wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 07:09 pm BST

PDB ID	:	6NKK
Title	:	Structure of PhqE Reductase/Diels-Alderase from Penicillium fellutanum in complex with NADP+ and premalbrancheamide
Authors	:	Newmister, S.A.; Dan, Q.; Smith, J.L.; Sherman, D.H.
Deposited on	:	2019-01-07
Resolution	:	2.30 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:

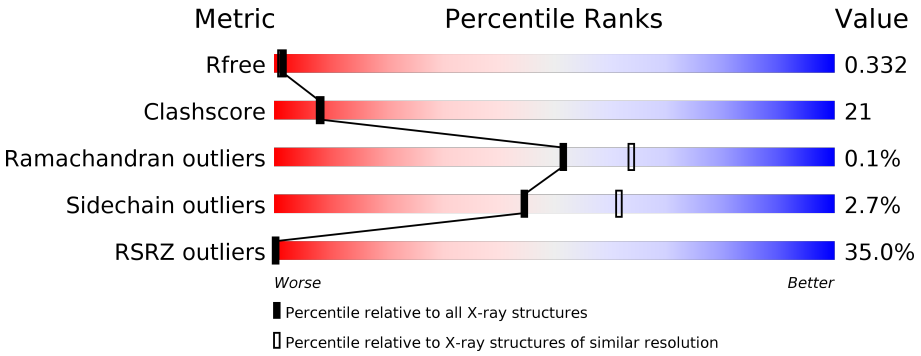
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	265	14% 73% 23%
1	B	265	12% 77% 19%
1	C	265	20% 66% 29%
1	D	265	23% 66% 28%
1	E	265	54% 55% 39%
1	F	265	80% 49% 43% 5%

2 Entry composition (i)

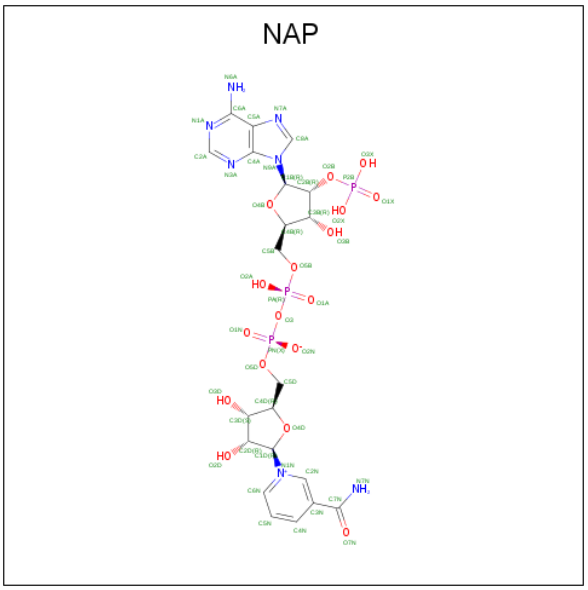
There are 4 unique types of molecules in this entry. The entry contains 11722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Short chain dehydrogenase.

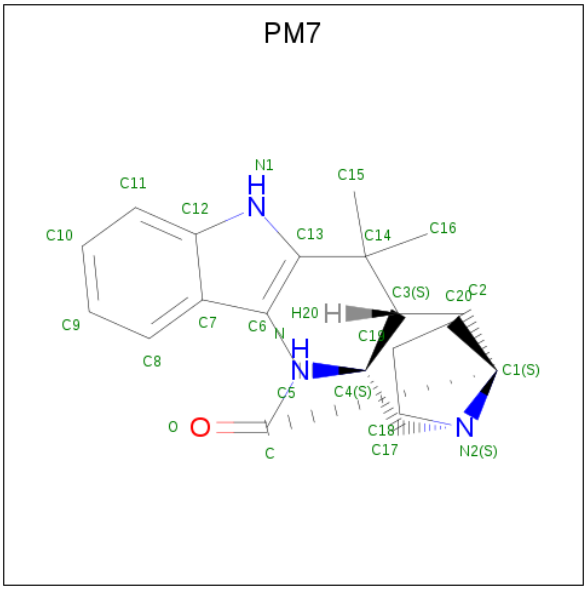
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1866	1167	321	366	12			
1	B	257	Total	C	N	O	S	0	0	0
			1866	1167	321	366	12			
1	C	256	Total	C	N	O	S	0	0	0
			1859	1163	320	364	12			
1	D	257	Total	C	N	O	S	0	0	0
			1866	1167	321	366	12			
1	E	256	Total	C	N	O	S	0	0	0
			1859	1163	320	364	12			
1	F	256	Total	C	N	O	S	0	0	0
			1859	1163	320	364	12			

- 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	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (5aS,12aS,13aS)-12,12-dimethyl-2,3,11,12,12a,13-hexahydro-1H,5H,6H-5a,13a-(epiminomethano)indolizino[7,6-b]carbazol-14-one (three-letter code: PM7) (formula: $C_{21}H_{25}N_3O$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	21	3	1		
3	B	1	Total	C	N	O	0	0
			25	21	3	1		
3	C	1	Total	C	N	O	0	0
			25	21	3	1		
3	D	1	Total	C	N	O	0	0
			25	21	3	1		
3	E	1	Total	C	N	O	0	0
			25	21	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			25	21	3	1		

- Molecule 4 is water.

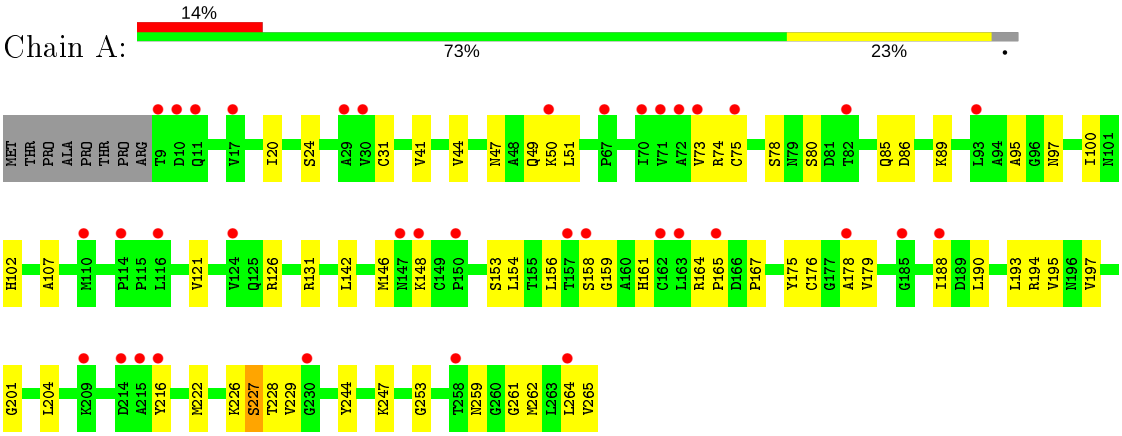
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	36	Total	O	0	0
			36	36		
4	C	22	Total	O	0	0
			22	22		
4	D	18	Total	O	0	0
			18	18		
4	E	1	Total	O	0	0
			1	1		

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.

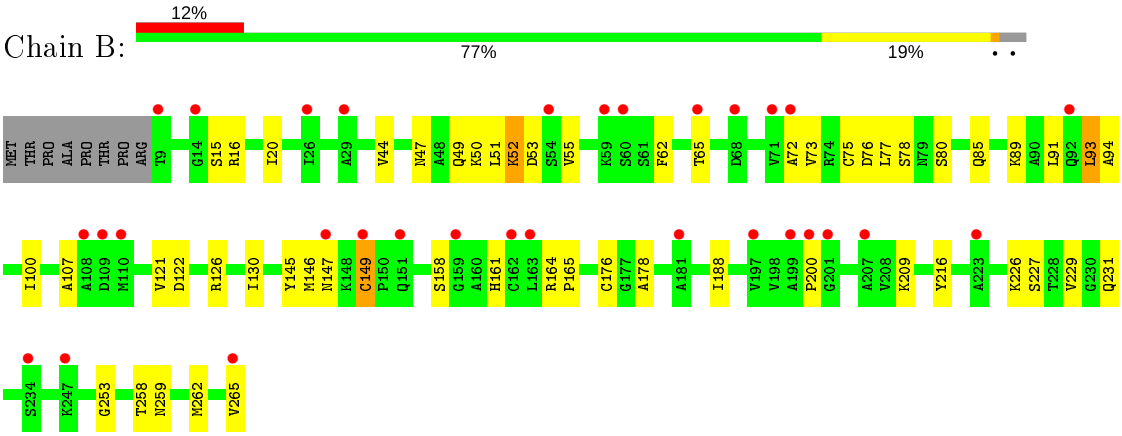
- Molecule 1: Short chain dehydrogenase

Chain A:



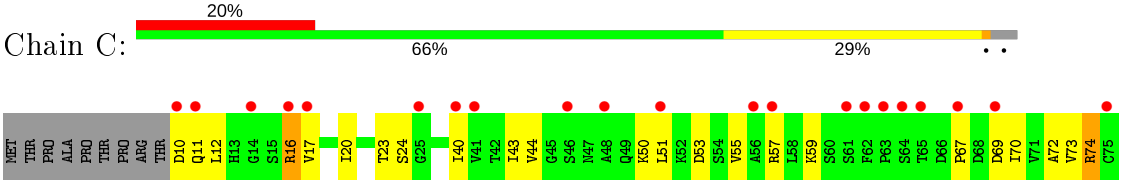
- Molecule 1: Short chain dehydrogenase

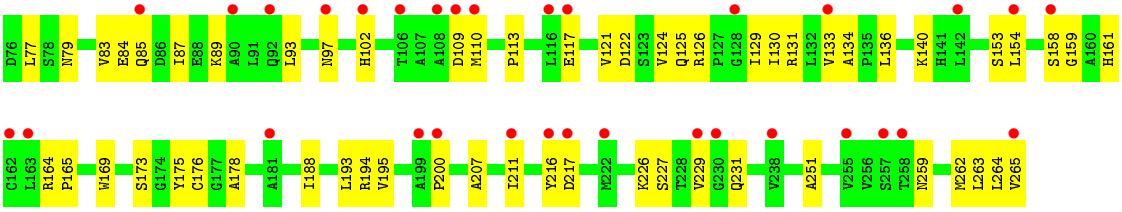
Chain B:



- Molecule 1: Short chain dehydrogenase

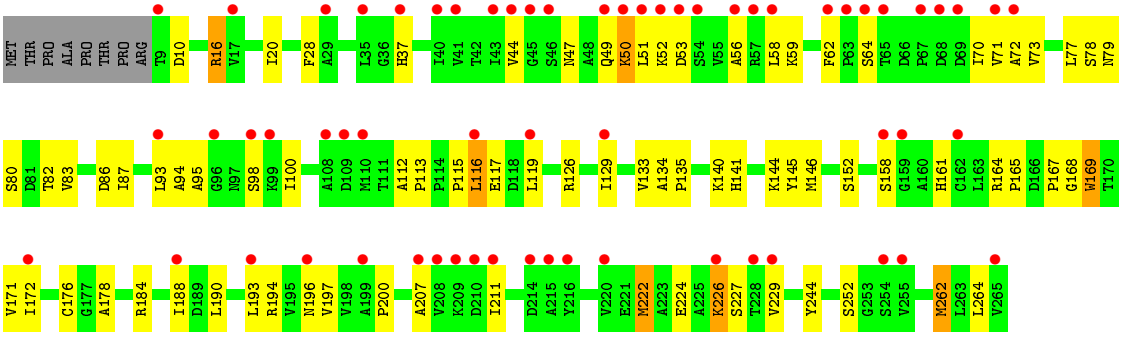
Chain C:





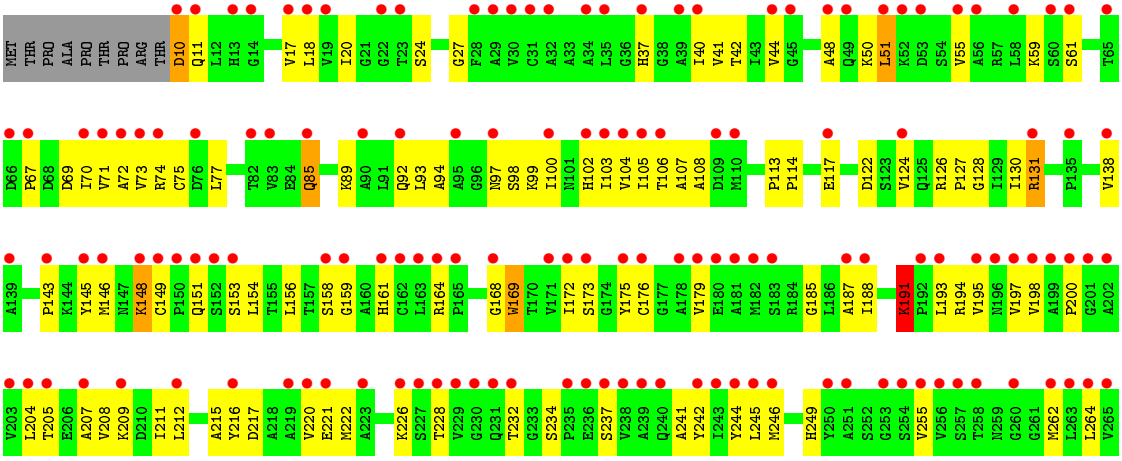
• Molecule 1: Short chain dehydrogenase

Chain D:



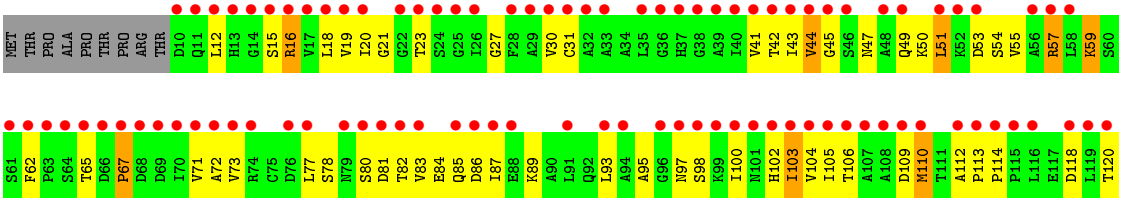
• Molecule 1: Short chain dehydrogenase

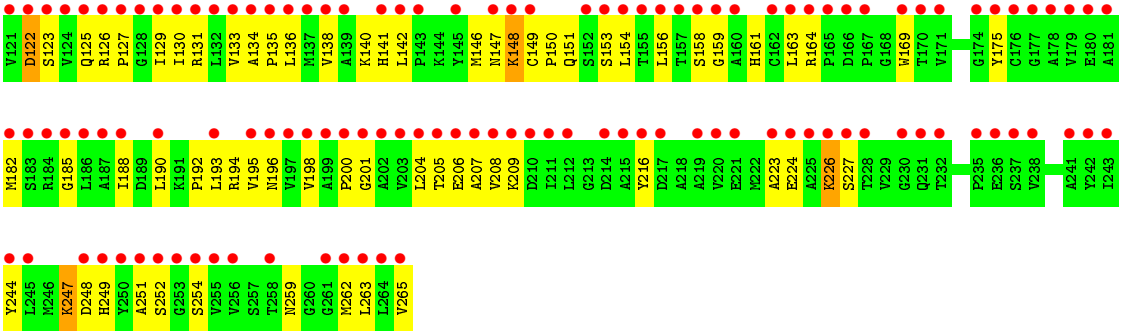
Chain E:



• Molecule 1: Short chain dehydrogenase

Chain F:




V121 D122 S123 V124 Q125 R126 P127 G128 I129 I130 R131 L132 V133 A134 P135 L136 M137 V138 A139 K140 H141 L142 P143 K144 Y145 M146 N147 K148 C149 P150 Q151 S152 S153 L154 T155 L156 T157 S158 G159 A160 H161 C162 L163 R164 P165 D166 P167 G168 W169 T170 V171 G174 Y175 C176 G177 A178 V179 E180 A181
M182 S183 R184 G185 L186 A187 I188 D189 L190 K191 P192 L193 R194 V195 N196 V197 V198 A199 P200 G201 A202 V203 L204 T205 E206 A207 V208 K209 D210 I211 L212 G213 D214 A215 Y216 D217 A218 A219 V220 E221 M222 A223 E224 A225 K226 S227 T228 V229 G230 Q231 T232 P235 E236 S237 V238 A241 Y242 I243
Y244 L245 M246 K247 D248 H249 Y250 A251 S252 G253 S254 V255 V256 S257 T258 N259 G260 G261 M262 L263 L264 V265

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.59Å 117.25Å 64.81Å 90.00° 107.96° 90.00°	Depositor
Resolution (Å)	46.38 – 2.30 46.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.38-2.30) 99.3 (46.38-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.293 , 0.336 0.293 , 0.332	Depositor DCC
R_{free} test set	3153 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11722	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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, PM7

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	0.60	0/1895	0.64	0/2580
1	B	0.44	0/1895	0.63	1/2580 (0.0%)
1	C	0.42	0/1888	0.63	0/2570
1	D	0.61	3/1895 (0.2%)	0.73	3/2580 (0.1%)
1	E	0.57	1/1888 (0.1%)	0.93	12/2570 (0.5%)
1	F	0.61	0/1888	1.09	11/2570 (0.4%)
All	All	0.55	4/11349 (0.0%)	0.80	27/15450 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	169	TRP	CB-CG	-6.87	1.37	1.50
1	D	168	GLY	C-O	-5.66	1.14	1.23
1	D	169	TRP	C-O	-5.49	1.12	1.23
1	D	169	TRP	CG-CD1	-5.16	1.29	1.36

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	182	MET	CB-CG-SD	-10.83	79.91	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	110	MET	CA-CB-CG	9.58	129.59	113.30
1	D	116	LEU	CA-CB-CG	8.87	135.69	115.30
1	F	110	MET	CB-CG-SD	8.18	136.93	112.40
1	E	51	LEU	CA-CB-CG	8.17	134.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	PRO	Peptide
1	D	167	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1866	0	1899	47	0
1	B	1866	0	1899	42	0
1	C	1859	0	1892	73	0
1	D	1866	0	1899	69	0
1	E	1859	0	1892	114	0
1	F	1859	0	1892	167	1
2	A	48	0	23	3	0
2	B	48	0	25	2	0
2	C	48	0	23	2	0
2	D	48	0	23	2	0
2	E	48	0	25	5	0
2	F	48	0	22	12	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	25	0	0	0	0
3	E	25	0	0	0	0
3	F	25	0	0	3	0
4	A	32	0	0	1	0
4	B	36	0	0	2	0
4	C	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	18	0	0	0	0
4	E	1	0	0	0	0
All	All	11722	0	11514	492	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 21.

The worst 5 of 492 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:F:47:ASN:CB	1:F:50:LYS:HD2	1.72	1.18
2:F:801:NAP:O4B	2:F:801:NAP:C1B	1.63	1.17
1:C:73:VAL:HG11	1:C:93:LEU:HD12	1.27	1.12
1:F:81:ASP:O	1:F:82:THR:HB	1.48	1.11
1:B:50:LYS:NZ	2:B:801:NAP:O1X	1.82	1.10

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:F:125:GLN:OE1	1:F:125:GLN:OE1[2_556]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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	255/265 (96%)	250 (98%)	5 (2%)	0	100	100
1	B	255/265 (96%)	246 (96%)	9 (4%)	0	100	100
1	C	254/265 (96%)	248 (98%)	6 (2%)	0	100	100
1	D	255/265 (96%)	246 (96%)	8 (3%)	1 (0%)	34	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	254/265 (96%)	248 (98%)	6 (2%)	0	100	100
1	F	254/265 (96%)	242 (95%)	12 (5%)	0	100	100
All	All	1527/1590 (96%)	1480 (97%)	46 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	50	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/211 (97%)	198 (97%)	6 (3%)	42	58
1	B	204/211 (97%)	198 (97%)	6 (3%)	42	58
1	C	203/211 (96%)	197 (97%)	6 (3%)	41	57
1	D	204/211 (97%)	200 (98%)	4 (2%)	55	72
1	E	203/211 (96%)	199 (98%)	4 (2%)	55	72
1	F	203/211 (96%)	196 (97%)	7 (3%)	37	51
All	All	1221/1266 (96%)	1188 (97%)	33 (3%)	44	61

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	74	ARG
1	D	62	PHE
1	F	163	LEU
1	C	122	ASP
1	C	126	ARG

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

Mol	Chain	Res	Type
1	E	37	HIS
1	E	249	HIS
1	F	102	HIS
1	E	11	GLN
1	F	79	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PM7	F	802	-	26,30,30	5.40	13 (50%)	30,51,51	2.21	6 (20%)
3	PM7	A	802	-	26,30,30	5.35	12 (46%)	30,51,51	1.82	6 (20%)
2	NAP	A	801	-	45,52,52	4.47	14 (31%)	56,80,80	1.99	6 (10%)
3	PM7	B	802	-	26,30,30	5.36	12 (46%)	30,51,51	1.86	7 (23%)
3	PM7	C	802	-	26,30,30	5.37	12 (46%)	30,51,51	1.84	6 (20%)
2	NAP	E	801	-	45,52,52	1.70	12 (26%)	56,80,80	1.66	15 (26%)
2	NAP	F	801	-	45,52,52	4.63	15 (33%)	56,80,80	2.14	11 (19%)
2	NAP	C	801	-	45,52,52	4.49	14 (31%)	56,80,80	2.01	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	D	801	-	45,52,52	4.51	14 (31%)	56,80,80	2.04	8 (14%)
3	PM7	D	802	-	26,30,30	5.37	12 (46%)	30,51,51	1.81	6 (20%)
2	NAP	B	801	-	45,52,52	2.30	19 (42%)	56,80,80	1.62	13 (23%)
3	PM7	E	802	-	26,30,30	5.35	12 (46%)	30,51,51	2.00	7 (23%)

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	A	801	-	-	13/31/67/67	0/5/5/5
2	NAP	B	801	-	-	11/31/67/67	0/5/5/5
2	NAP	E	801	-	-	8/31/67/67	0/5/5/5
2	NAP	F	801	-	-	13/31/67/67	0/5/5/5
2	NAP	C	801	-	-	12/31/67/67	0/5/5/5
2	NAP	D	801	-	-	12/31/67/67	0/5/5/5

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	O4B-C1B	16.17	1.63	1.41
2	D	801	NAP	O4B-C1B	15.72	1.63	1.41
2	F	801	NAP	O4D-C1D	15.37	1.62	1.41
2	C	801	NAP	O4B-C1B	15.33	1.62	1.41
2	F	801	NAP	C2D-C1D	-15.29	1.30	1.53

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	NAP	C5A-C6A-N6A	9.55	134.86	120.35
2	F	801	NAP	C5A-C6A-N6A	9.53	134.84	120.35
2	D	801	NAP	C5A-C6A-N6A	9.50	134.79	120.35
2	A	801	NAP	C5A-C6A-N6A	9.17	134.29	120.35
2	F	801	NAP	N6A-C6A-N1A	-6.76	104.55	118.57

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C5B-O5B-PA-O1A
2	A	801	NAP	C5B-O5B-PA-O2A
2	A	801	NAP	PN-O3-PA-O5B
2	A	801	NAP	C5D-O5D-PN-O1N
2	A	801	NAP	C5D-O5D-PN-O2N

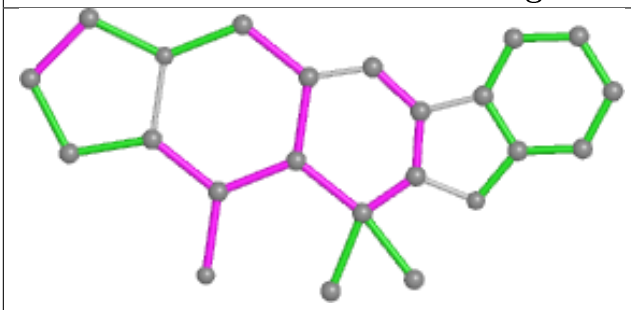
There are no ring outliers.

7 monomers are involved in 29 short contacts:

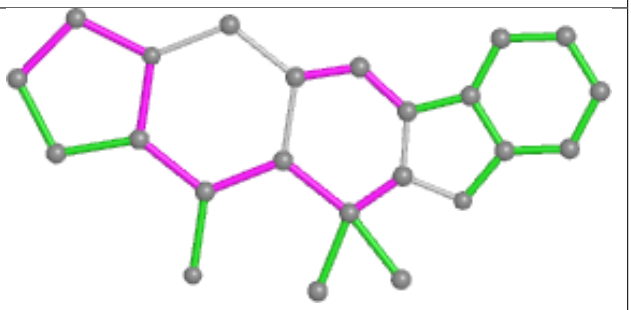
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	802	PM7	3	0
2	A	801	NAP	3	0
2	E	801	NAP	5	0
2	F	801	NAP	12	0
2	C	801	NAP	2	0
2	D	801	NAP	2	0
2	B	801	NAP	2	0

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.

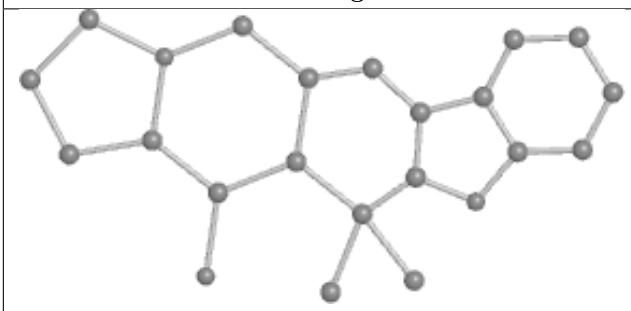
Ligand PM7 F 802



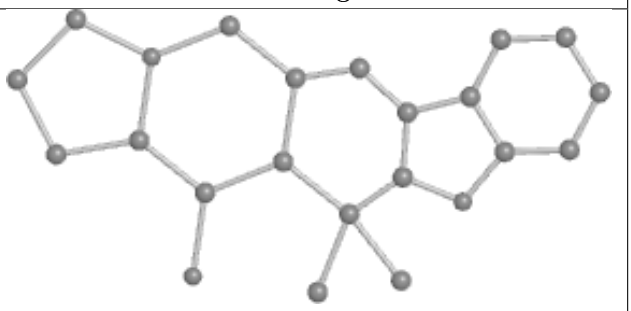
Bond lengths



Bond angles

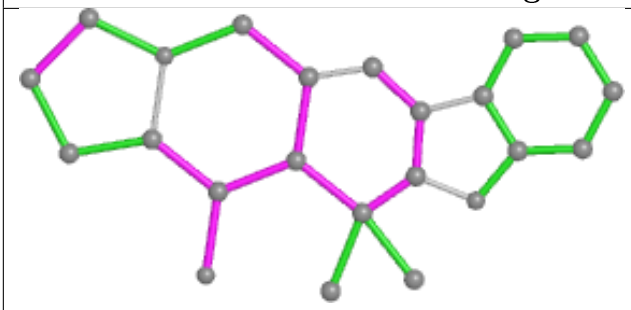


Torsions

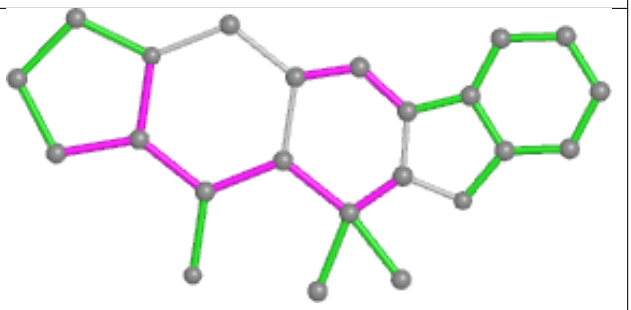


Rings

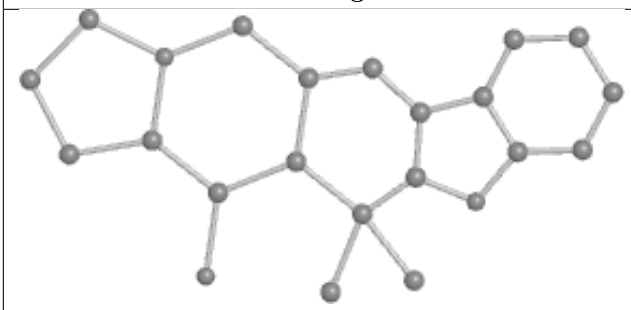
Ligand PM7 A 802



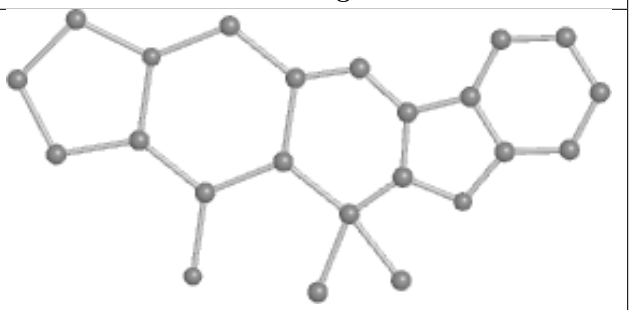
Bond lengths



Bond angles

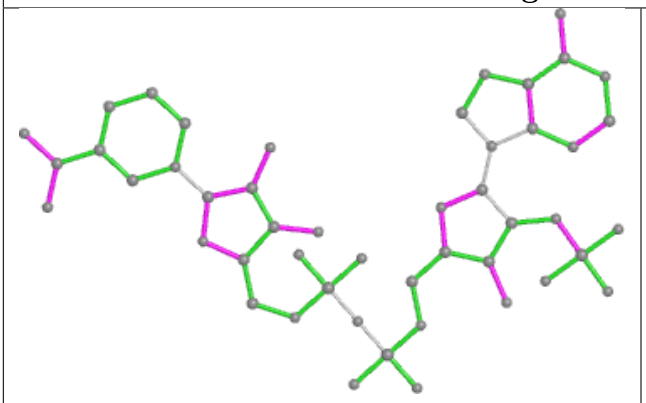


Torsions

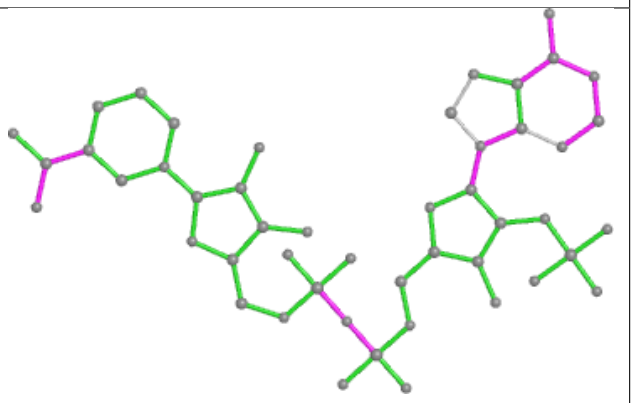


Rings

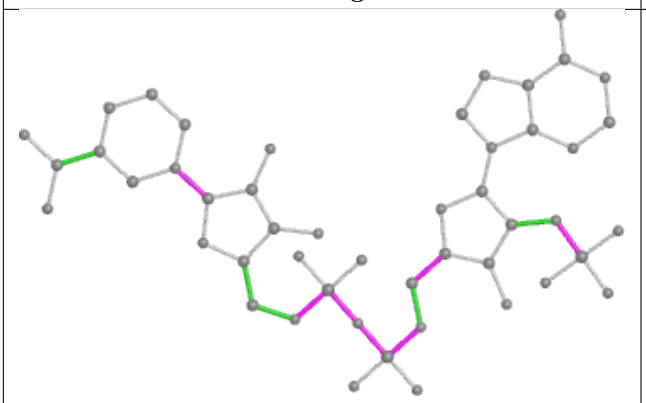
Ligand NAP A 801



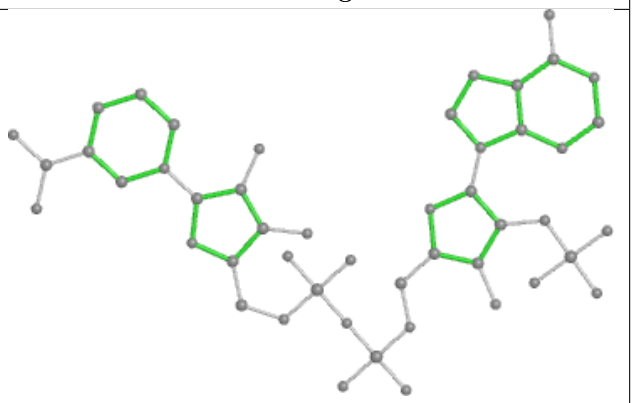
Bond lengths



Bond angles

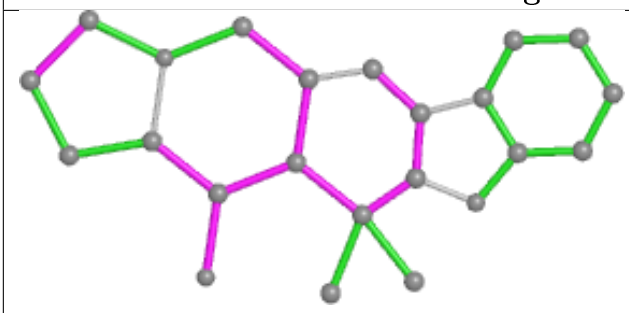


Torsions



Rings

Ligand PM7 B 802



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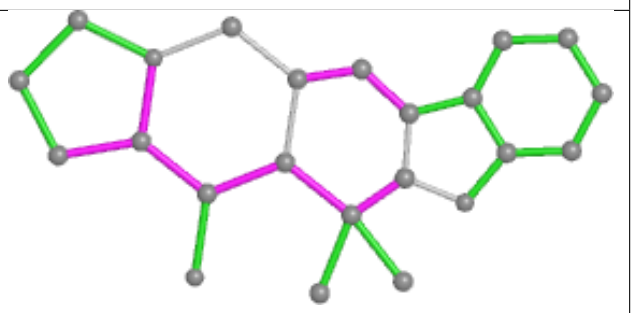
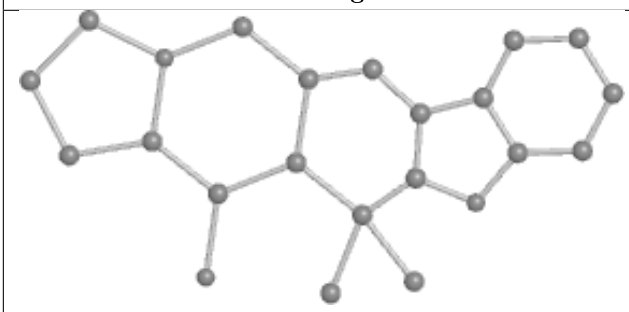


Bond angles



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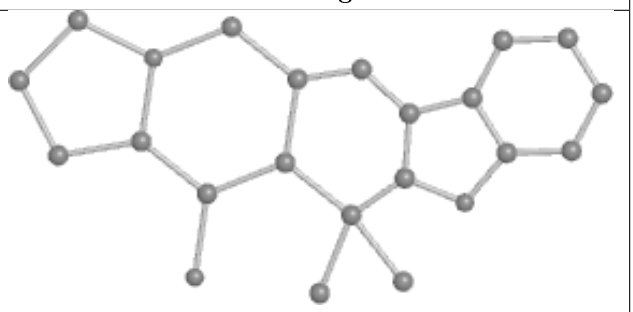
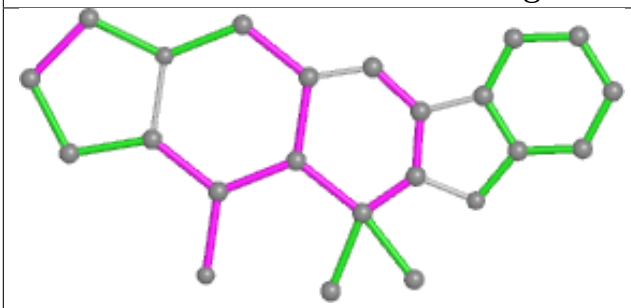


Rings

Ligand PM7 C 802



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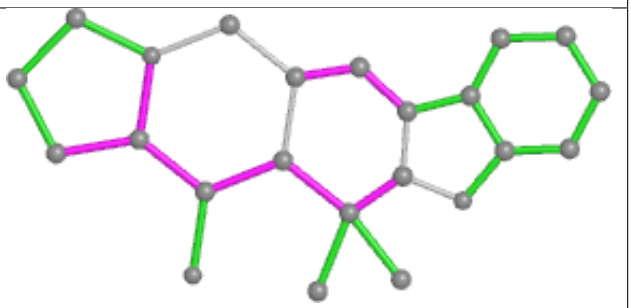
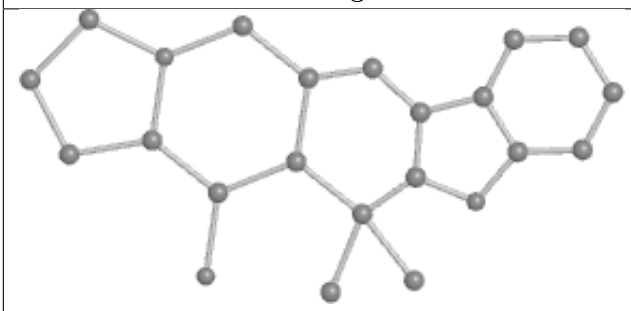
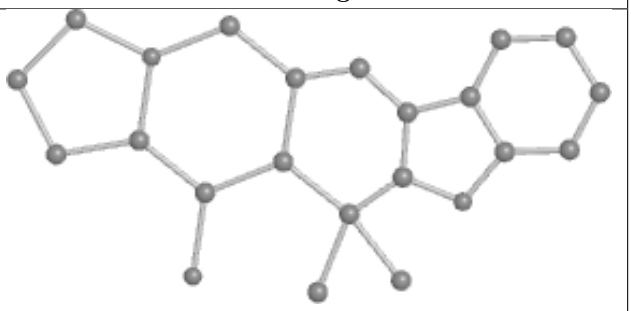


Bond angles

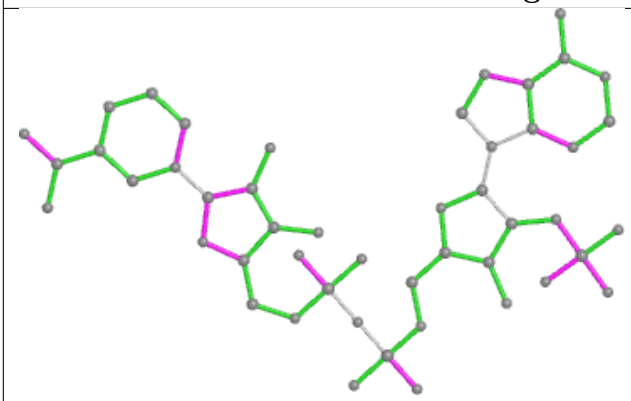


Torsions



Rings

Ligand NAP E 801



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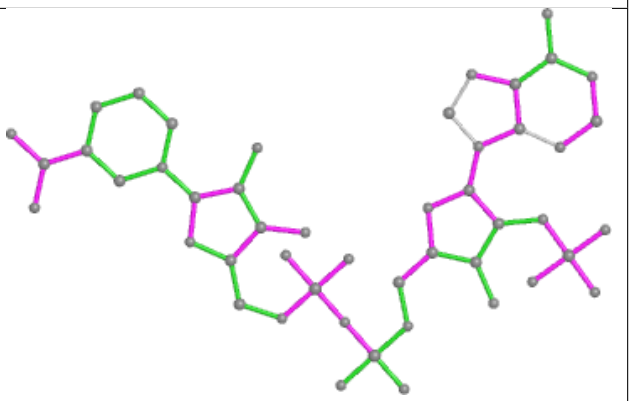
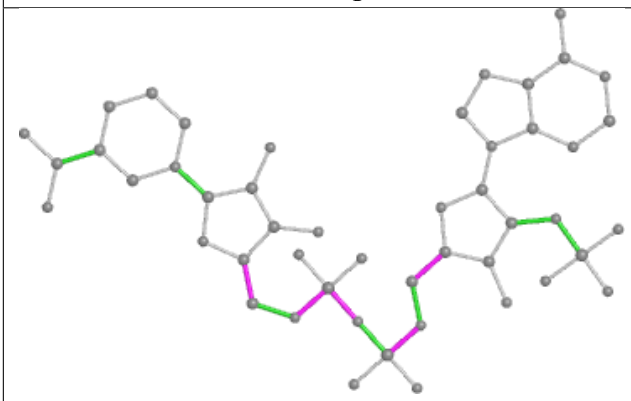
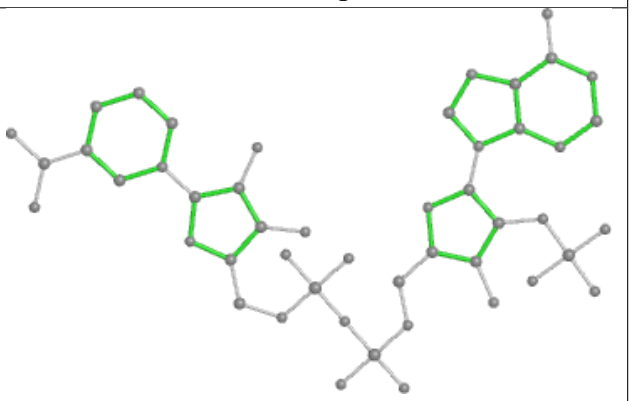


Bond angles

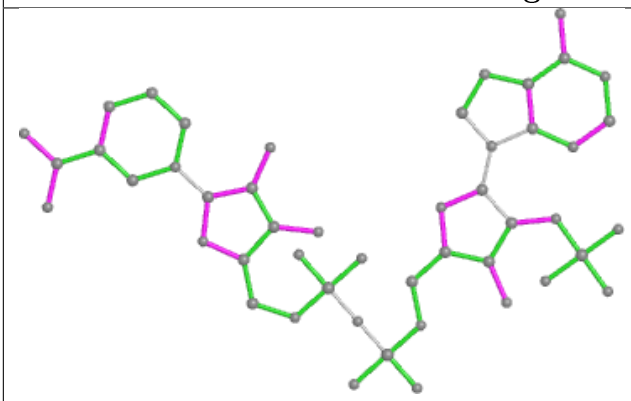


Torsions

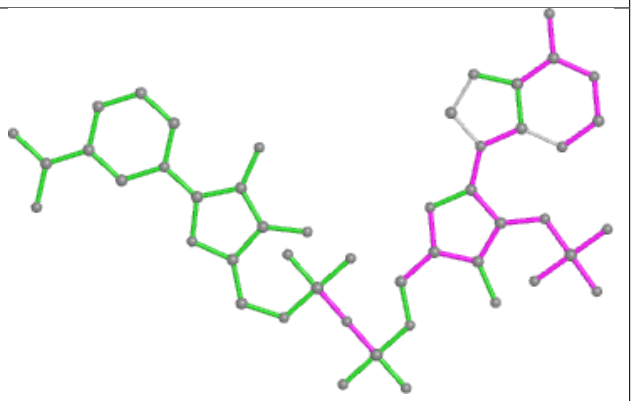


Rings

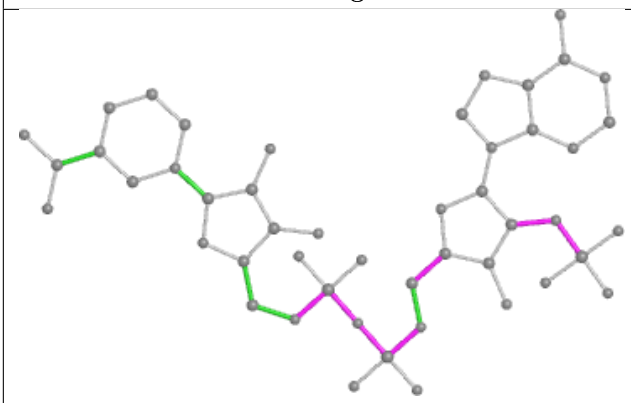
Ligand NAP F 801



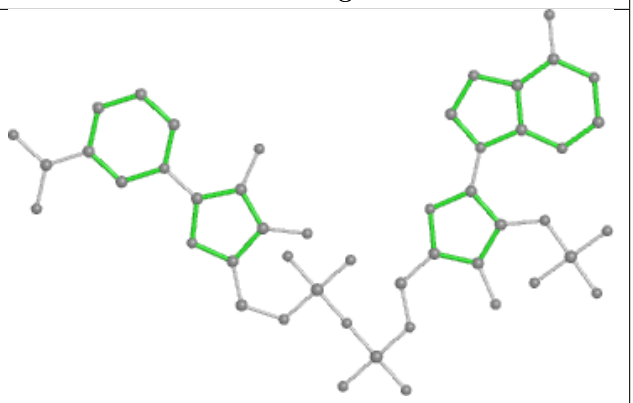
Bond lengths



Bond angles

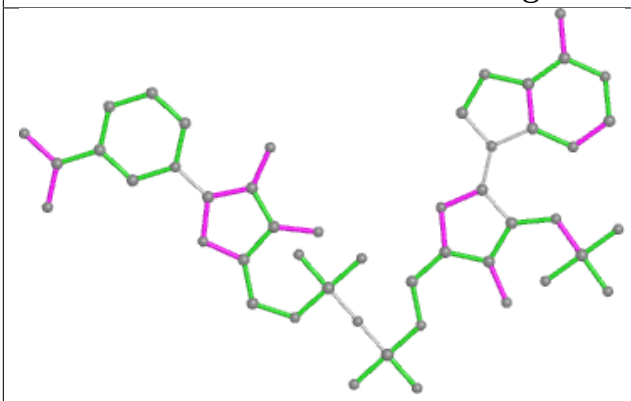


Torsions



Rings

Ligand NAP C 801



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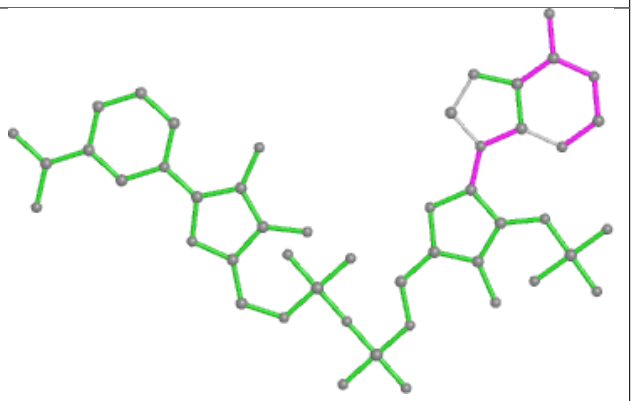

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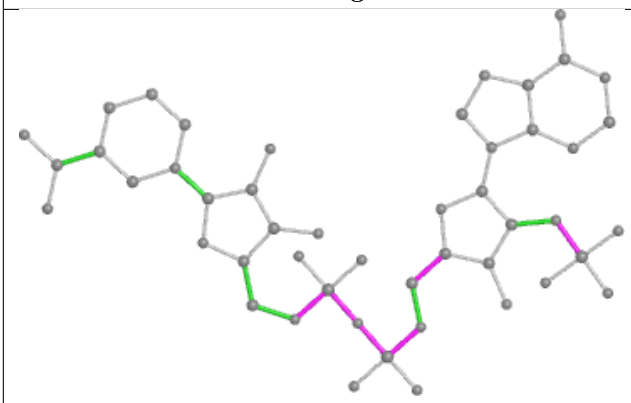
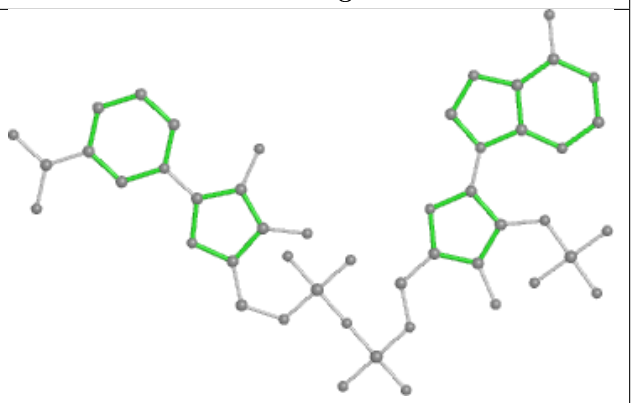
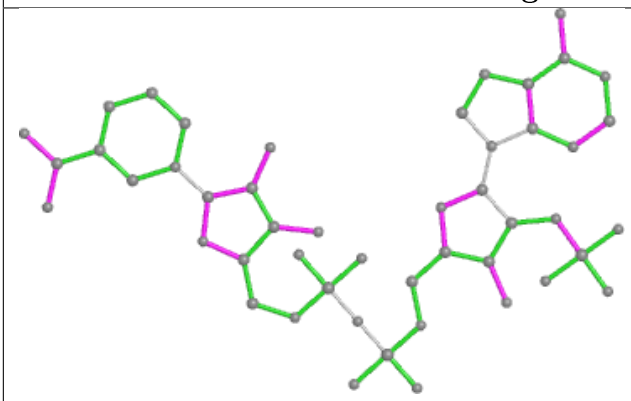


Torsions

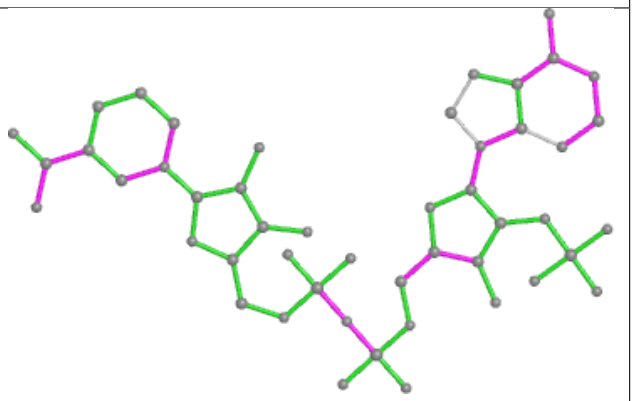


Rings

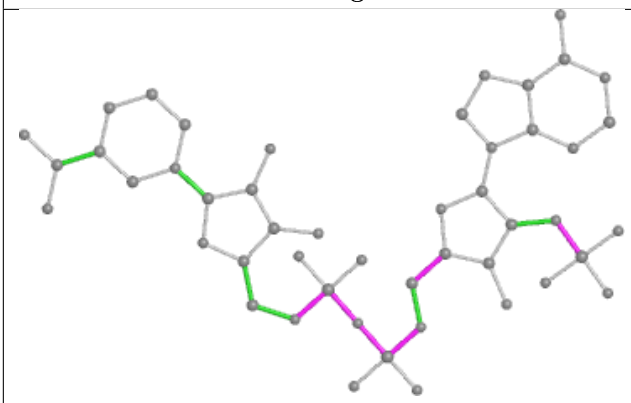
Ligand NAP D 801



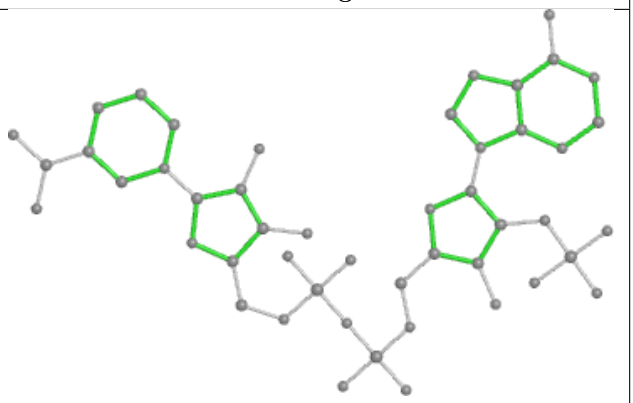
Bond lengths



Bond angles

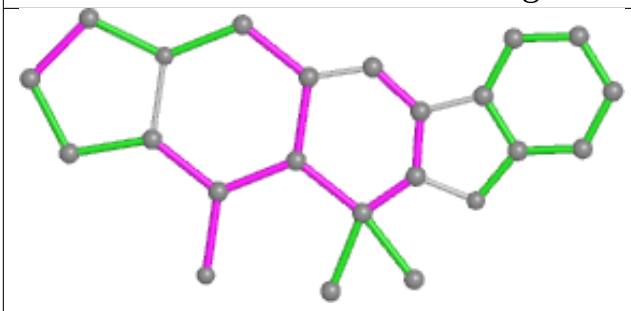


Torsions

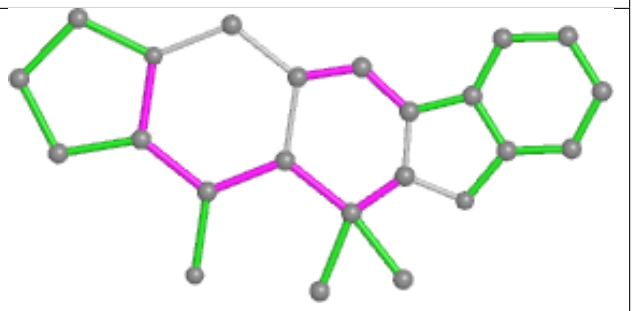


Rings

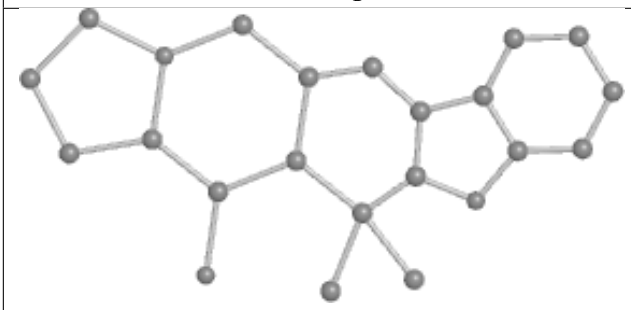
Ligand PM7 D 802



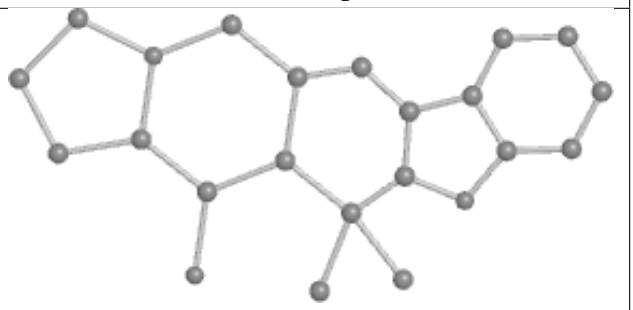
Bond lengths



Bond angles

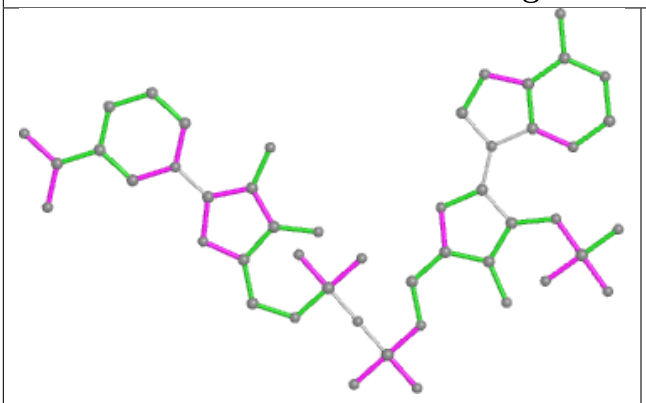


Torsions



Rings

Ligand NAP B 801



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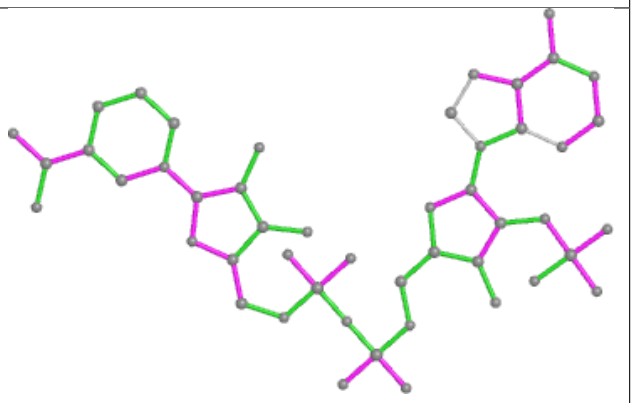
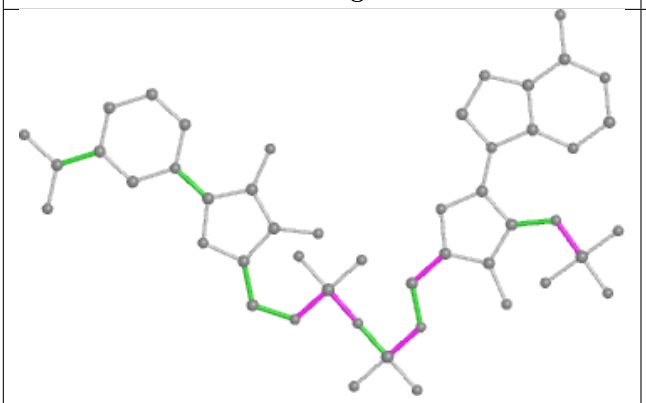
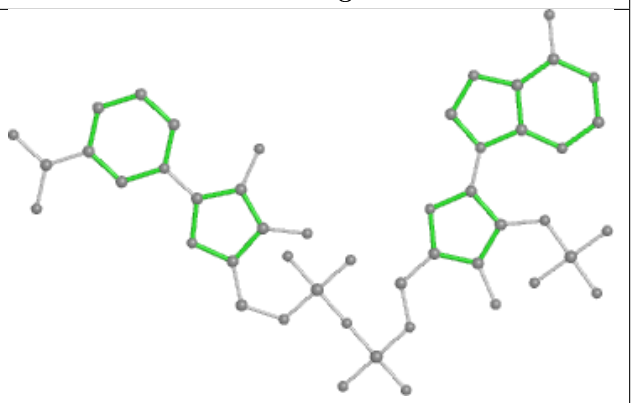


Bond angles

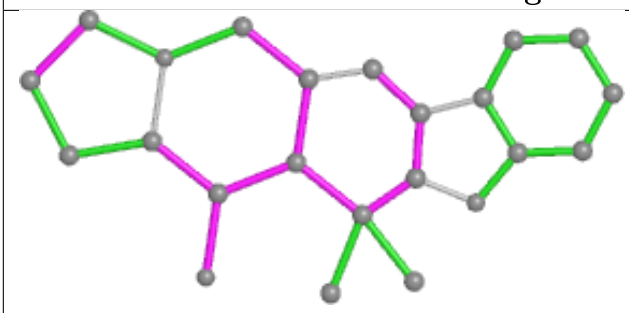


Torsions

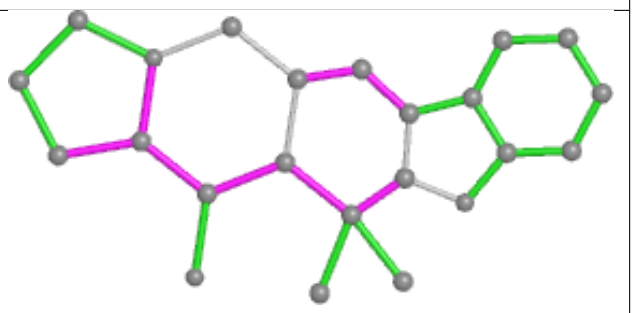


Rings

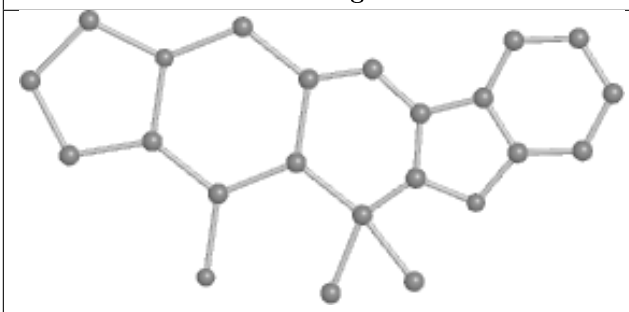
Ligand PM7 E 802



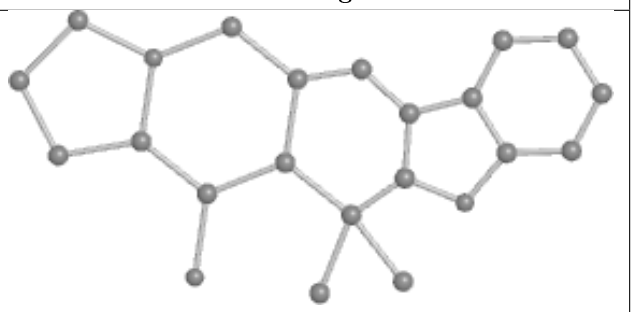
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	257/265 (96%)	1.18	37 (14%)	2	3	32, 54, 78, 119	0
1	B	257/265 (96%)	1.14	31 (12%)	4	6	31, 50, 79, 114	0
1	C	256/265 (96%)	1.39	53 (20%)	1	1	32, 63, 105, 123	0
1	D	257/265 (96%)	1.47	62 (24%)	0	0	36, 63, 105, 141	0
1	E	256/265 (96%)	2.61	143 (55%)	0	0	55, 88, 123, 154	0
1	F	256/265 (96%)	4.23	212 (82%)	0	0	82, 117, 150, 176	0
All	All	1539/1590 (96%)	2.00	538 (34%)	0	0	31, 67, 130, 176	0

The worst 5 of 538 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	130	ILE	23.7
1	F	255	VAL	14.0
1	F	19	VAL	13.8
1	E	240	GLN	12.4
1	F	119	LEU	10.7

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

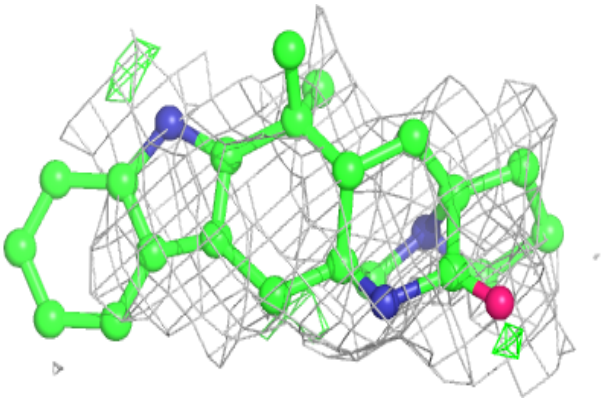
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

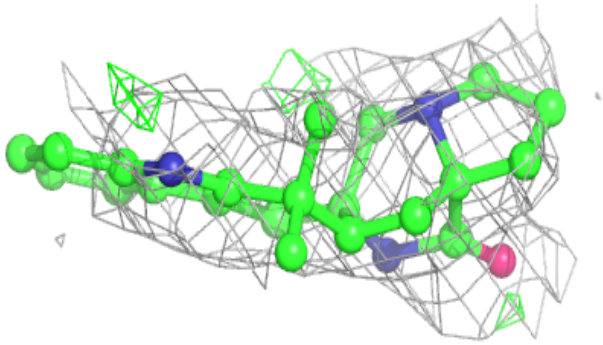
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PM7	F	802	25/25	0.54	0.37	72,94,107,112	0
2	NAP	F	801	48/48	0.76	0.27	77,100,116,121	0
3	PM7	E	802	25/25	0.81	0.39	80,90,106,107	0
2	NAP	C	801	48/48	0.84	0.21	42,58,83,85	0
3	PM7	A	802	25/25	0.84	0.22	51,60,68,74	0
3	PM7	D	802	25/25	0.85	0.24	59,63,69,70	0
3	PM7	B	802	25/25	0.86	0.19	33,47,51,60	0
2	NAP	E	801	48/48	0.86	0.17	63,78,89,97	0
3	PM7	C	802	25/25	0.86	0.20	51,61,72,74	0
2	NAP	A	801	48/48	0.87	0.18	35,51,62,69	0
2	NAP	D	801	48/48	0.88	0.17	42,63,76,77	0
2	NAP	B	801	48/48	0.93	0.15	33,44,60,65	0

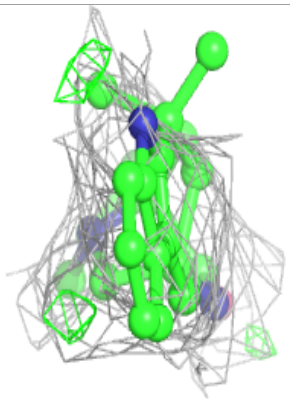
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PM7 F 802:

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

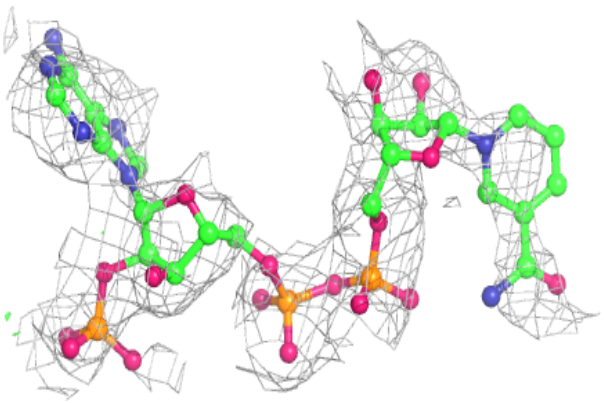


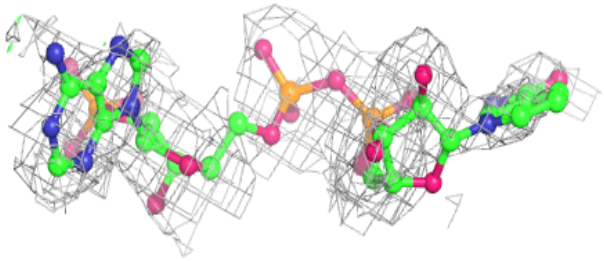


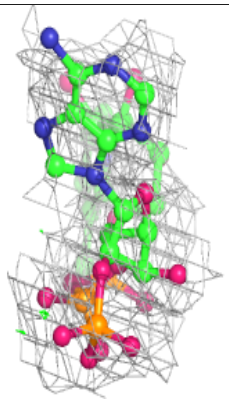


Electron density around NAP F 801:

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

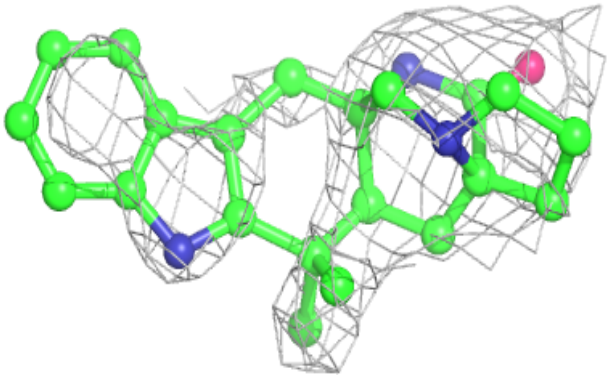


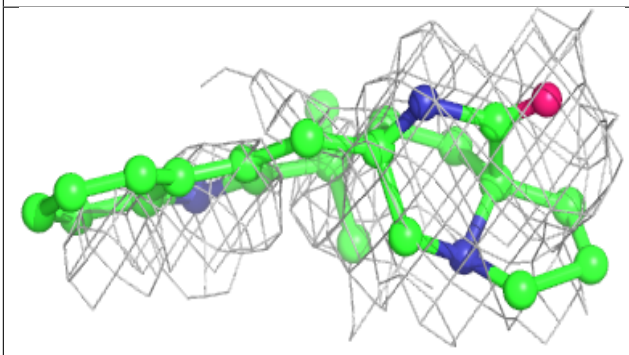


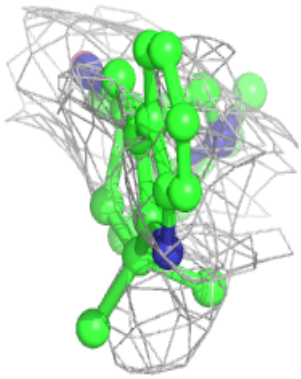


Electron density around PM7 E 802:

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

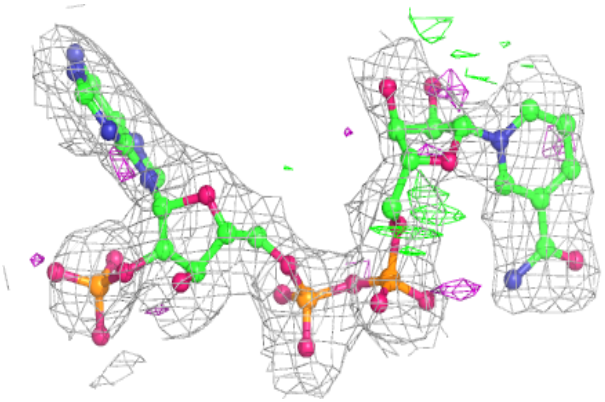


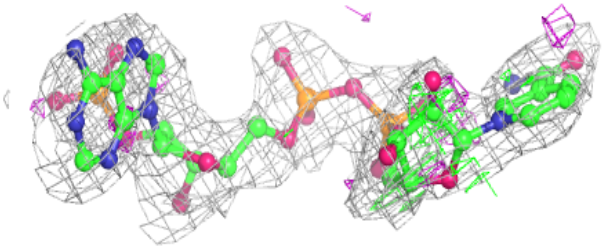


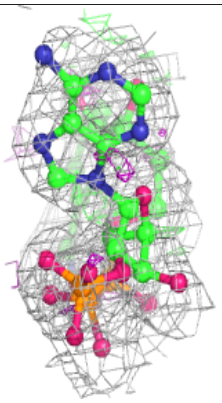


Electron density around NAP C 801:

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

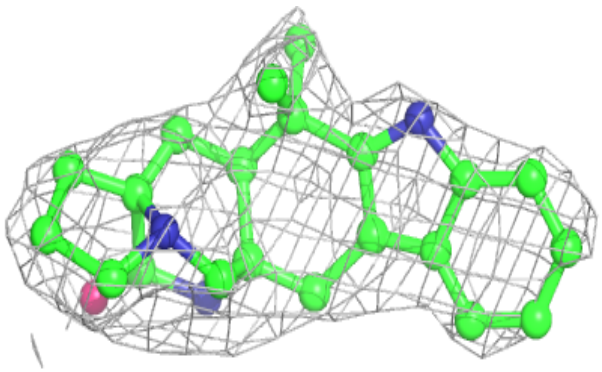


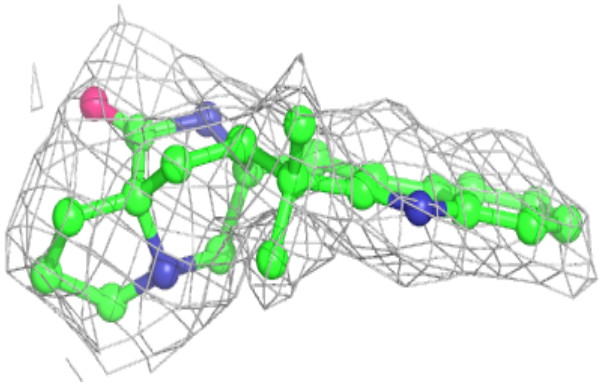


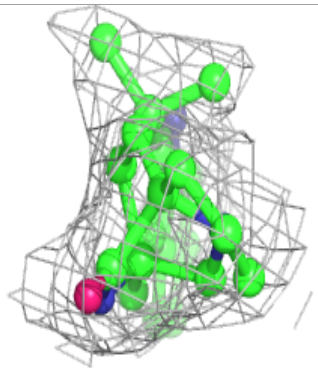


Electron density around PM7 A 802:

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

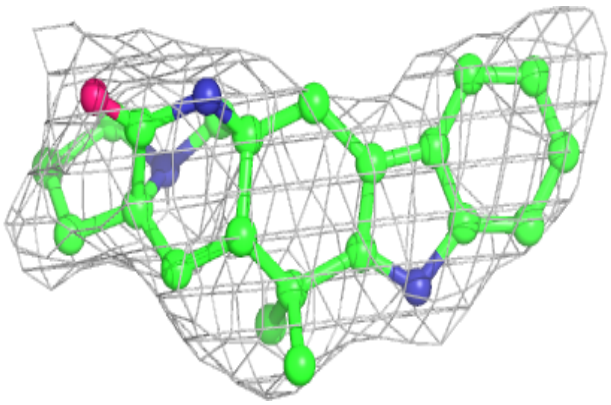


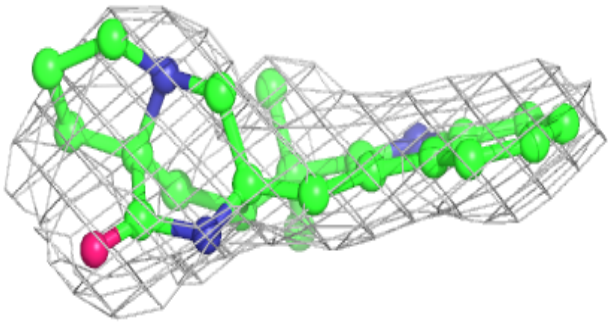


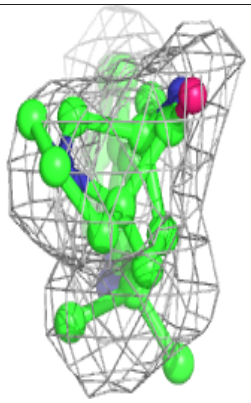


Electron density around PM7 D 802:

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

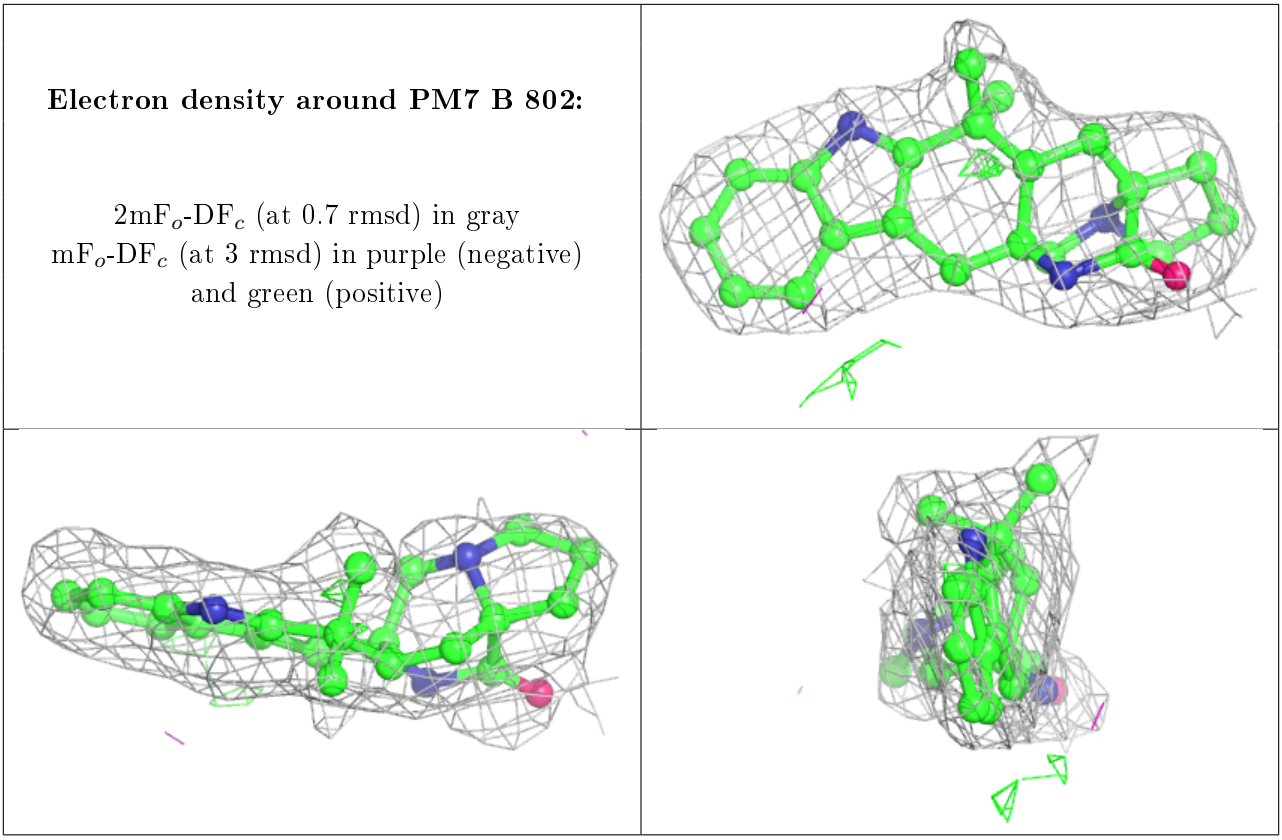






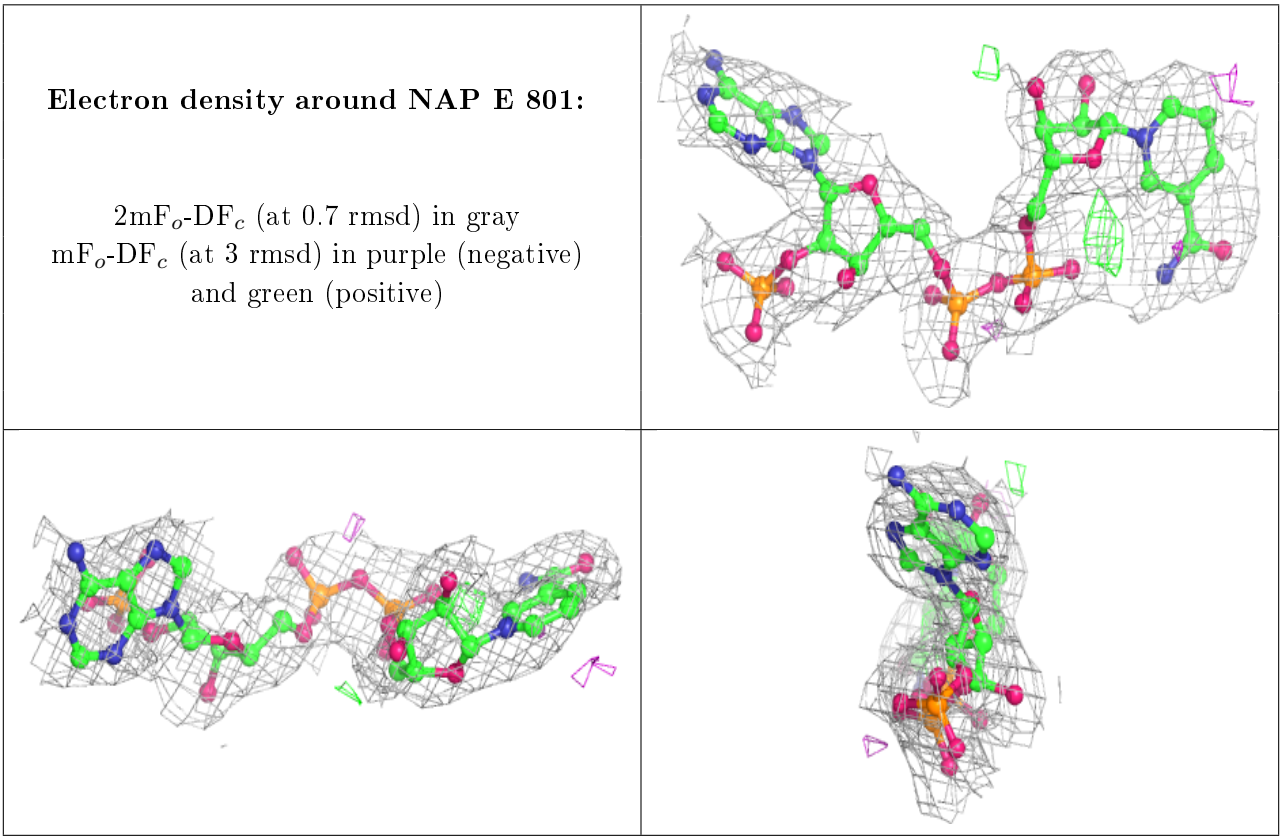
Electron density around PM7 B 802:

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



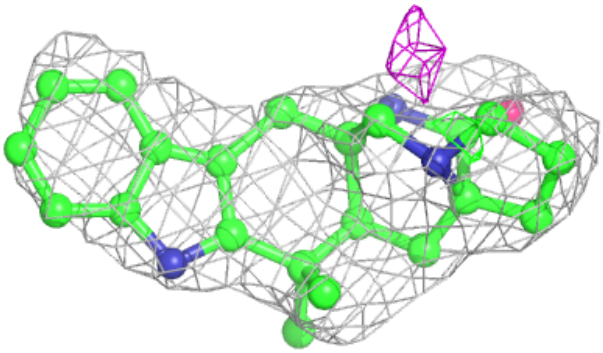
Electron density around NAP E 801:

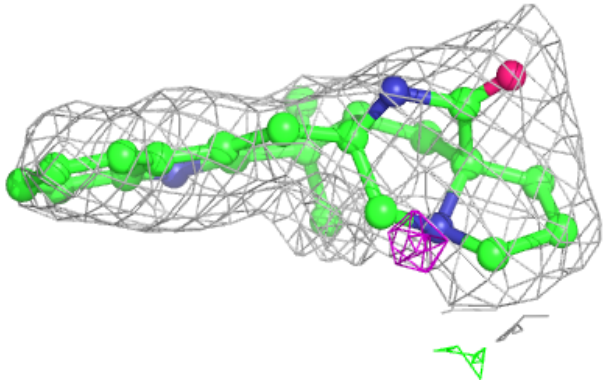
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

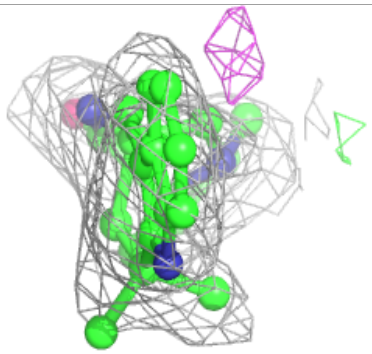


Electron density around PM7 C 802:

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

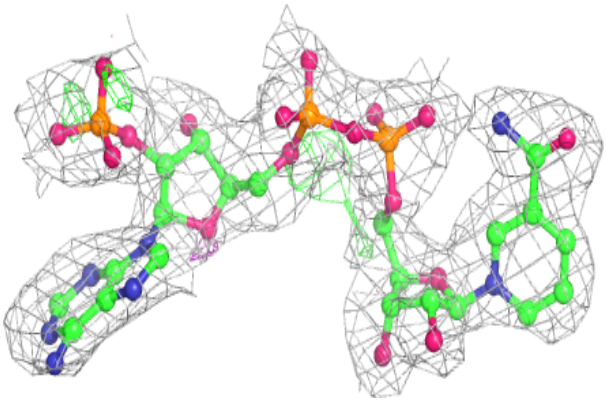


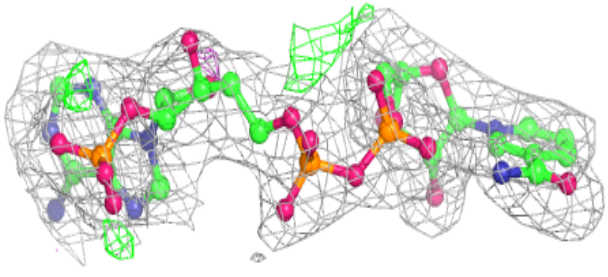


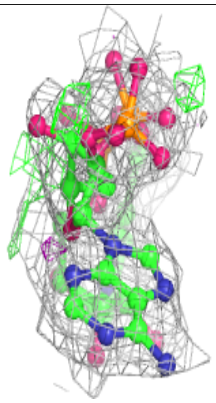


Electron density around NAP A 801:

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

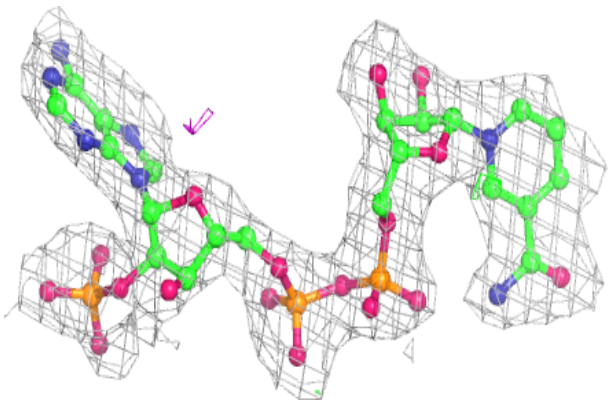


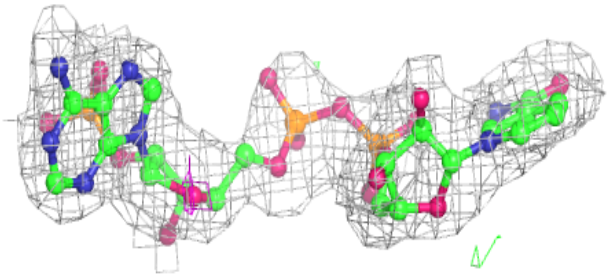


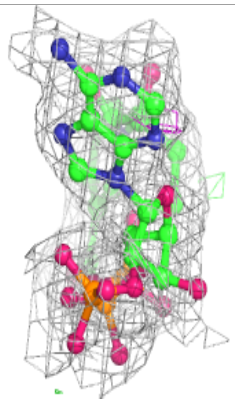


Electron density around NAP D 801:

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

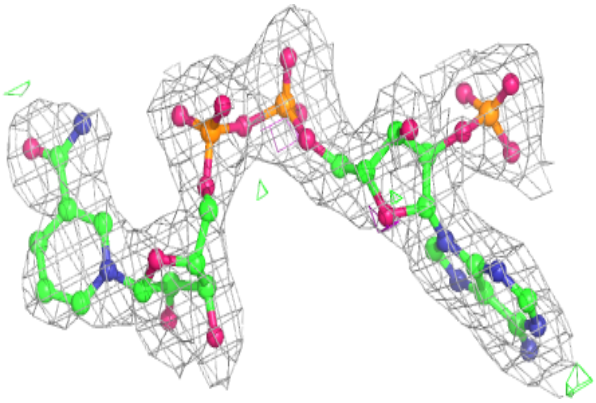


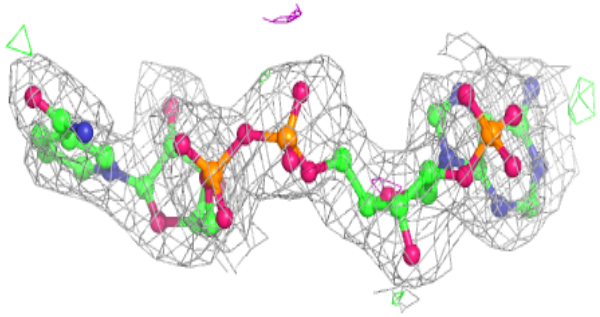


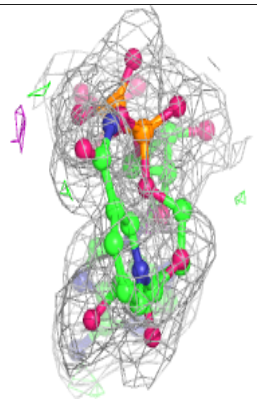


Electron density around NAP B 801:

$2mF_o$-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.