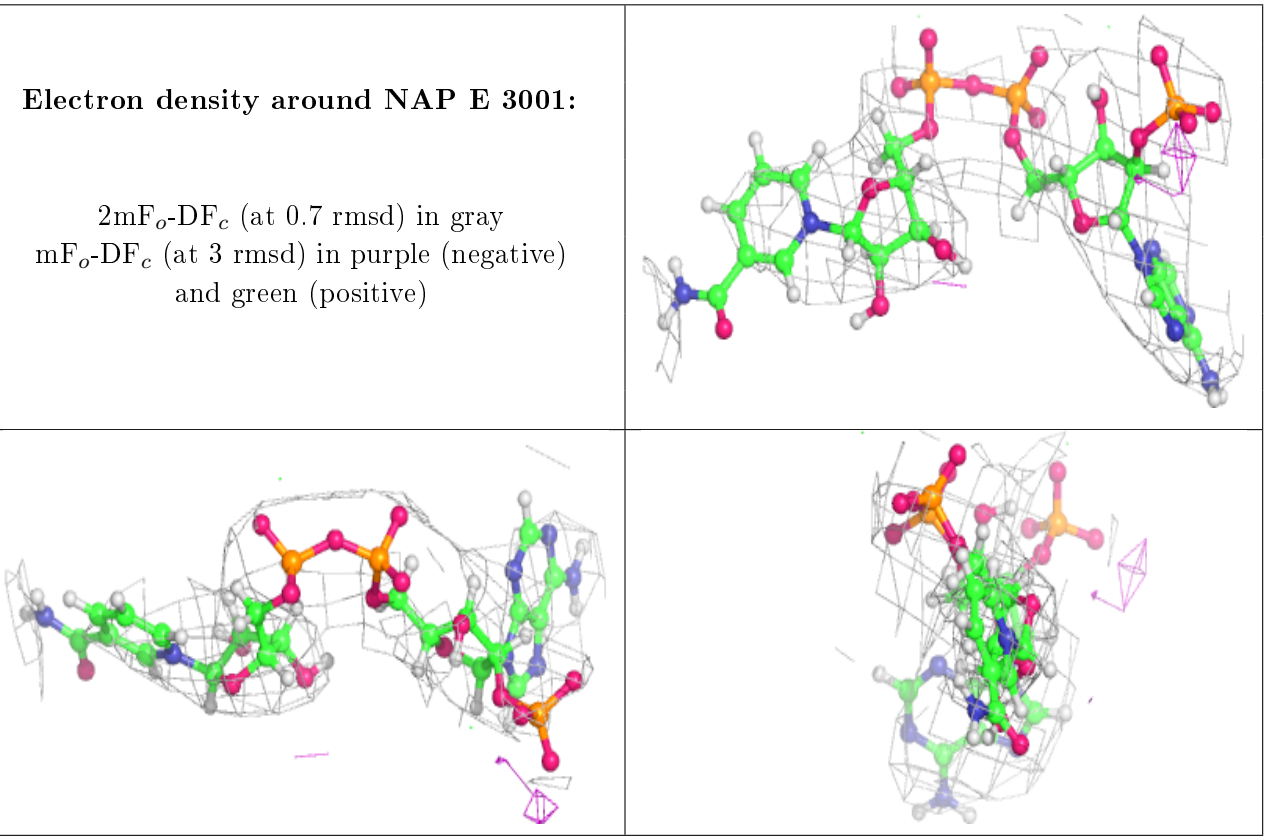
Electron density around NAP B 3002:

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



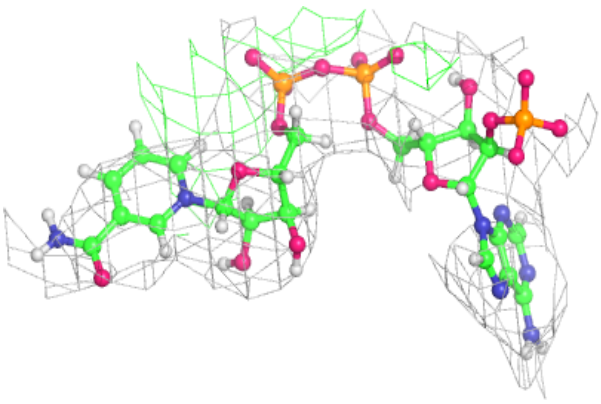
Electron density around NAP E 3001:

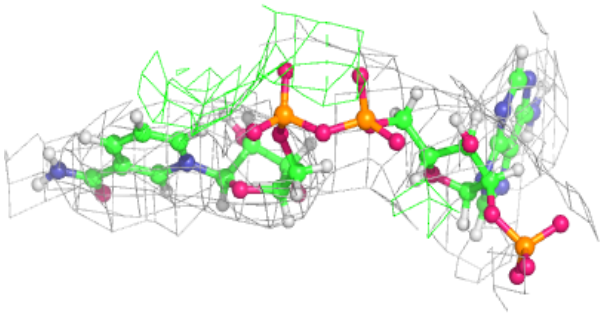
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

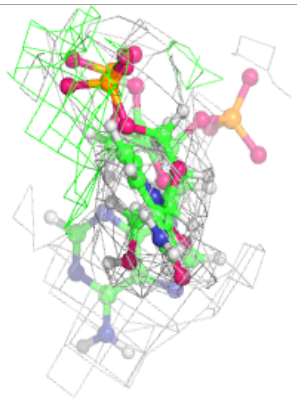


Electron density around NAP H 3001:

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

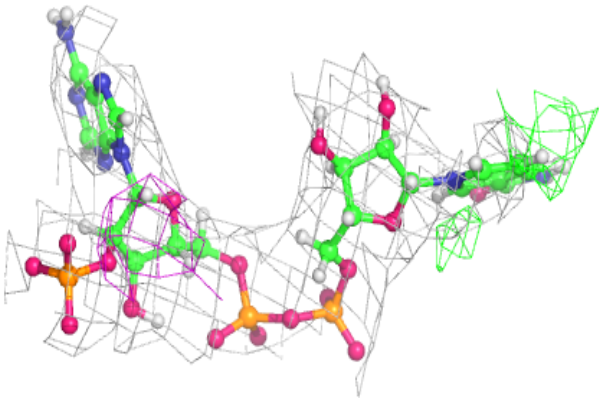


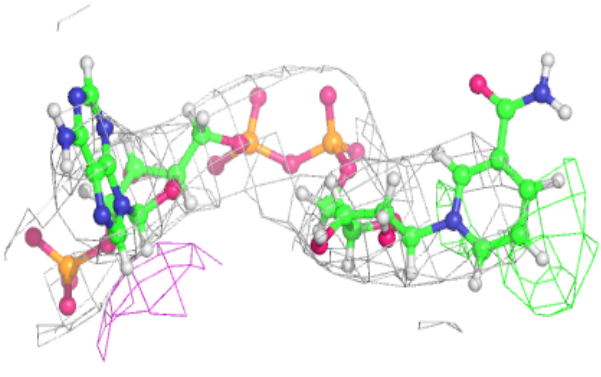




Electron density around NAP F 3001:

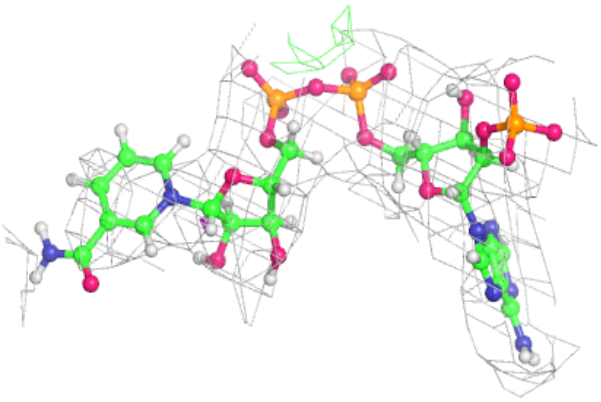
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

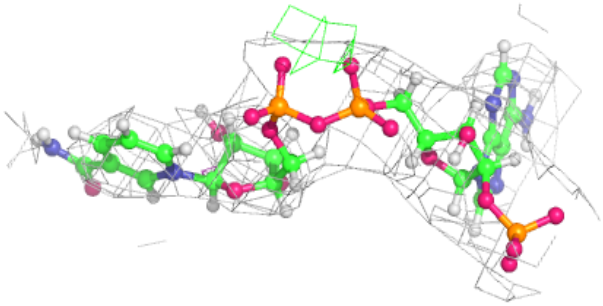


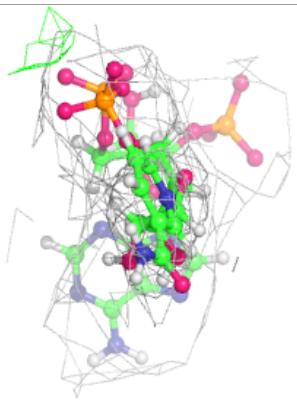


Electron density around NAP I 3001:

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

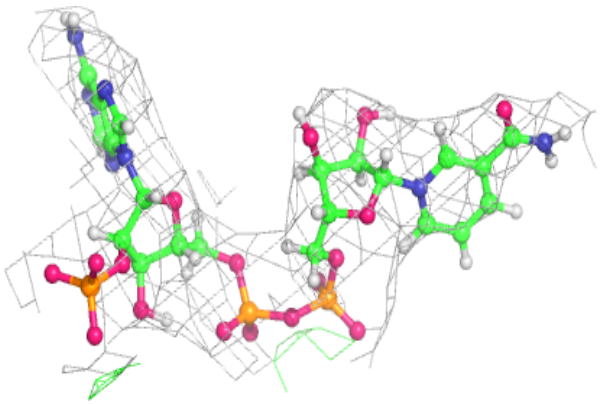


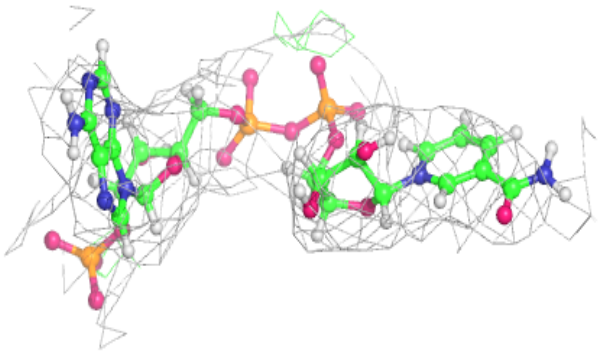


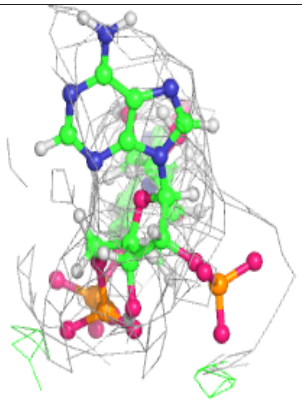


Electron density around NAP M 3001:

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

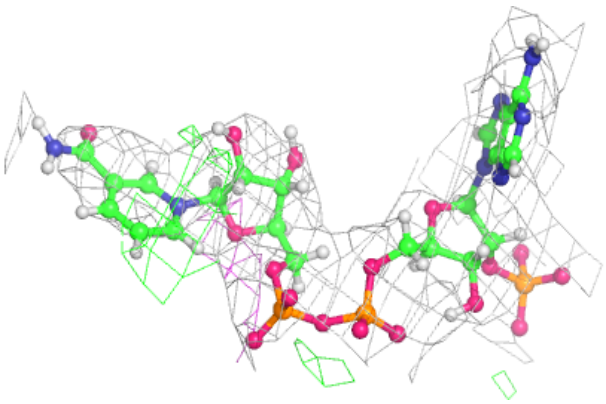


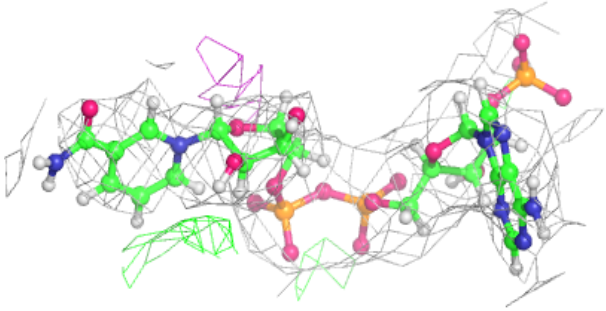


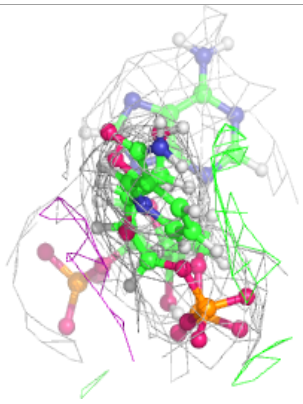


Electron density around NAP N 3001:

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

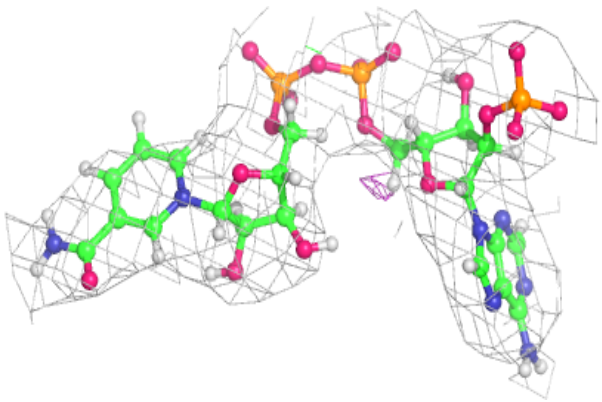


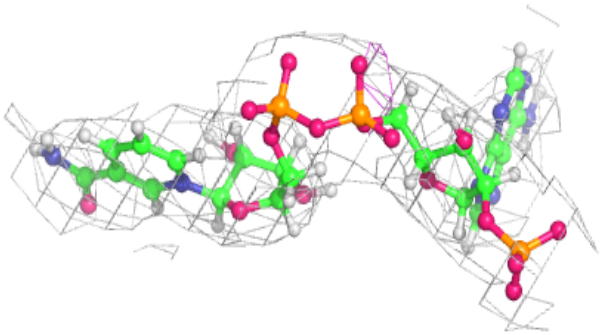


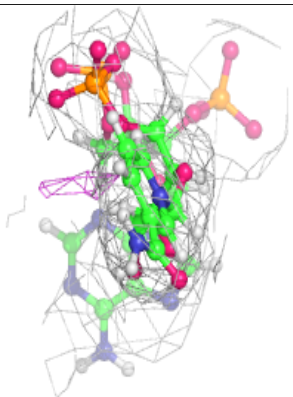


Electron density around NAP G 3001:

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

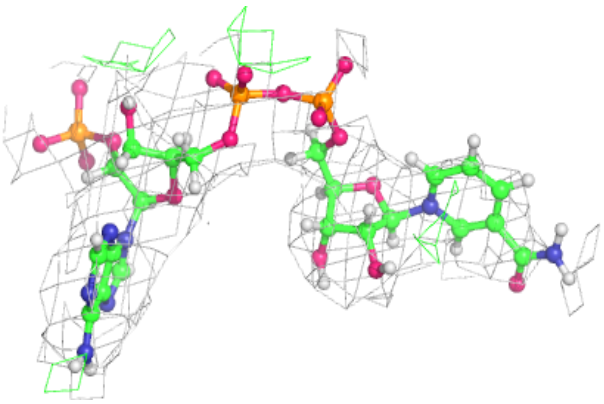


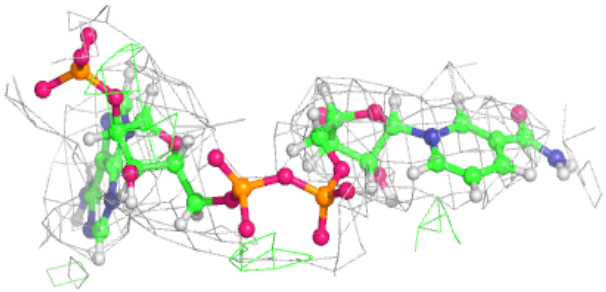


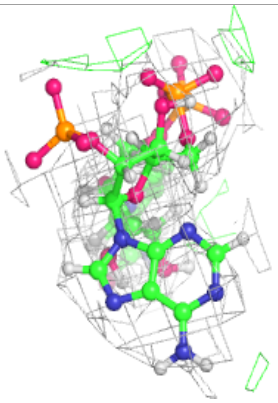


Electron density around NAP D 3001:

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

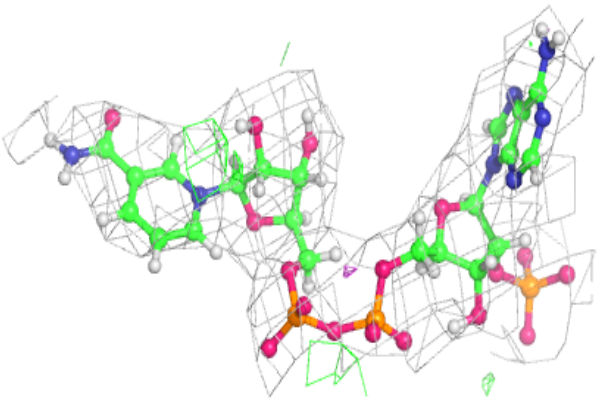


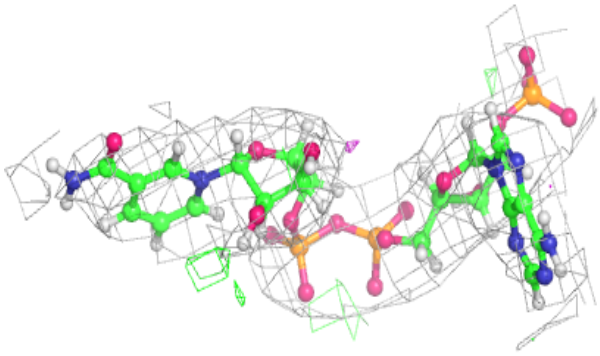




Electron density around NAP C 3001:

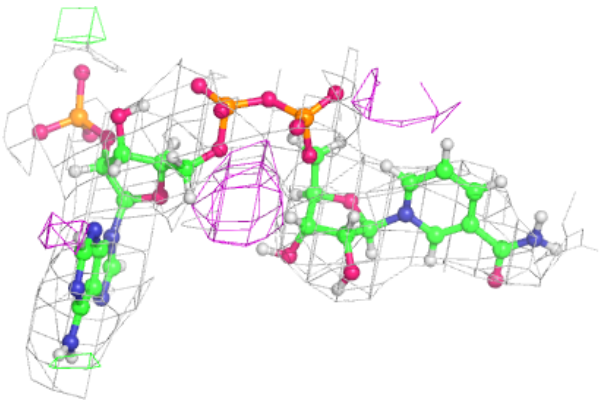
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

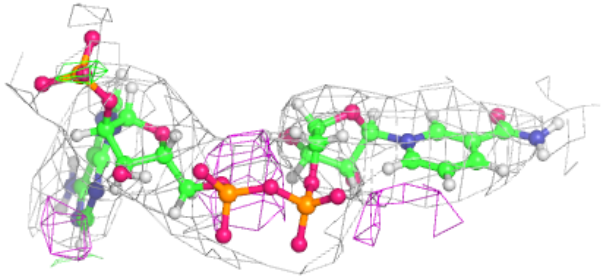


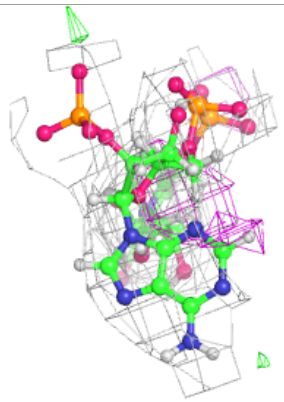


Electron density around NAP L 3001:

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

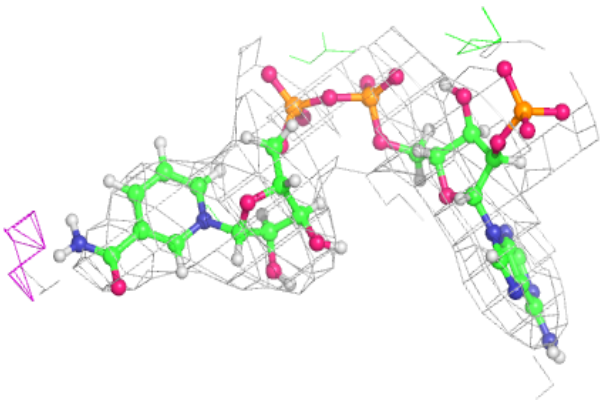


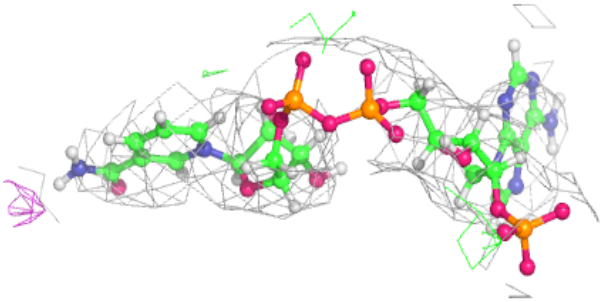




Electron density around NAP O 3001:

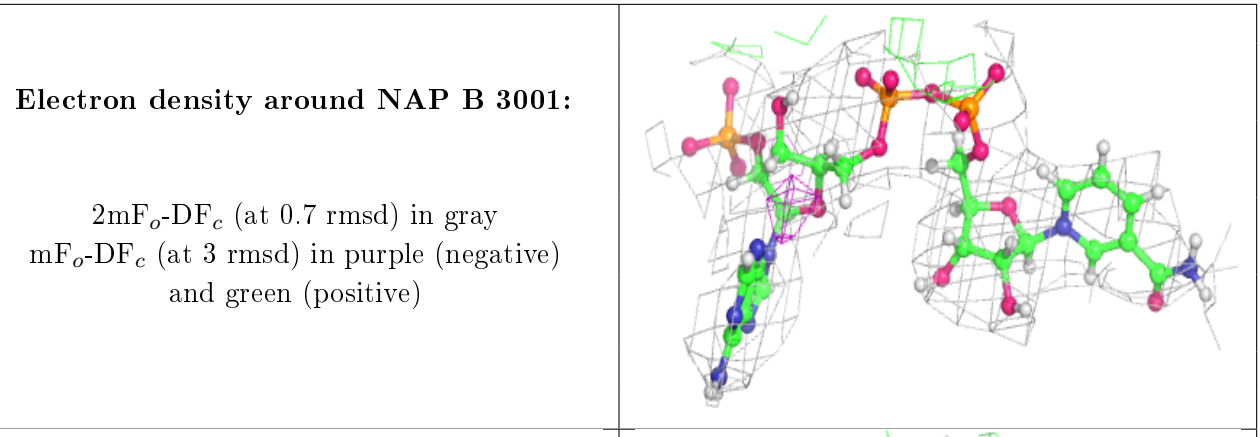
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





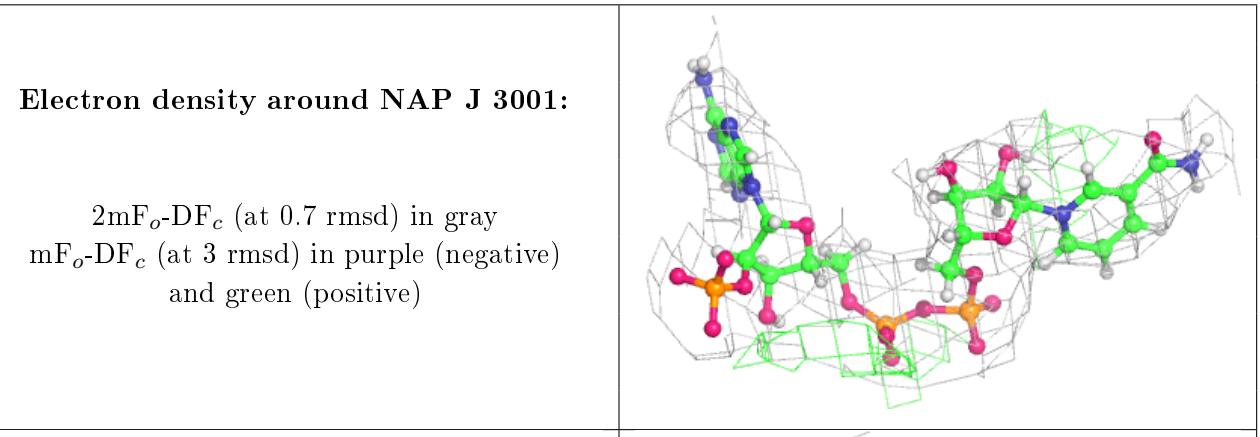
Electron density around NAP B 3001:

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



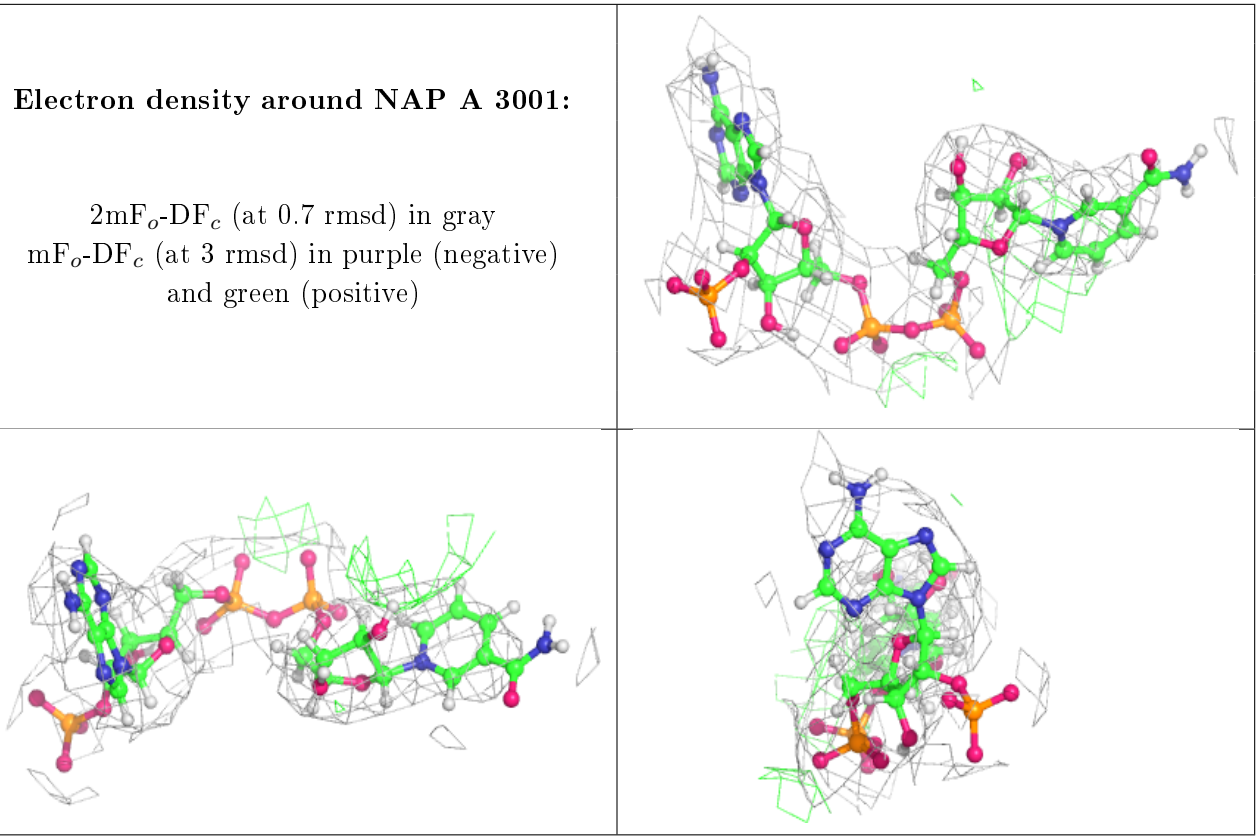
Electron density around NAP J 3001:

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



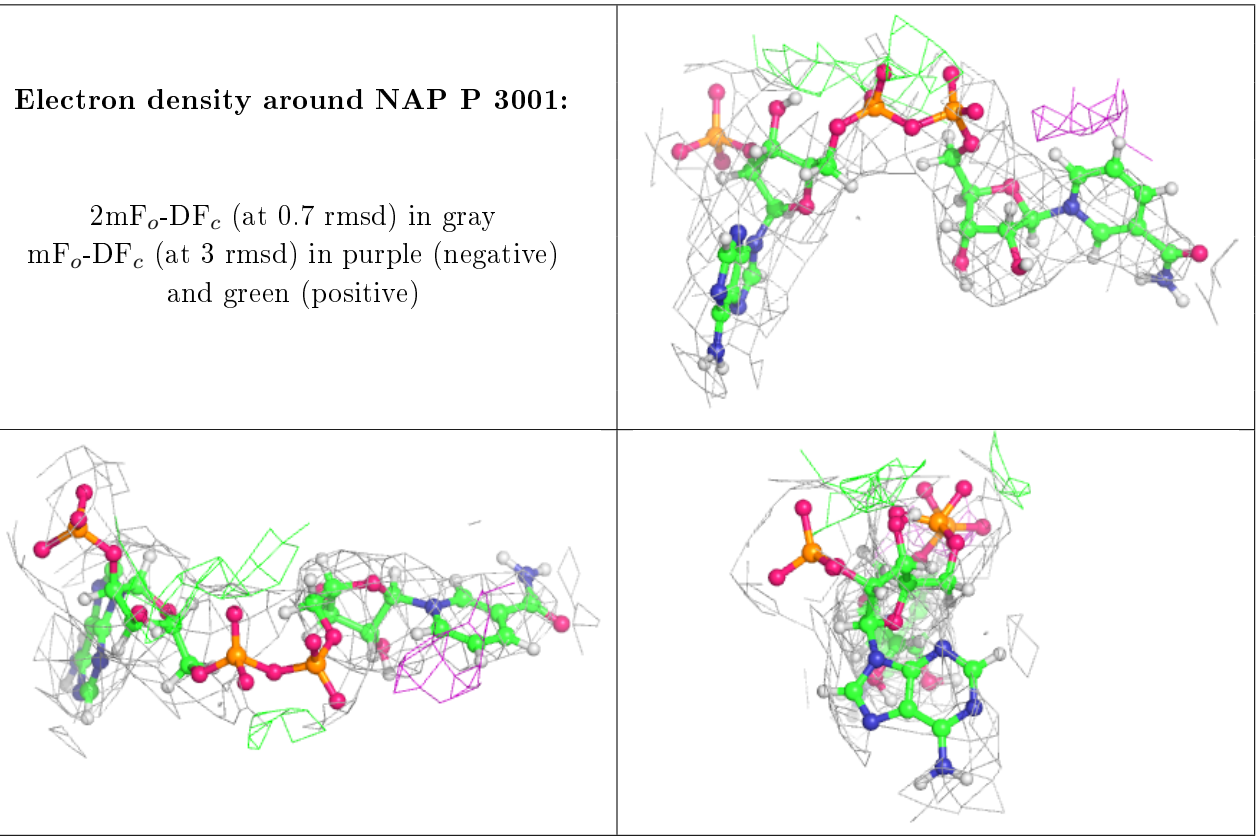
Electron density around NAP A 3001:

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



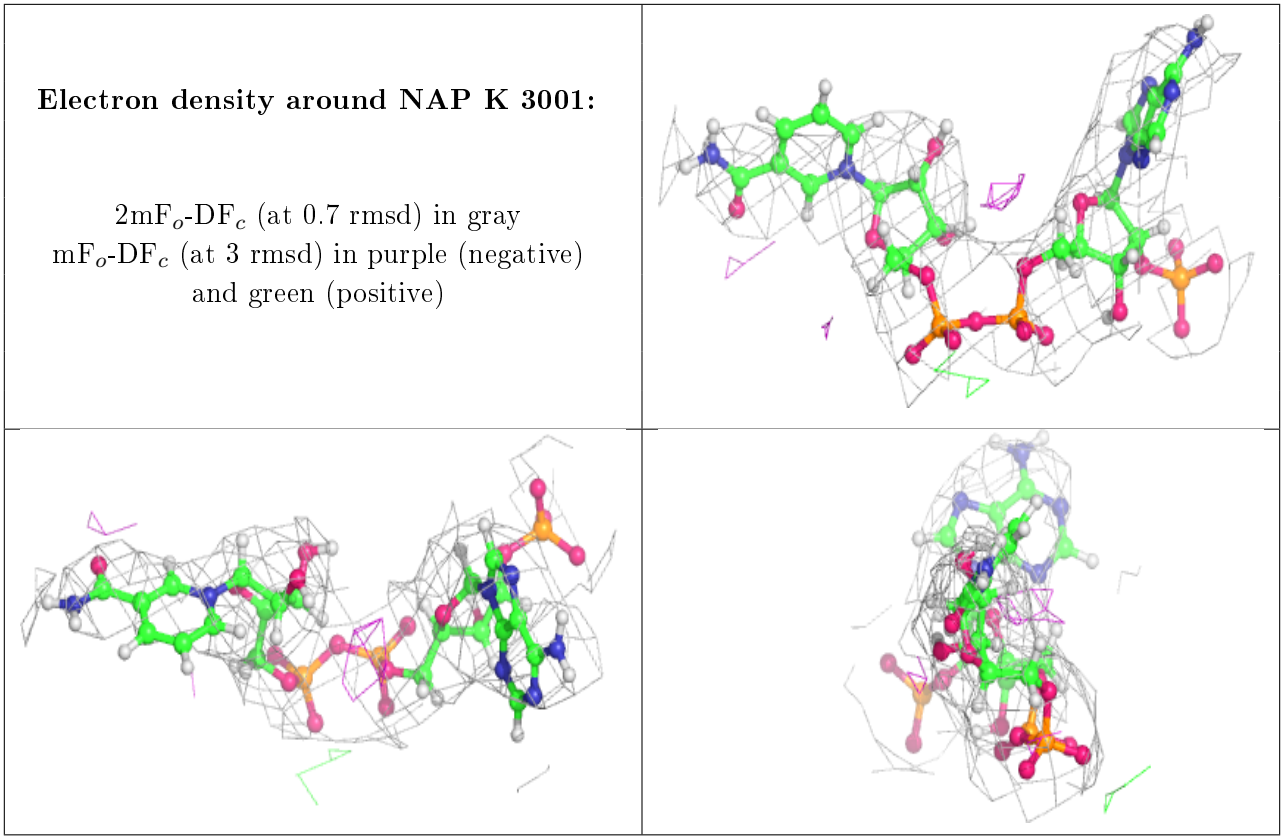
Electron density around NAP P 3001:

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



Electron density around NAP K 3001:

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



6.5 Other polymers (i)

There are no such residues in this entry.