wwPDB X-ray Structure Validation Summary Report (i)

Apr 18, 2026 – 04:26 PM UTC

PDB ID	:	4D42 / pdb_00004d42
Title	:	Crystal structure of S. aureus FabI in complex with NADP and 4-fluoro- 5-hexyl-2-phenoxyphenol
Authors	:	Schiebel, J.; Chang, A.; Tonge, P.J.; Sotriffer, C.A.; Kisker, C.
Deposited on	:	2014-10-26
Resolution	:	2.02 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

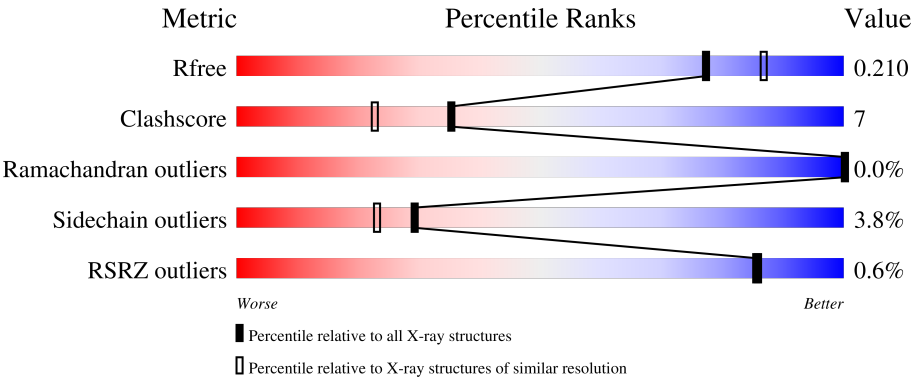
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.02 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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	77% 13% 10%
1	B	282	% 78% 11% • 10%
1	C	282	77% 13% • 10%
1	D	282	% 73% 16% • 10%
1	E	282	79% 11% 10%

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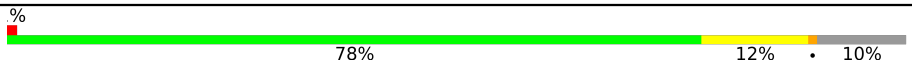
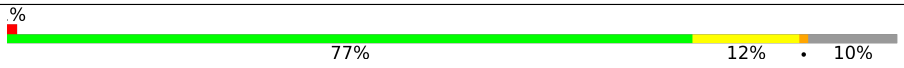
Mol	Chain	Length	Quality of chain
1	F	282	
1	G	282	
1	H	282	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLU	A	1258	-	-	X	-
2	GLU	B	1259	-	-	X	-
2	GLU	C	1259	-	-	X	-
2	GLU	E	1259	-	-	X	-
2	GLU	F	1259	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18217 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	11	0
			2049	1289	358	397	5			
1	B	255	Total	C	N	O	S	0	13	0
			2057	1293	357	402	5			
1	C	255	Total	C	N	O	S	0	11	0
			2045	1285	357	398	5			
1	D	255	Total	C	N	O	S	0	6	0
			2002	1261	350	387	4			
1	E	254	Total	C	N	O	S	0	12	0
			2044	1284	356	399	5			
1	F	255	Total	C	N	O	S	0	12	0
			2055	1294	359	397	5			
1	G	254	Total	C	N	O	S	0	7	0
			2001	1261	350	386	4			
1	H	254	Total	C	N	O	S	0	4	0
			1979	1246	343	386	4			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP Q7A6D8
A	-24	LYS	-	expression tag	UNP Q7A6D8
A	-23	HIS	-	expression tag	UNP Q7A6D8
A	-22	HIS	-	expression tag	UNP Q7A6D8
A	-21	HIS	-	expression tag	UNP Q7A6D8
A	-20	HIS	-	expression tag	UNP Q7A6D8
A	-19	HIS	-	expression tag	UNP Q7A6D8
A	-18	HIS	-	expression tag	UNP Q7A6D8
A	-17	PRO	-	expression tag	UNP Q7A6D8
A	-16	MET	-	expression tag	UNP Q7A6D8
A	-15	SER	-	expression tag	UNP Q7A6D8
A	-14	ASP	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	TYR	-	expression tag	UNP Q7A6D8
A	-12	ASP	-	expression tag	UNP Q7A6D8
A	-11	ILE	-	expression tag	UNP Q7A6D8
A	-10	PRO	-	expression tag	UNP Q7A6D8
A	-9	THR	-	expression tag	UNP Q7A6D8
A	-8	THR	-	expression tag	UNP Q7A6D8
A	-7	GLU	-	expression tag	UNP Q7A6D8
A	-6	ASN	-	expression tag	UNP Q7A6D8
A	-5	LEU	-	expression tag	UNP Q7A6D8
A	-4	TYR	-	expression tag	UNP Q7A6D8
A	-3	PHE	-	expression tag	UNP Q7A6D8
A	-2	GLN	-	expression tag	UNP Q7A6D8
A	-1	GLY	-	expression tag	UNP Q7A6D8
A	0	ALA	-	expression tag	UNP Q7A6D8
A	2	VAL	LEU	engineered mutation	UNP Q7A6D8
B	-25	MET	-	expression tag	UNP Q7A6D8
B	-24	LYS	-	expression tag	UNP Q7A6D8
B	-23	HIS	-	expression tag	UNP Q7A6D8
B	-22	HIS	-	expression tag	UNP Q7A6D8
B	-21	HIS	-	expression tag	UNP Q7A6D8
B	-20	HIS	-	expression tag	UNP Q7A6D8
B	-19	HIS	-	expression tag	UNP Q7A6D8
B	-18	HIS	-	expression tag	UNP Q7A6D8
B	-17	PRO	-	expression tag	UNP Q7A6D8
B	-16	MET	-	expression tag	UNP Q7A6D8
B	-15	SER	-	expression tag	UNP Q7A6D8
B	-14	ASP	-	expression tag	UNP Q7A6D8
B	-13	TYR	-	expression tag	UNP Q7A6D8
B	-12	ASP	-	expression tag	UNP Q7A6D8
B	-11	ILE	-	expression tag	UNP Q7A6D8
B	-10	PRO	-	expression tag	UNP Q7A6D8
B	-9	THR	-	expression tag	UNP Q7A6D8
B	-8	THR	-	expression tag	UNP Q7A6D8
B	-7	GLU	-	expression tag	UNP Q7A6D8
B	-6	ASN	-	expression tag	UNP Q7A6D8
B	-5	LEU	-	expression tag	UNP Q7A6D8
B	-4	TYR	-	expression tag	UNP Q7A6D8
B	-3	PHE	-	expression tag	UNP Q7A6D8
B	-2	GLN	-	expression tag	UNP Q7A6D8
B	-1	GLY	-	expression tag	UNP Q7A6D8
B	0	ALA	-	expression tag	UNP Q7A6D8
B	2	VAL	LEU	engineered mutation	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-25	MET	-	expression tag	UNP Q7A6D8
C	-24	LYS	-	expression tag	UNP Q7A6D8
C	-23	HIS	-	expression tag	UNP Q7A6D8
C	-22	HIS	-	expression tag	UNP Q7A6D8
C	-21	HIS	-	expression tag	UNP Q7A6D8
C	-20	HIS	-	expression tag	UNP Q7A6D8
C	-19	HIS	-	expression tag	UNP Q7A6D8
C	-18	HIS	-	expression tag	UNP Q7A6D8
C	-17	PRO	-	expression tag	UNP Q7A6D8
C	-16	MET	-	expression tag	UNP Q7A6D8
C	-15	SER	-	expression tag	UNP Q7A6D8
C	-14	ASP	-	expression tag	UNP Q7A6D8
C	-13	TYR	-	expression tag	UNP Q7A6D8
C	-12	ASP	-	expression tag	UNP Q7A6D8
C	-11	ILE	-	expression tag	UNP Q7A6D8
C	-10	PRO	-	expression tag	UNP Q7A6D8
C	-9	THR	-	expression tag	UNP Q7A6D8
C	-8	THR	-	expression tag	UNP Q7A6D8
C	-7	GLU	-	expression tag	UNP Q7A6D8
C	-6	ASN	-	expression tag	UNP Q7A6D8
C	-5	LEU	-	expression tag	UNP Q7A6D8
C	-4	TYR	-	expression tag	UNP Q7A6D8
C	-3	PHE	-	expression tag	UNP Q7A6D8
C	-2	GLN	-	expression tag	UNP Q7A6D8
C	-1	GLY	-	expression tag	UNP Q7A6D8
C	0	ALA	-	expression tag	UNP Q7A6D8
C	2	VAL	LEU	engineered mutation	UNP Q7A6D8
D	-25	MET	-	expression tag	UNP Q7A6D8
D	-24	LYS	-	expression tag	UNP Q7A6D8
D	-23	HIS	-	expression tag	UNP Q7A6D8
D	-22	HIS	-	expression tag	UNP Q7A6D8
D	-21	HIS	-	expression tag	UNP Q7A6D8
D	-20	HIS	-	expression tag	UNP Q7A6D8
D	-19	HIS	-	expression tag	UNP Q7A6D8
D	-18	HIS	-	expression tag	UNP Q7A6D8
D	-17	PRO	-	expression tag	UNP Q7A6D8
D	-16	MET	-	expression tag	UNP Q7A6D8
D	-15	SER	-	expression tag	UNP Q7A6D8
D	-14	ASP	-	expression tag	UNP Q7A6D8
D	-13	TYR	-	expression tag	UNP Q7A6D8
D	-12	ASP	-	expression tag	UNP Q7A6D8
D	-11	ILE	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	-	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8
D	-7	GLU	-	expression tag	UNP Q7A6D8
D	-6	ASN	-	expression tag	UNP Q7A6D8
D	-5	LEU	-	expression tag	UNP Q7A6D8
D	-4	TYR	-	expression tag	UNP Q7A6D8
D	-3	PHE	-	expression tag	UNP Q7A6D8
D	-2	GLN	-	expression tag	UNP Q7A6D8
D	-1	GLY	-	expression tag	UNP Q7A6D8
D	0	ALA	-	expression tag	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8
E	-25	MET	-	expression tag	UNP Q7A6D8
E	-24	LYS	-	expression tag	UNP Q7A6D8
E	-23	HIS	-	expression tag	UNP Q7A6D8
E	-22	HIS	-	expression tag	UNP Q7A6D8
E	-21	HIS	-	expression tag	UNP Q7A6D8
E	-20	HIS	-	expression tag	UNP Q7A6D8
E	-19	HIS	-	expression tag	UNP Q7A6D8
E	-18	HIS	-	expression tag	UNP Q7A6D8
E	-17	PRO	-	expression tag	UNP Q7A6D8
E	-16	MET	-	expression tag	UNP Q7A6D8
E	-15	SER	-	expression tag	UNP Q7A6D8
E	-14	ASP	-	expression tag	UNP Q7A6D8
E	-13	TYR	-	expression tag	UNP Q7A6D8
E	-12	ASP	-	expression tag	UNP Q7A6D8
E	-11	ILE	-	expression tag	UNP Q7A6D8
E	-10	PRO	-	expression tag	UNP Q7A6D8
E	-9	THR	-	expression tag	UNP Q7A6D8
E	-8	THR	-	expression tag	UNP Q7A6D8
E	-7	GLU	-	expression tag	UNP Q7A6D8
E	-6	ASN	-	expression tag	UNP Q7A6D8
E	-5	LEU	-	expression tag	UNP Q7A6D8
E	-4	TYR	-	expression tag	UNP Q7A6D8
E	-3	PHE	-	expression tag	UNP Q7A6D8
E	-2	GLN	-	expression tag	UNP Q7A6D8
E	-1	GLY	-	expression tag	UNP Q7A6D8
E	0	ALA	-	expression tag	UNP Q7A6D8
E	2	VAL	LEU	engineered mutation	UNP Q7A6D8
F	-25	MET	-	expression tag	UNP Q7A6D8
F	-24	LYS	-	expression tag	UNP Q7A6D8
F	-23	HIS	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-22	HIS	-	expression tag	UNP Q7A6D8
F	-21	HIS	-	expression tag	UNP Q7A6D8
F	-20	HIS	-	expression tag	UNP Q7A6D8
F	-19	HIS	-	expression tag	UNP Q7A6D8
F	-18	HIS	-	expression tag	UNP Q7A6D8
F	-17	PRO	-	expression tag	UNP Q7A6D8
F	-16	MET	-	expression tag	UNP Q7A6D8
F	-15	SER	-	expression tag	UNP Q7A6D8
F	-14	ASP	-	expression tag	UNP Q7A6D8
F	-13	TYR	-	expression tag	UNP Q7A6D8
F	-12	ASP	-	expression tag	UNP Q7A6D8
F	-11	ILE	-	expression tag	UNP Q7A6D8
F	-10	PRO	-	expression tag	UNP Q7A6D8
F	-9	THR	-	expression tag	UNP Q7A6D8
F	-8	THR	-	expression tag	UNP Q7A6D8
F	-7	GLU	-	expression tag	UNP Q7A6D8
F	-6	ASN	-	expression tag	UNP Q7A6D8
F	-5	LEU	-	expression tag	UNP Q7A6D8
F	-4	TYR	-	expression tag	UNP Q7A6D8
F	-3	PHE	-	expression tag	UNP Q7A6D8
F	-2	GLN	-	expression tag	UNP Q7A6D8
F	-1	GLY	-	expression tag	UNP Q7A6D8
F	0	ALA	-	expression tag	UNP Q7A6D8
F	2	VAL	LEU	engineered mutation	UNP Q7A6D8
G	-25	MET	-	expression tag	UNP Q7A6D8
G	-24	LYS	-	expression tag	UNP Q7A6D8
G	-23	HIS	-	expression tag	UNP Q7A6D8
G	-22	HIS	-	expression tag	UNP Q7A6D8
G	-21	HIS	-	expression tag	UNP Q7A6D8
G	-20	HIS	-	expression tag	UNP Q7A6D8
G	-19	HIS	-	expression tag	UNP Q7A6D8
G	-18	HIS	-	expression tag	UNP Q7A6D8
G	-17	PRO	-	expression tag	UNP Q7A6D8
G	-16	MET	-	expression tag	UNP Q7A6D8
G	-15	SER	-	expression tag	UNP Q7A6D8
G	-14	ASP	-	expression tag	UNP Q7A6D8
G	-13	TYR	-	expression tag	UNP Q7A6D8
G	-12	ASP	-	expression tag	UNP Q7A6D8
G	-11	ILE	-	expression tag	UNP Q7A6D8
G	-10	PRO	-	expression tag	UNP Q7A6D8
G	-9	THR	-	expression tag	UNP Q7A6D8
G	-8	THR	-	expression tag	UNP Q7A6D8

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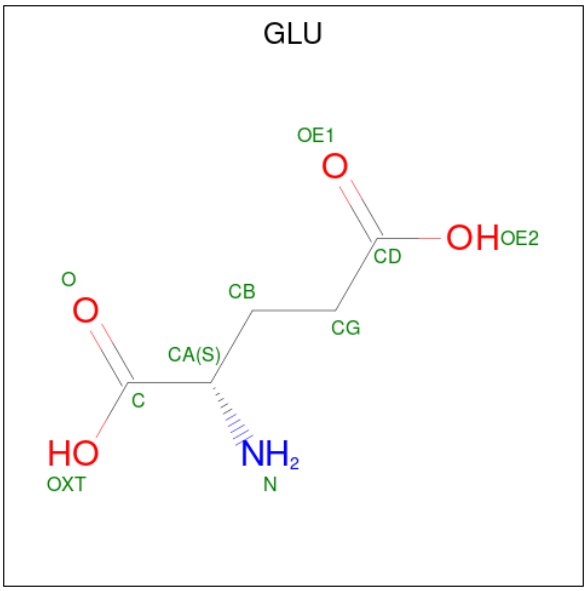
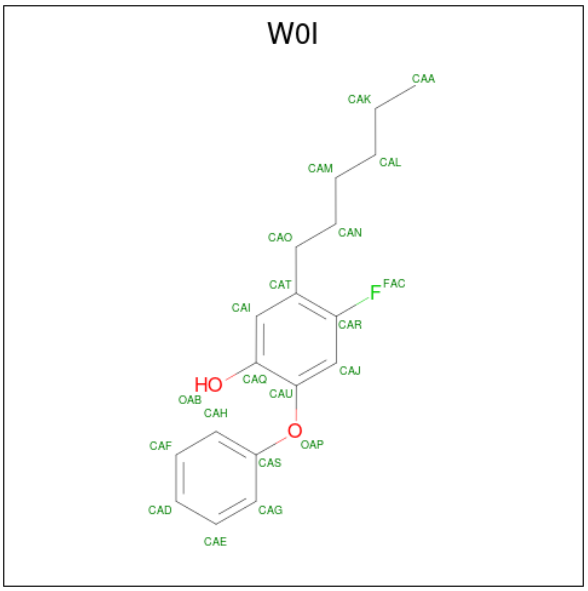
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8
G	0	ALA	-	expression tag	UNP Q7A6D8
G	2	VAL	LEU	engineered mutation	UNP Q7A6D8
H	-25	MET	-	expression tag	UNP Q7A6D8
H	-24	LYS	-	expression tag	UNP Q7A6D8
H	-23	HIS	-	expression tag	UNP Q7A6D8
H	-22	HIS	-	expression tag	UNP Q7A6D8
H	-21	HIS	-	expression tag	UNP Q7A6D8
H	-20	HIS	-	expression tag	UNP Q7A6D8
H	-19	HIS	-	expression tag	UNP Q7A6D8
H	-18	HIS	-	expression tag	UNP Q7A6D8
H	-17	PRO	-	expression tag	UNP Q7A6D8
H	-16	MET	-	expression tag	UNP Q7A6D8
H	-15	SER	-	expression tag	UNP Q7A6D8
H	-14	ASP	-	expression tag	UNP Q7A6D8
H	-13	TYR	-	expression tag	UNP Q7A6D8
H	-12	ASP	-	expression tag	UNP Q7A6D8
H	-11	ILE	-	expression tag	UNP Q7A6D8
H	-10	PRO	-	expression tag	UNP Q7A6D8
H	-9	THR	-	expression tag	UNP Q7A6D8
H	-8	THR	-	expression tag	UNP Q7A6D8
H	-7	GLU	-	expression tag	UNP Q7A6D8
H	-6	ASN	-	expression tag	UNP Q7A6D8
H	-5	LEU	-	expression tag	UNP Q7A6D8
H	-4	TYR	-	expression tag	UNP Q7A6D8
H	-3	PHE	-	expression tag	UNP Q7A6D8
H	-2	GLN	-	expression tag	UNP Q7A6D8
H	-1	GLY	-	expression tag	UNP Q7A6D8
H	0	ALA	-	expression tag	UNP Q7A6D8
H	2	VAL	LEU	engineered mutation	UNP Q7A6D8

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



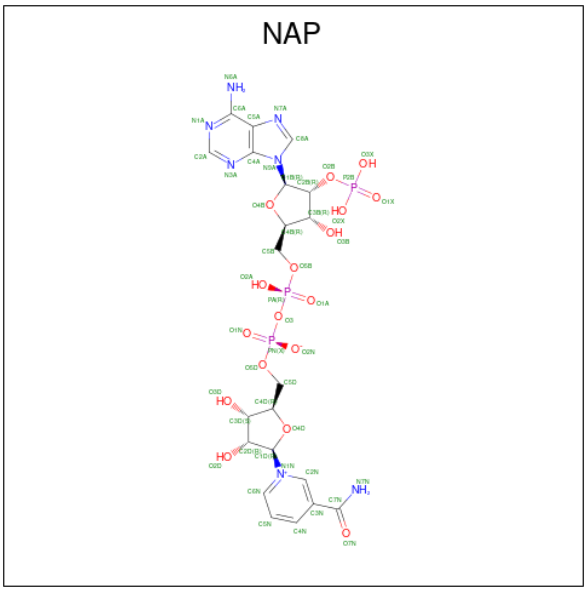
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 10 5 1 4	0	0
2	B	1	Total C N O 10 5 1 4	0	0
2	C	1	Total C N O 10 5 1 4	0	0
2	E	1	Total C N O 10 5 1 4	0	0
2	F	1	Total C N O 10 5 1 4	0	0
2	G	1	Total C N O 10 5 1 4	0	0

- Molecule 3 is 4-fluoro-5-hexyl-2-phenoxyphenol (CCD ID: W0I) (formula: $C_{18}H_{21}FO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F O 21 18 1 2	0	0
3	B	1	Total C F O 21 18 1 2	0	0
3	C	1	Total C F O 21 18 1 2	0	0
3	D	1	Total C F O 21 18 1 2	0	0
3	E	1	Total C F O 21 18 1 2	0	0
3	F	1	Total C F O 21 18 1 2	0	0
3	G	1	Total C F O 21 18 1 2	0	0
3	H	1	Total C F O 21 18 1 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	B	179	Total	O	0	0
			179	179		
5	C	189	Total	O	0	0
			189	189		
5	D	125	Total	O	0	0
			125	125		

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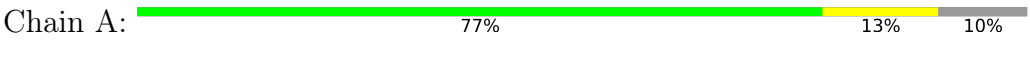
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	207	Total O 207 207	0	0
5	F	169	Total O 169 169	0	0
5	G	160	Total O 160 160	0	0
5	H	129	Total O 129 129	0	0

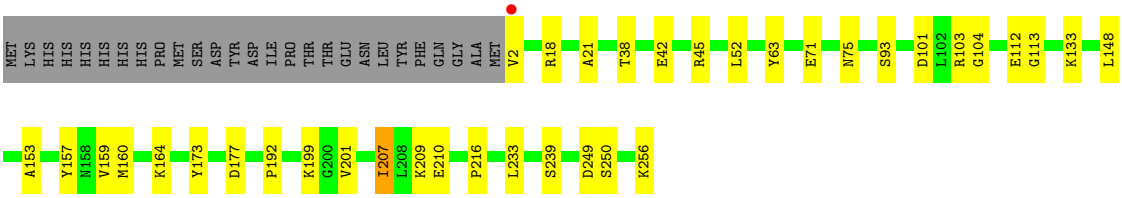
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain A:

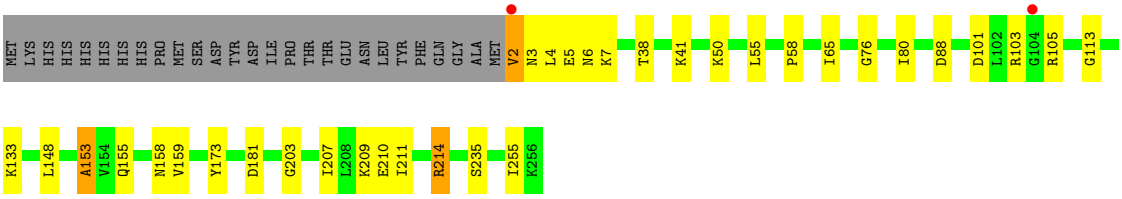




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain B:

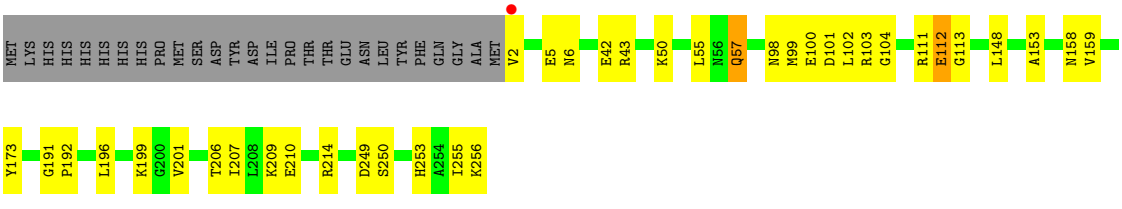




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain C:

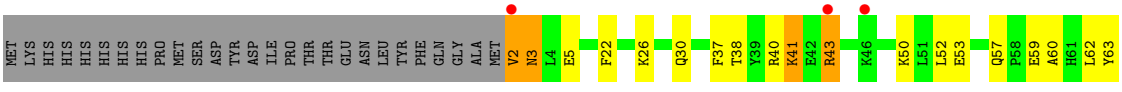




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain D:



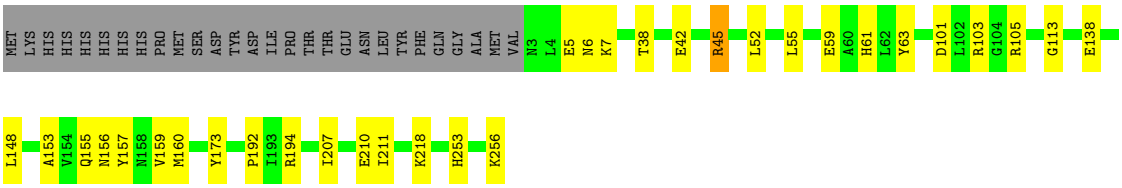




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain E:

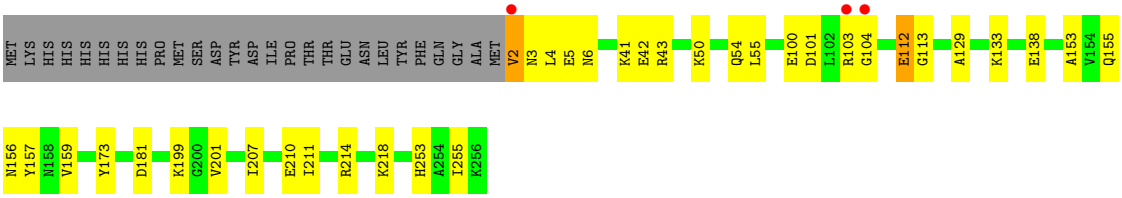




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain F:

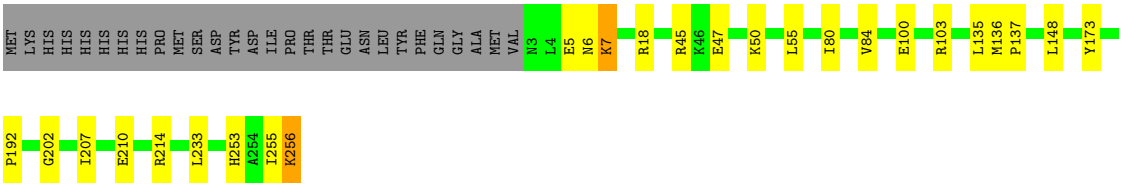




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain G:

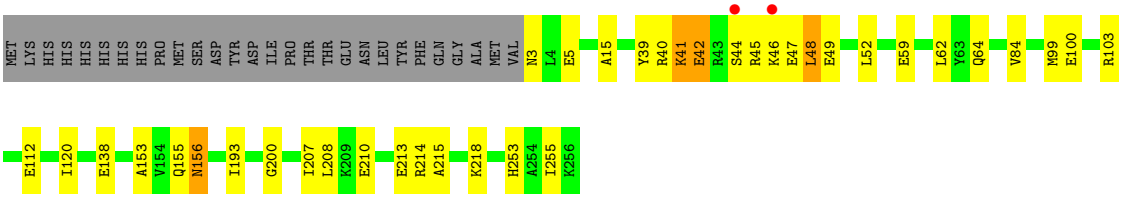




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.35Å 94.86Å 94.90Å 98.19° 97.22° 112.46°	Depositor
Resolution (Å)	38.44 – 2.02 38.44 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.44-2.02) 97.8 (38.44-2.02)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.145 , 0.185 0.177 , 0.210	Depositor DCC
R_{free} test set	9096 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18217	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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, W0I

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	0.82	0/2088	1.04	1/2810 (0.0%)
1	B	0.78	1/2096 (0.0%)	1.00	0/2821
1	C	0.71	0/2078	0.99	3/2797 (0.1%)
1	D	0.74	0/2041	1.05	4/2748 (0.1%)
1	E	0.81	0/2080	1.09	0/2799
1	F	0.79	1/2097 (0.0%)	1.00	3/2821 (0.1%)
1	G	0.72	0/2043	1.02	0/2749
1	H	0.71	0/2012	1.04	1/2710 (0.0%)
All	All	0.76	2/16535 (0.0%)	1.03	12/22255 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	129	ALA	CA-CB	5.61	1.62	1.53
1	B	153	ALA	CA-CB	-5.43	1.46	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	57	GLN	CA-C-N	-7.96	111.62	120.45
1	D	57	GLN	C-N-CA	-7.96	111.62	120.45
1	A	239	SER	N-CA-C	5.88	118.47	111.71
1	H	59	GLU	N-CA-C	5.87	118.78	109.50
1	F	138	GLU	N-CA-C	5.78	119.31	112.72

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	2049	0	2073	42	1
1	B	2057	0	2073	30	0
1	C	2045	0	2061	58	0
1	D	2002	0	2029	42	0
1	E	2044	0	2058	31	0
1	F	2055	0	2086	45	0
1	G	2001	0	2033	18	0
1	H	1979	0	1994	19	0
2	A	10	0	5	4	0
2	B	10	0	5	9	0
2	C	10	0	5	10	0
2	E	10	0	5	4	0
2	F	10	0	5	11	0
2	G	10	0	5	2	0
3	A	21	0	20	2	0
3	B	21	0	20	1	0
3	C	21	0	20	2	0
3	D	21	0	21	1	0
3	E	21	0	20	1	0
3	F	21	0	20	2	0
3	G	21	0	20	0	0
3	H	21	0	21	0	0
4	A	48	0	25	0	0
4	B	48	0	25	0	0
4	C	48	0	25	1	0
4	D	48	0	25	4	0
4	E	48	0	25	0	0
4	F	48	0	25	1	0
4	G	48	0	25	1	0
4	H	48	0	25	2	0
5	A	215	0	0	7	0
5	B	179	0	0	5	0
5	C	189	0	0	11	0
5	D	125	0	0	5	0
5	E	207	0	0	3	1
5	F	169	0	0	6	0
5	G	160	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	129	0	0	3	0
All	All	18217	0	16799	250	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 7.

The worst 5 of 250 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:C:104[B]:GLY:HA3	5:C:2104:HOH:O	1.30	1.31
1:A:2:VAL:HG12	1:D:2:VAL:HG13	1.16	1.15
1:B:103[A]:ARG:NH1	2:B:1259:GLU:HG3	1.70	1.07
1:C:98:ASN:HB3	1:C:100[B]:GLU:HG2	1.36	1.04
1:A:18[A]:ARG:HH22	1:A:199:LYS:HZ2	0.96	0.95

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:A:42[A]:GLU:OE2	5:E:2120:HOH:O[1_554]	1.95	0.25

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	264/282 (94%)	252 (96%)	12 (4%)	0	100	100
1	B	266/282 (94%)	254 (96%)	12 (4%)	0	100	100
1	C	264/282 (94%)	256 (97%)	8 (3%)	0	100	100
1	D	259/282 (92%)	249 (96%)	10 (4%)	0	100	100
1	E	264/282 (94%)	256 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	265/282 (94%)	251 (95%)	14 (5%)	0	100 100
1	G	259/282 (92%)	251 (97%)	8 (3%)	0	100 100
1	H	256/282 (91%)	240 (94%)	15 (6%)	1 (0%)	30 22
All	All	2097/2256 (93%)	2009 (96%)	87 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	156	ASN

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	219/234 (94%)	214 (98%)	5 (2%)	44 43
1	B	220/234 (94%)	212 (96%)	8 (4%)	31 26
1	C	218/234 (93%)	212 (97%)	6 (3%)	38 35
1	D	214/234 (92%)	204 (95%)	10 (5%)	23 16
1	E	218/234 (93%)	215 (99%)	3 (1%)	59 61
1	F	220/234 (94%)	213 (97%)	7 (3%)	34 30
1	G	214/234 (92%)	206 (96%)	8 (4%)	30 24
1	H	211/234 (90%)	196 (93%)	15 (7%)	13 7
All	All	1734/1872 (93%)	1672 (96%)	62 (4%)	29 26

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	255	ILE
1	H	84	VAL
1	F	55	LEU
1	H	64	GLN
1	H	207	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	253	HIS
1	G	156	ASN
1	H	253	HIS
1	H	3	ASN
1	H	30	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	W0I	D	1258	-	22,22,22	0.69	0	28,28,28	1.23	2 (7%)
4	NAP	F	1257	-	50,52,52	1.62	6 (12%)	71,80,80	1.78	17 (23%)
2	GLU	B	1259	-	8,9,9	1.04	0	8,11,11	1.20	1 (12%)
4	NAP	C	1257	-	50,52,52	1.55	3 (6%)	71,80,80	1.74	14 (19%)
2	GLU	A	1258	-	8,9,9	1.17	0	8,11,11	1.08	0
4	NAP	E	1257	-	50,52,52	1.59	8 (16%)	71,80,80	1.88	14 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLU	E	1259	-	8,9,9	1.07	0	8,11,11	0.94	0
3	W0I	B	1258	-	22,22,22	0.76	0	28,28,28	1.22	4 (14%)
2	GLU	C	1259	-	8,9,9	1.18	0	8,11,11	0.84	0
2	GLU	G	1259	-	8,9,9	1.13	0	8,11,11	0.99	0
4	NAP	A	1260	-	50,52,52	1.53	6 (12%)	71,80,80	1.81	15 (21%)
3	W0I	G	1258	-	22,22,22	0.86	0	28,28,28	1.36	5 (17%)
3	W0I	H	1258	-	22,22,22	0.82	0	28,28,28	1.21	4 (14%)
2	GLU	F	1259	-	8,9,9	1.13	0	8,11,11	0.96	0
3	W0I	F	1258	-	22,22,22	0.72	0	28,28,28	1.17	3 (10%)
3	W0I	E	1258	-	22,22,22	0.79	0	28,28,28	1.24	5 (17%)
4	NAP	G	1257	-	50,52,52	1.59	4 (8%)	71,80,80	1.74	19 (26%)
3	W0I	C	1258	-	22,22,22	1.00	0	28,28,28	1.44	5 (17%)
4	NAP	B	1257	-	50,52,52	1.64	7 (14%)	71,80,80	1.75	15 (21%)
4	NAP	D	1257	-	50,52,52	1.68	6 (12%)	71,80,80	1.63	17 (23%)
4	NAP	H	1257	-	50,52,52	1.56	4 (8%)	71,80,80	1.74	19 (26%)
3	W0I	A	1257	-	22,22,22	0.84	1 (4%)	28,28,28	1.20	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	W0I	D	1258	-	-	2/10/10/10	0/2/2/2
4	NAP	F	1257	-	-	6/35/67/67	0/5/5/5
2	GLU	B	1259	-	-	8/9/9/9	-
4	NAP	C	1257	-	-	7/35/67/67	0/5/5/5
2	GLU	A	1258	-	-	2/9/9/9	-
4	NAP	E	1257	-	-	7/35/67/67	0/5/5/5
2	GLU	E	1259	-	-	5/9/9/9	-
3	W0I	B	1258	-	-	0/10/10/10	0/2/2/2
2	GLU	C	1259	-	-	5/9/9/9	-
2	GLU	G	1259	-	-	2/9/9/9	-
4	NAP	A	1260	-	-	7/35/67/67	0/5/5/5
3	W0I	G	1258	-	-	2/10/10/10	0/2/2/2
3	W0I	H	1258	-	-	2/10/10/10	0/2/2/2
2	GLU	F	1259	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	W0I	F	1258	-	-	2/10/10/10	0/2/2/2
3	W0I	E	1258	-	-	1/10/10/10	0/2/2/2
4	NAP	G	1257	-	-	7/35/67/67	0/5/5/5
3	W0I	C	1258	-	-	2/10/10/10	0/2/2/2
4	NAP	B	1257	-	-	6/35/67/67	0/5/5/5
4	NAP	D	1257	-	-	8/35/67/67	0/5/5/5
4	NAP	H	1257	-	-	6/35/67/67	0/5/5/5
3	W0I	A	1257	-	-	3/10/10/10	0/2/2/2

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1257	NAP	O7N-C7N	8.69	1.40	1.24
4	G	1257	NAP	O7N-C7N	8.23	1.39	1.24
4	C	1257	NAP	O7N-C7N	8.20	1.39	1.24
4	H	1257	NAP	O7N-C7N	8.09	1.39	1.24
4	F	1257	NAP	O7N-C7N	7.52	1.38	1.24

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1257	NAP	C3N-C7N-N7N	7.25	126.68	117.74
4	H	1257	NAP	N3A-C2A-N1A	-6.27	119.10	128.58
4	F	1257	NAP	C3N-C7N-N7N	6.24	125.43	117.74
4	F	1257	NAP	N3A-C2A-N1A	-6.09	119.36	128.58
4	A	1260	NAP	C3N-C7N-N7N	5.96	125.08	117.74

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1258	GLU	N-CA-CB-CG
2	B	1259	GLU	O-C-CA-N
2	B	1259	GLU	N-CA-CB-CG
2	B	1259	GLU	C-CA-CB-CG
2	C	1259	GLU	N-CA-CB-CG

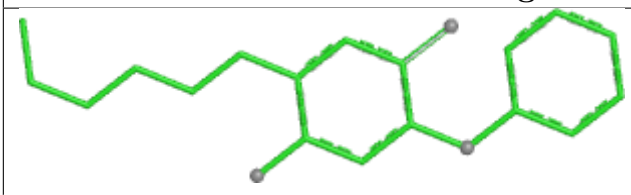
There are no ring outliers.

17 monomers are involved in 57 short contacts:

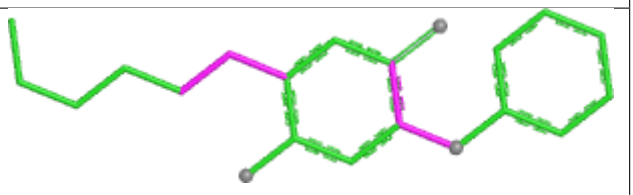
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1258	W0I	1	0
4	F	1257	NAP	1	0
2	B	1259	GLU	9	0
4	C	1257	NAP	1	0
2	A	1258	GLU	4	0
2	E	1259	GLU	4	0
3	B	1258	W0I	1	0
2	C	1259	GLU	10	0
2	G	1259	GLU	2	0
2	F	1259	GLU	11	0
3	F	1258	W0I	2	0
3	E	1258	W0I	1	0
4	G	1257	NAP	1	0
3	C	1258	W0I	2	0
4	D	1257	NAP	4	0
4	H	1257	NAP	2	0
3	A	1257	W0I	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.

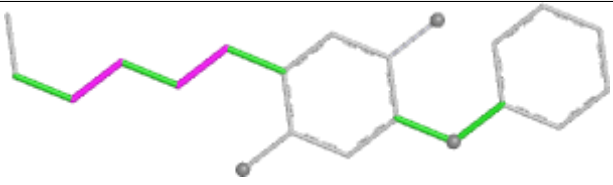
Ligand W0I D 1258



Bond lengths



Bond angles



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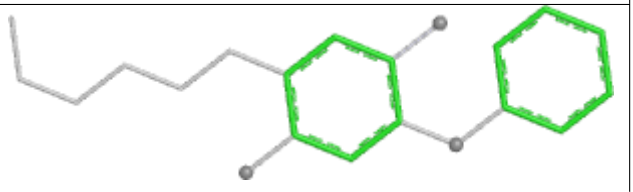
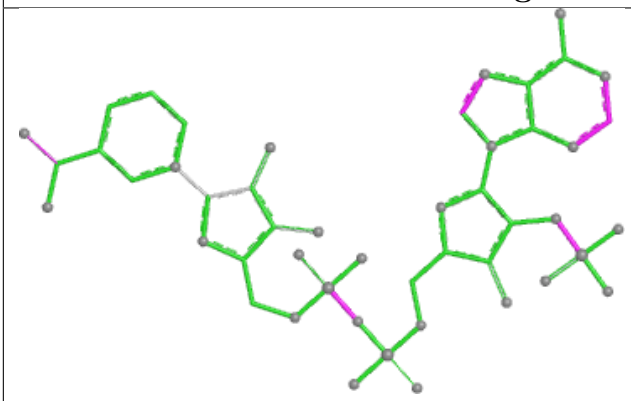


Rings

Ligand NAP F 1257



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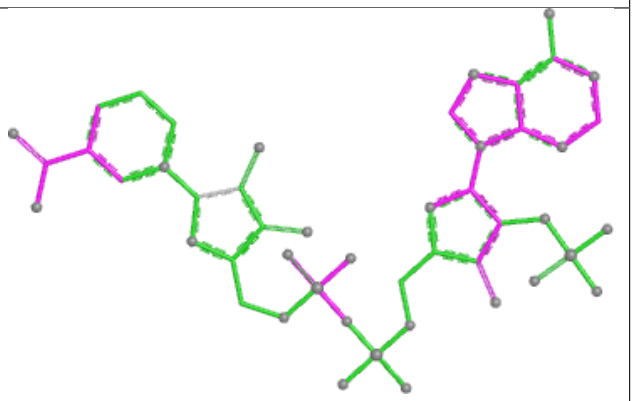

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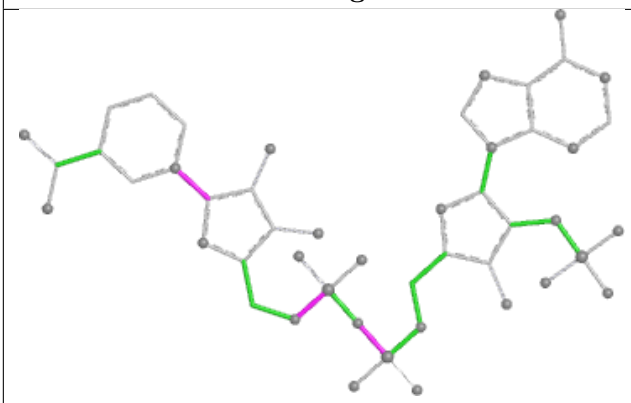

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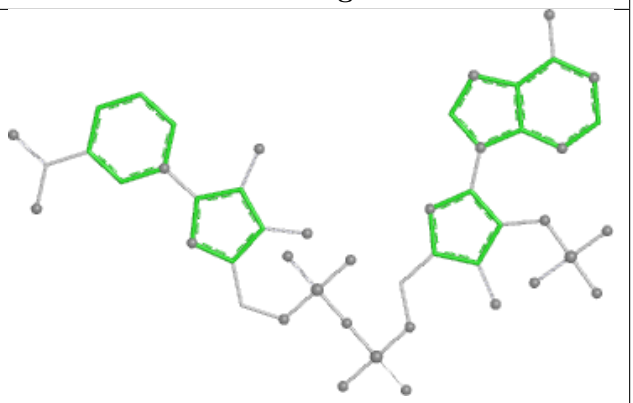
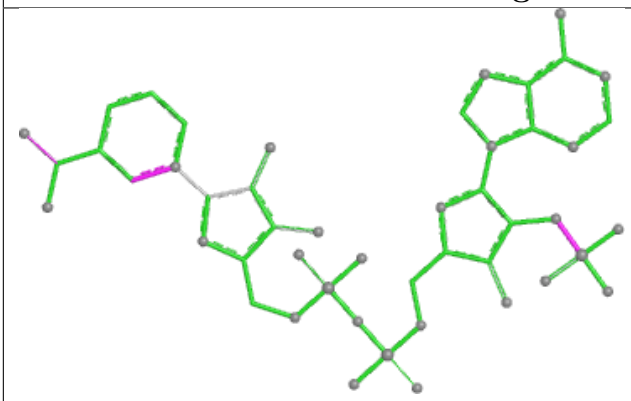


Rings

Ligand NAP C 1257



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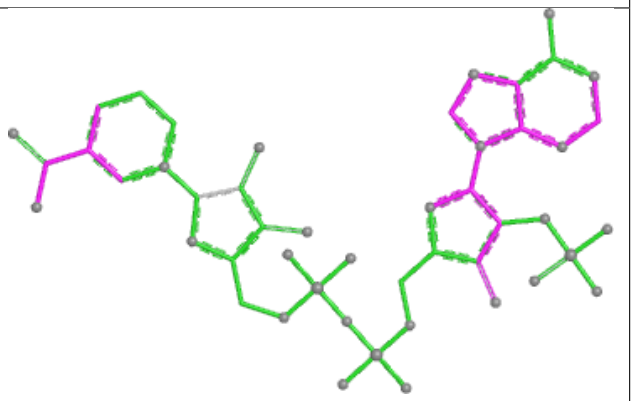

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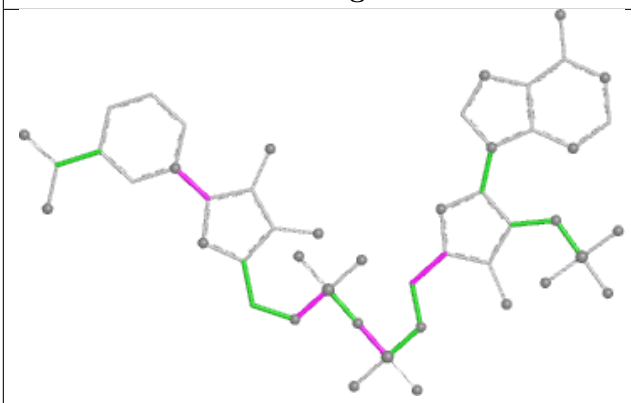

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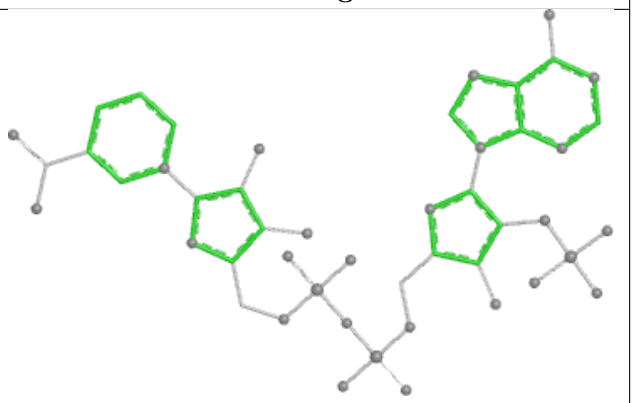
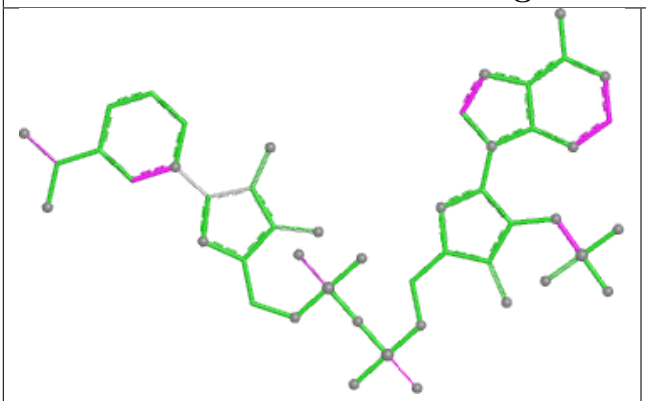


Rings

Ligand NAP E 1257



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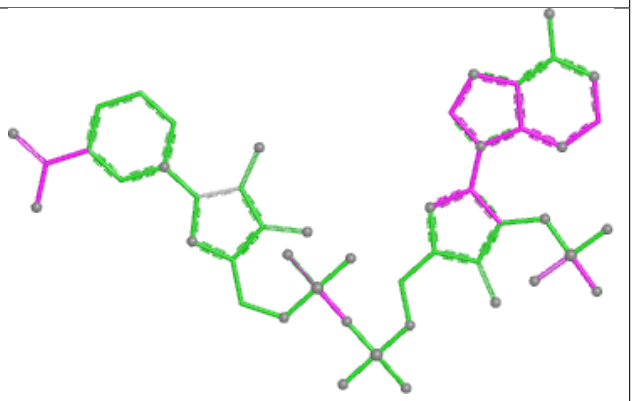

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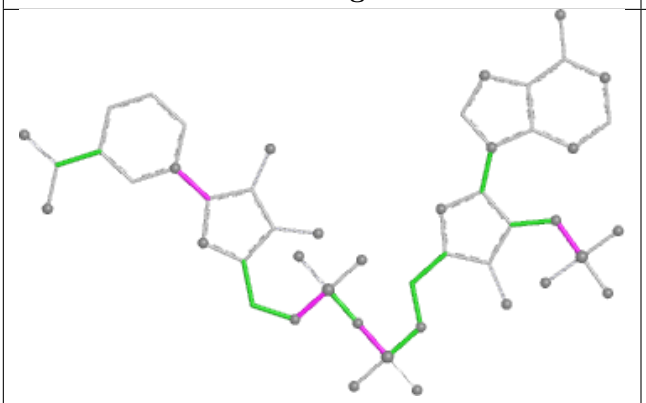

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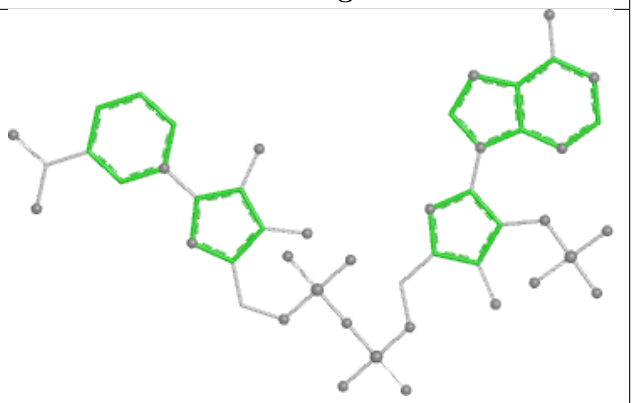
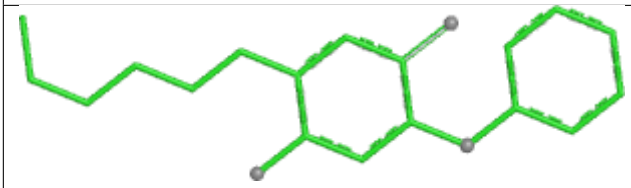


Rings

Ligand W0I B 1258



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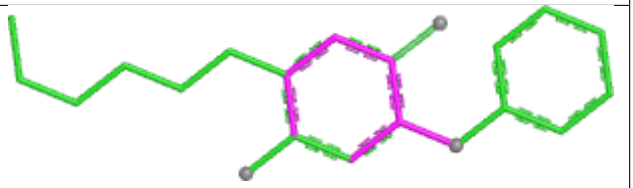

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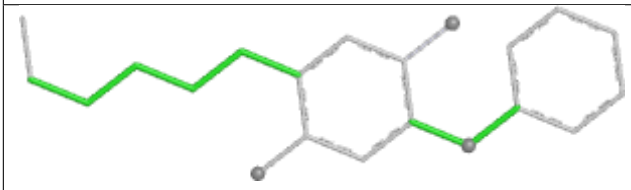

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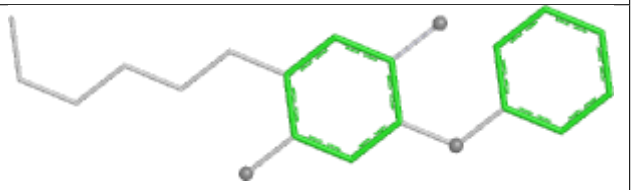
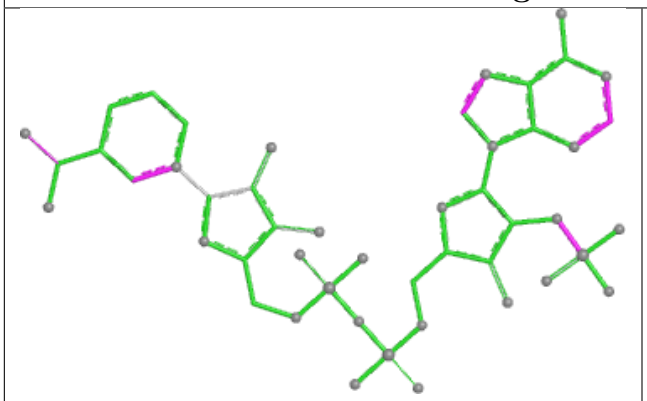


Rings

Ligand NAP A 1260



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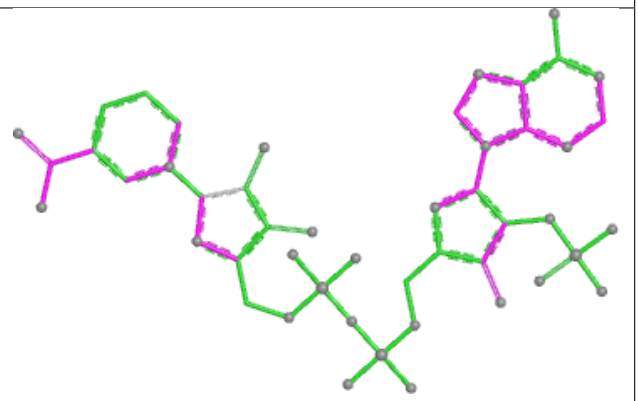

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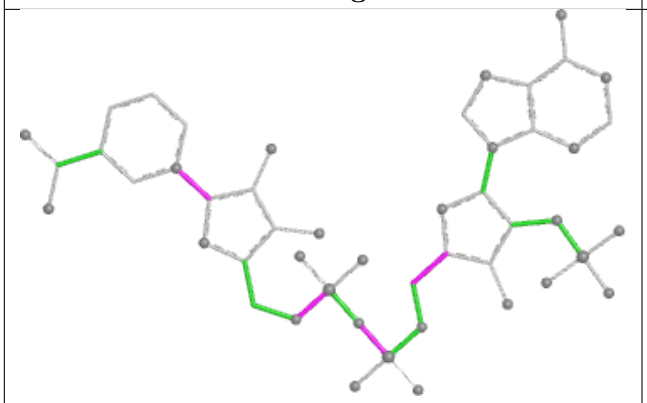

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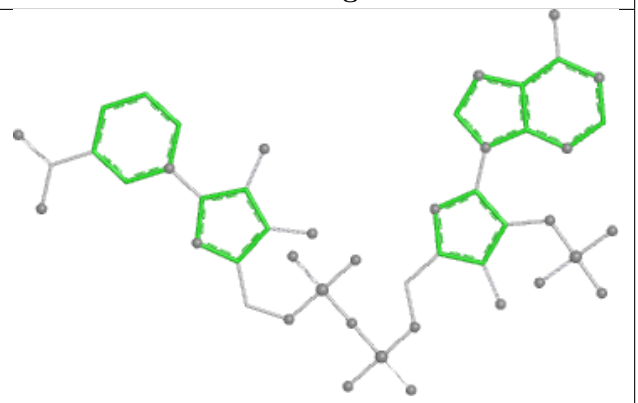
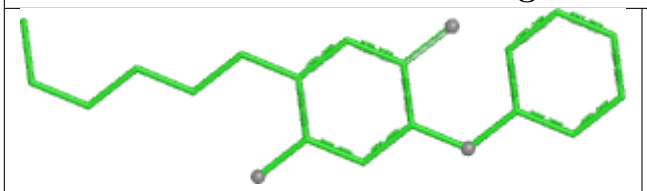


Rings

Ligand W0I G 1258



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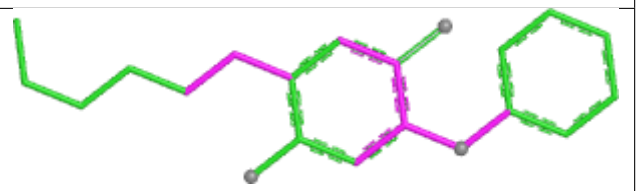

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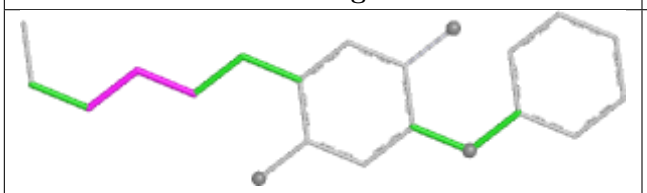

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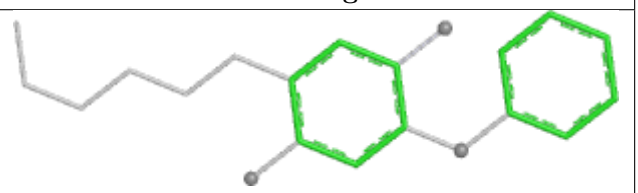
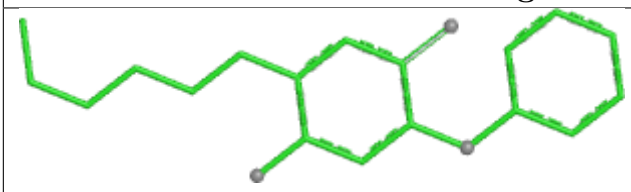


Rings

Ligand W0I H 1258



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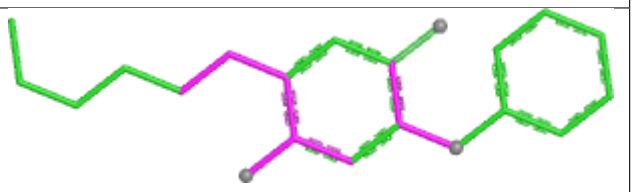

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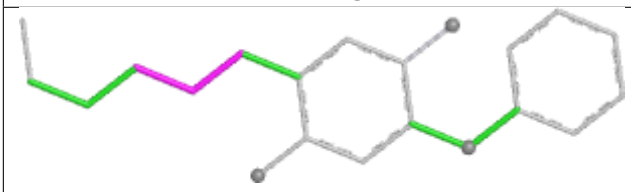

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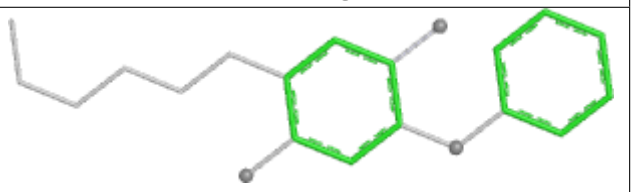
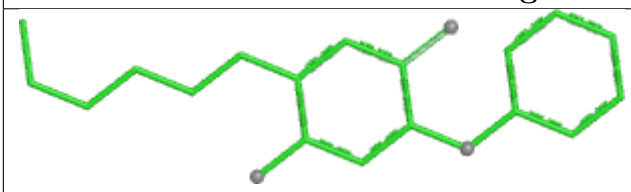


Rings

Ligand W0I F 1258



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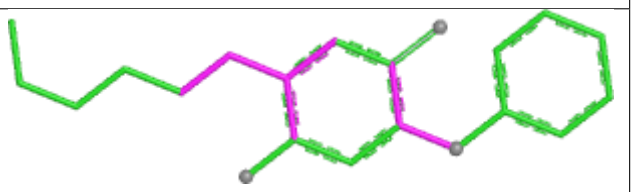

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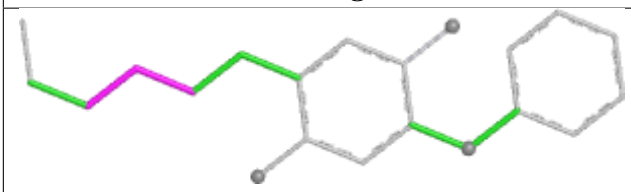

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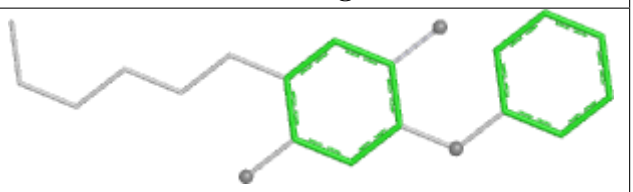
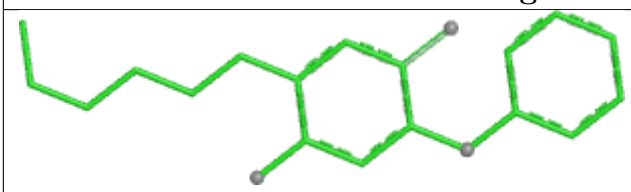


Rings

Ligand W0I E 1258



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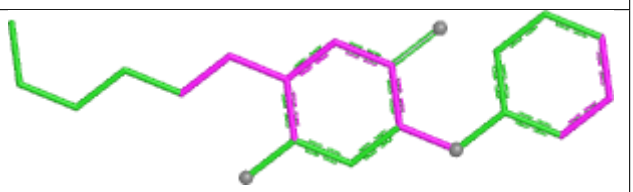

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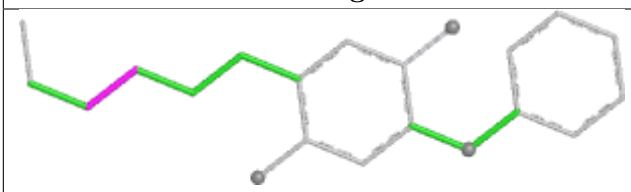

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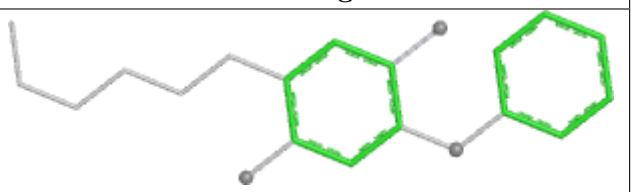
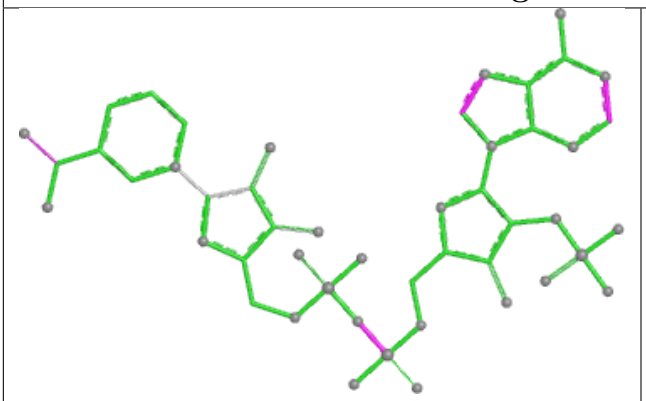


Rings

Ligand NAP G 1257



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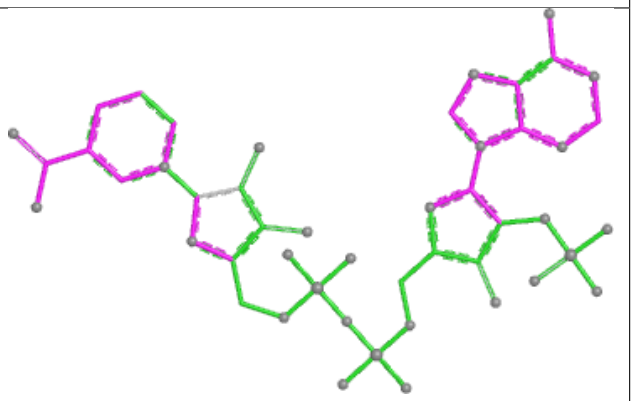

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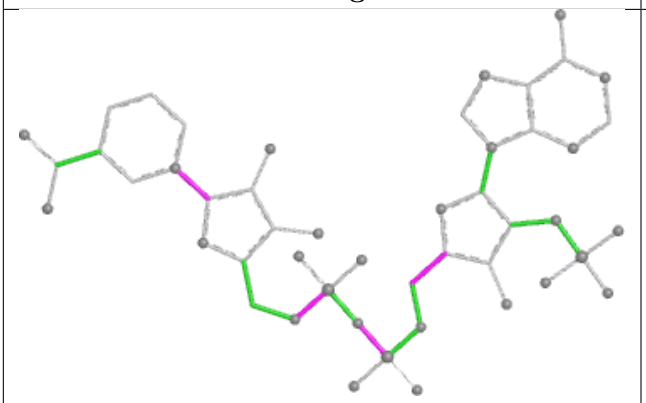

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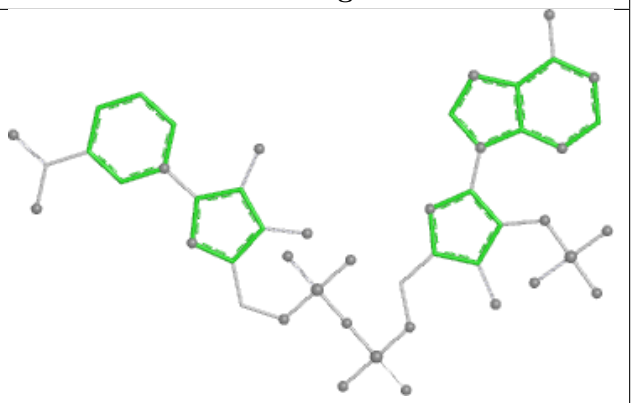
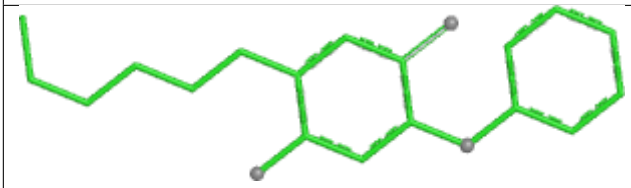


Rings

Ligand W0I C 1258



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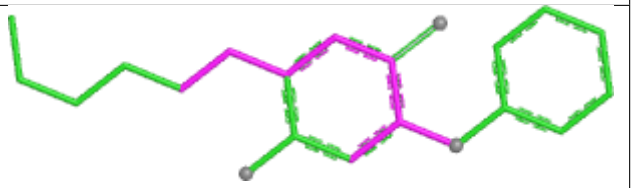

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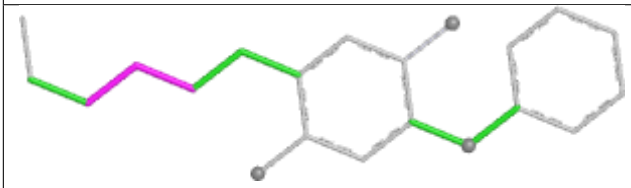

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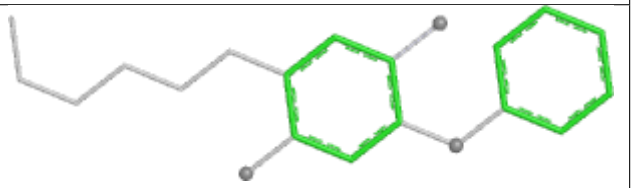
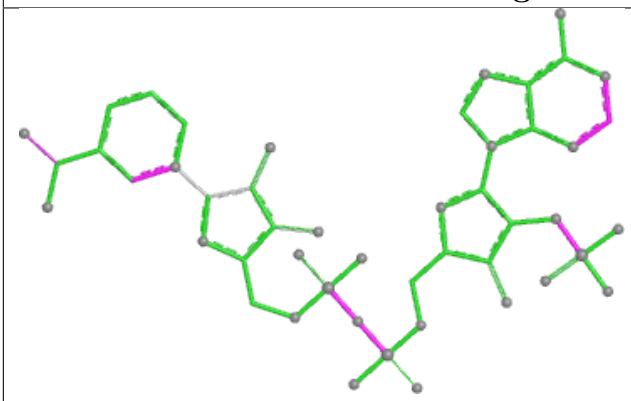


Rings

Ligand NAP B 1257



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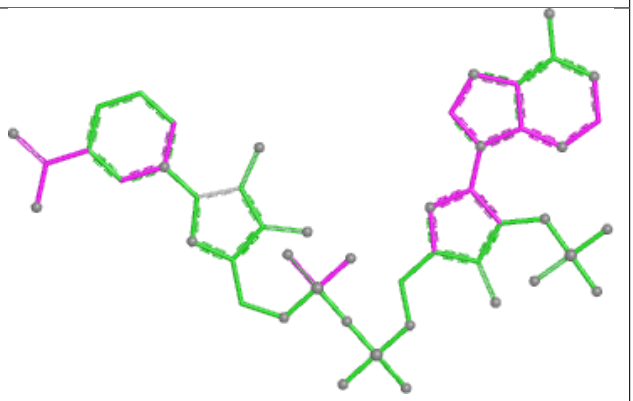

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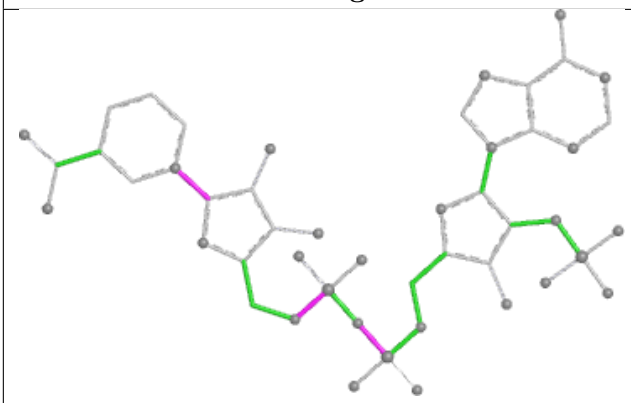

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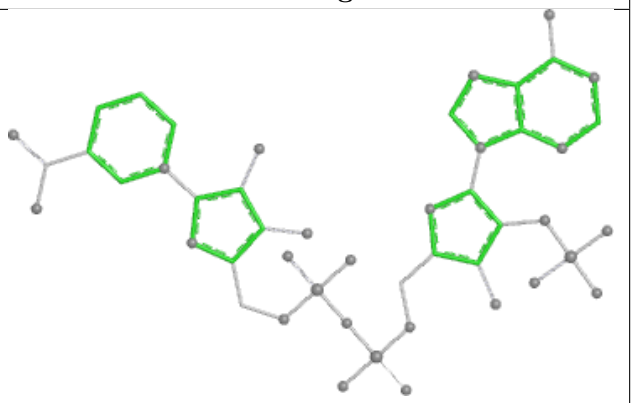
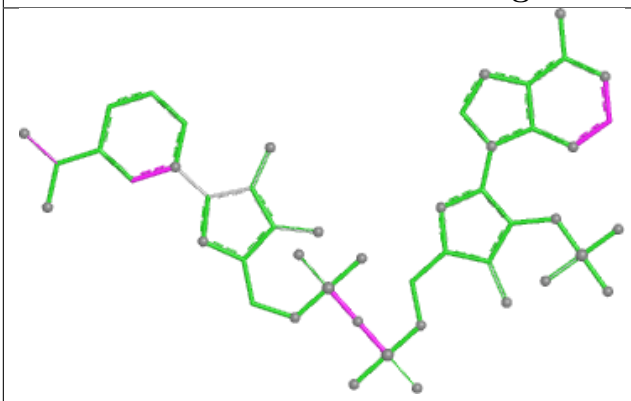


Rings

Ligand NAP D 1257



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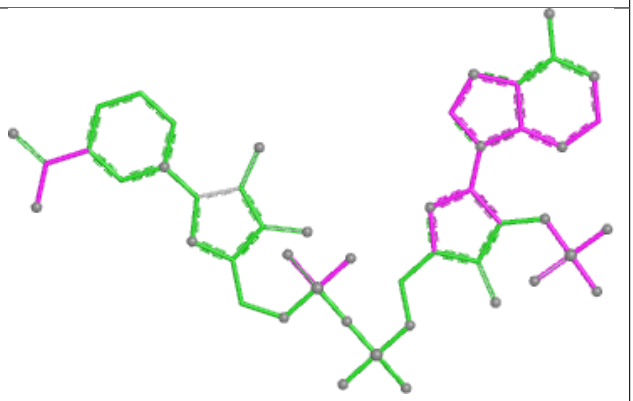

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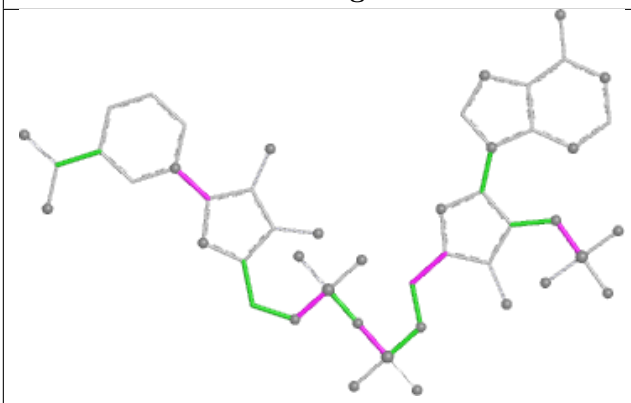

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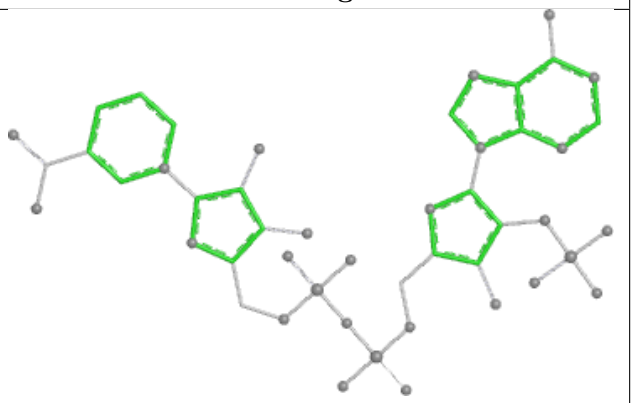
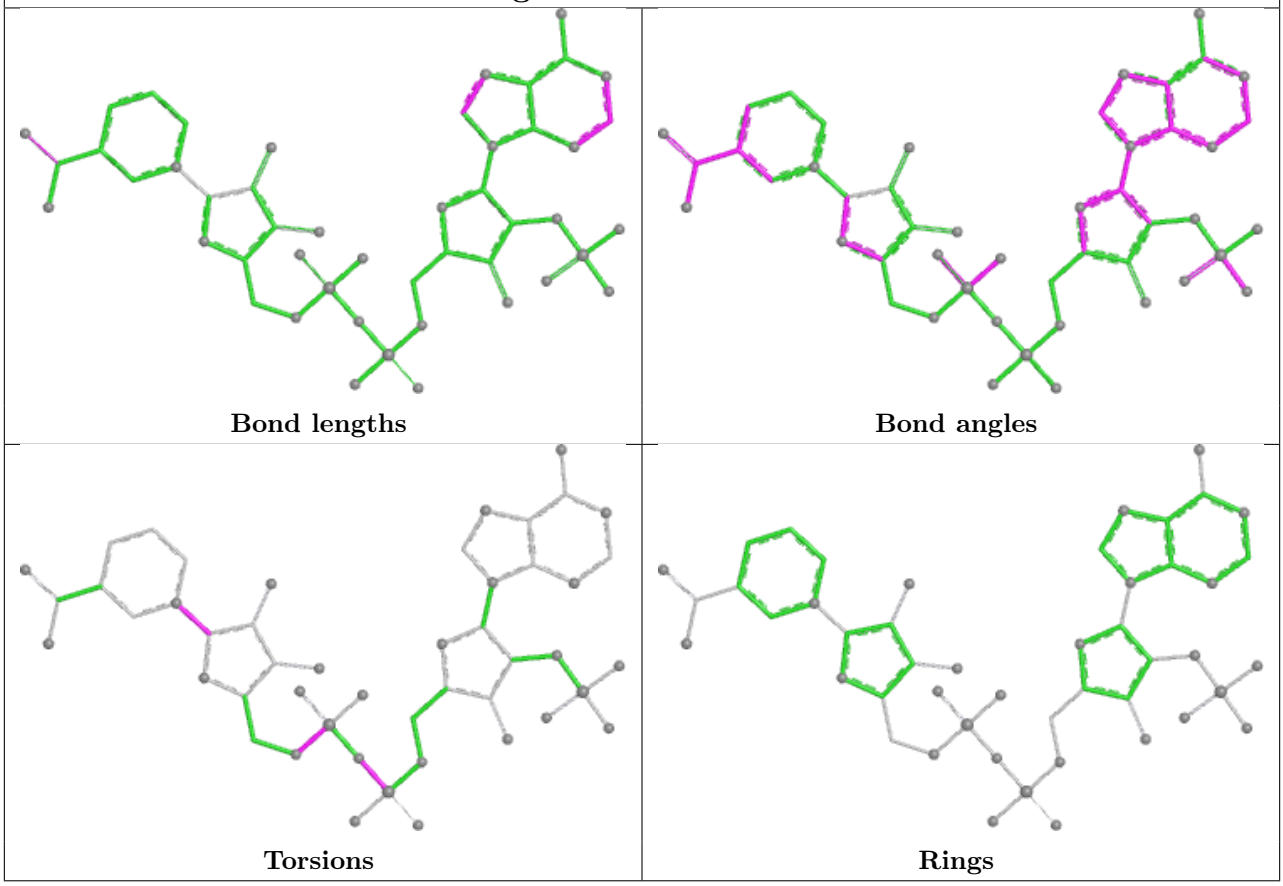
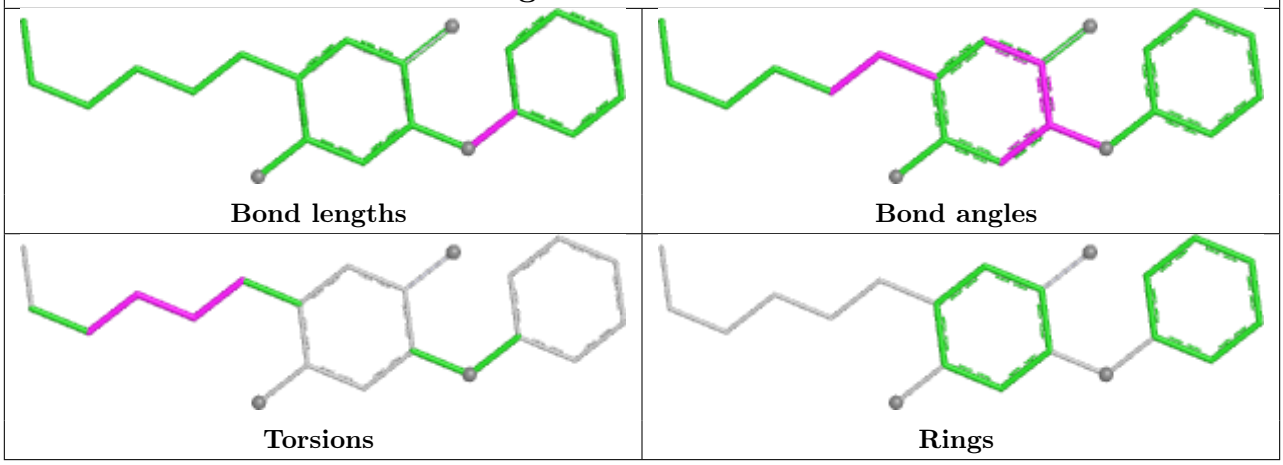


Rings

Ligand NAP H 1257



Ligand W0I A 1257



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, 95th 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	255/282 (90%)	-0.54	1 (0%) 88 89	12, 26, 51, 71	11 (4%)
1	B	255/282 (90%)	-0.51	2 (0%) 82 83	11, 28, 54, 68	13 (5%)
1	C	255/282 (90%)	-0.44	1 (0%) 88 89	12, 30, 55, 71	11 (4%)
1	D	255/282 (90%)	-0.31	3 (1%) 76 76	10, 34, 68, 80	6 (2%)
1	E	254/282 (90%)	-0.55	0 100 100	11, 26, 51, 61	12 (4%)
1	F	255/282 (90%)	-0.45	3 (1%) 76 76	14, 30, 55, 72	12 (4%)
1	G	254/282 (90%)	-0.48	0 100 100	13, 30, 54, 72	7 (2%)
1	H	254/282 (90%)	-0.36	2 (0%) 82 83	12, 33, 65, 92	4 (1%)
All	All	2037/2256 (90%)	-0.45	12 (0%) 85 86	10, 30, 57, 92	76 (3%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	VAL	5.7
1	C	2	VAL	5.5
1	B	104[A]	GLY	4.8
1	F	104[A]	GLY	4.7
1	F	2	VAL	3.9

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 oligosaccharides in this entry.

6.4 Ligands (i)

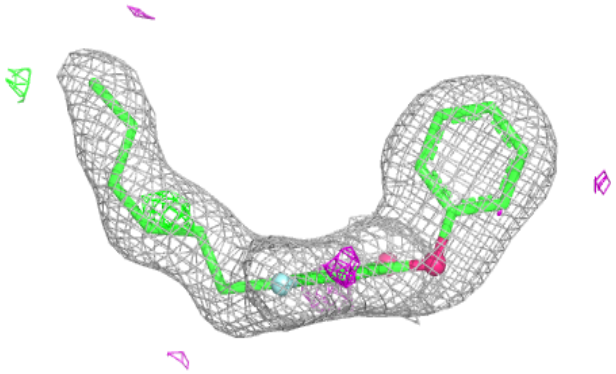
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

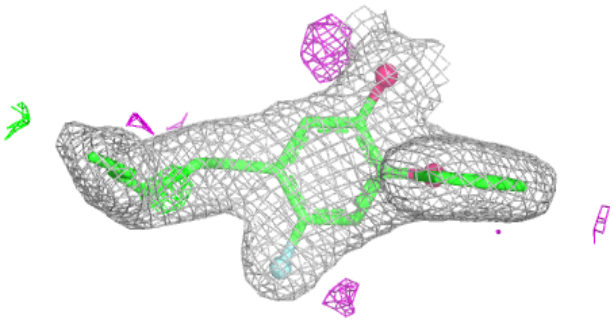
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLU	B	1259	10/10	0.67	0.22	89,90,93,96	0
2	GLU	A	1258	10/10	0.68	0.21	99,101,102,104	0
2	GLU	F	1259	10/10	0.70	0.19	102,103,103,103	0
2	GLU	E	1259	10/10	0.72	0.22	98,109,110,110	0
2	GLU	C	1259	10/10	0.72	0.18	89,92,94,94	0
2	GLU	G	1259	10/10	0.77	0.18	100,102,102,102	0
3	W0I	H	1258	21/21	0.94	0.09	30,36,40,42	0
3	W0I	D	1258	21/21	0.95	0.09	35,39,43,44	0
4	NAP	D	1257	48/48	0.95	0.07	29,33,49,52	0
3	W0I	B	1258	21/21	0.96	0.07	24,28,36,37	0
3	W0I	G	1258	21/21	0.96	0.07	23,28,38,40	0
4	NAP	H	1257	48/48	0.96	0.06	26,32,47,50	0
3	W0I	C	1258	21/21	0.97	0.07	24,29,38,42	0
3	W0I	A	1257	21/21	0.97	0.07	21,25,34,41	0
3	W0I	E	1258	21/21	0.97	0.06	22,25,32,33	0
3	W0I	F	1258	21/21	0.97	0.07	23,29,43,45	0
4	NAP	C	1257	48/48	0.98	0.05	22,28,35,37	0
4	NAP	A	1260	48/48	0.98	0.05	17,25,29,33	0
4	NAP	E	1257	48/48	0.98	0.05	18,24,30,35	0
4	NAP	F	1257	48/48	0.98	0.05	22,27,33,34	0
4	NAP	G	1257	48/48	0.98	0.05	18,28,33,41	0
4	NAP	B	1257	48/48	0.98	0.05	20,27,31,33	0

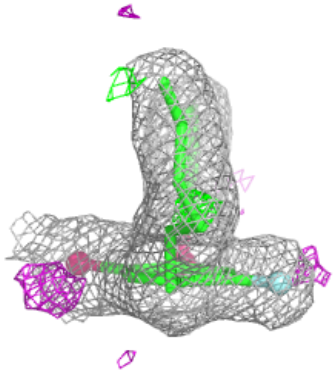
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W0I H 1258:

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

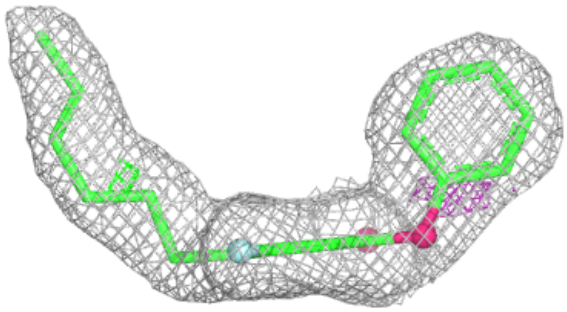


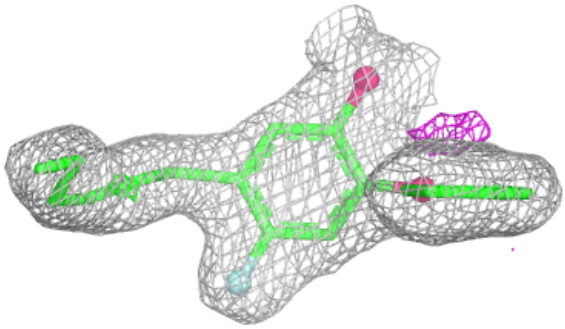


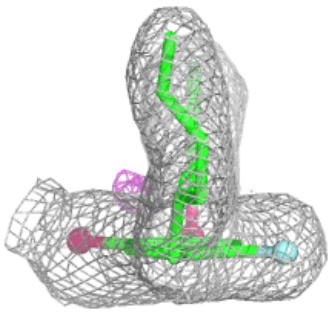


Electron density around W0I D 1258:

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

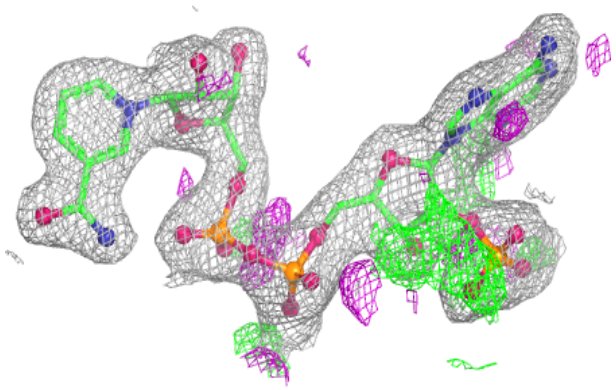


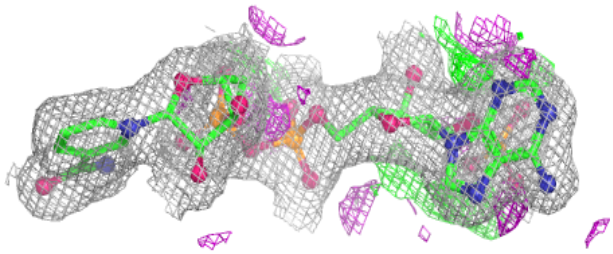


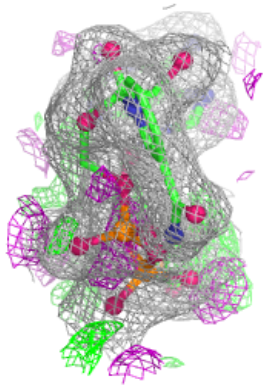


Electron density around NAP D 1257:

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

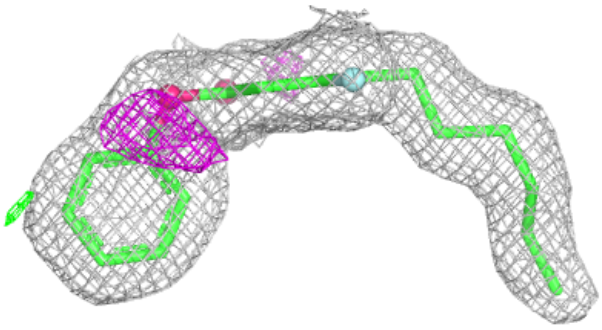


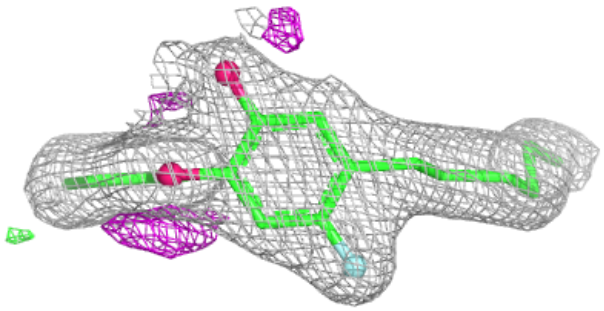


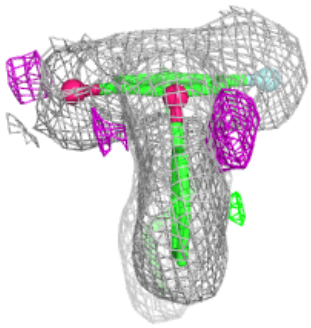


Electron density around W0I B 1258:

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

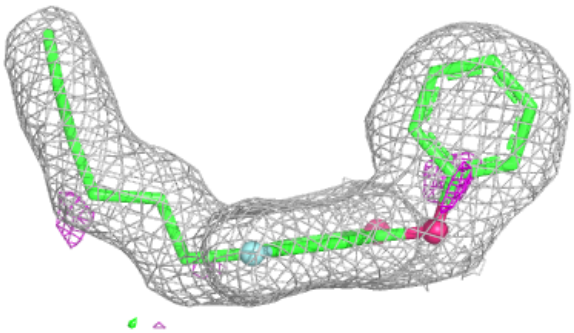


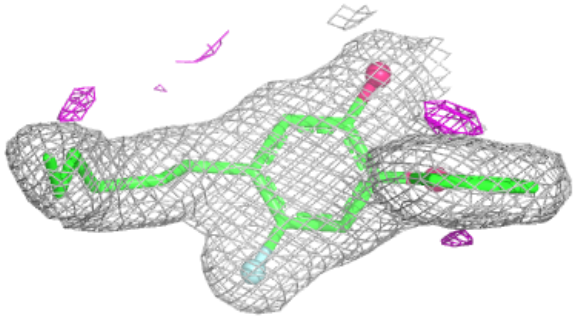


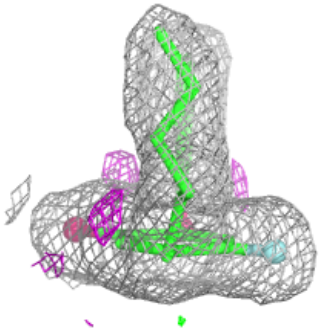


Electron density around W0I G 1258:

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

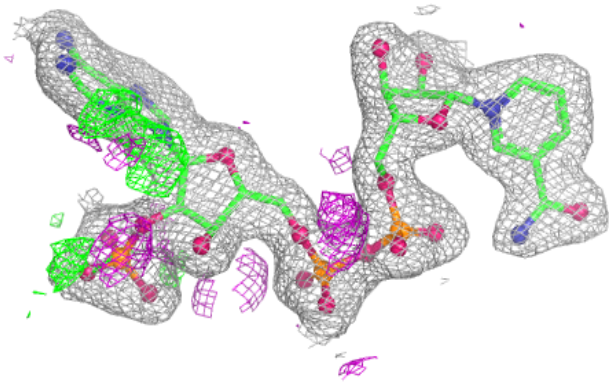


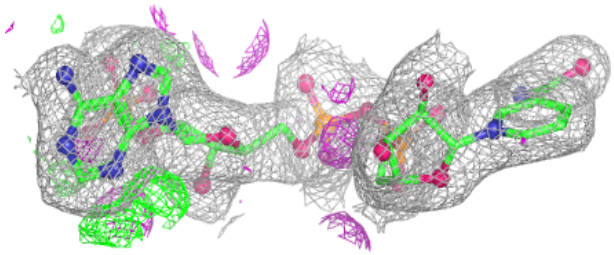


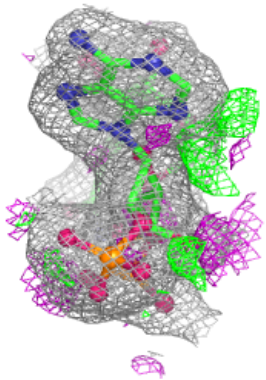


Electron density around NAP H 1257:

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

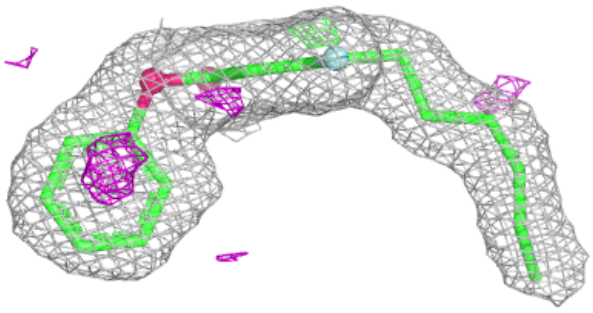


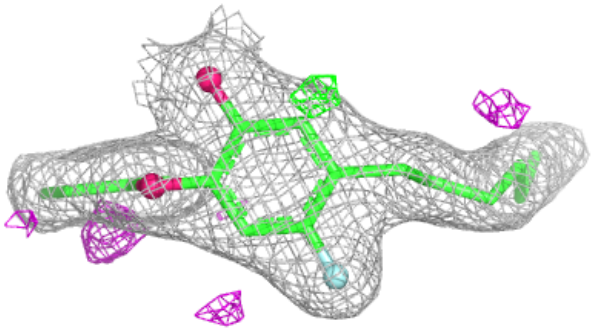


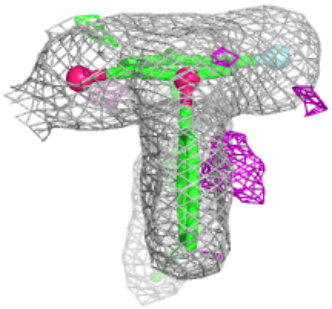


Electron density around W0I C 1258:

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







Electron density around W0I A 1257:

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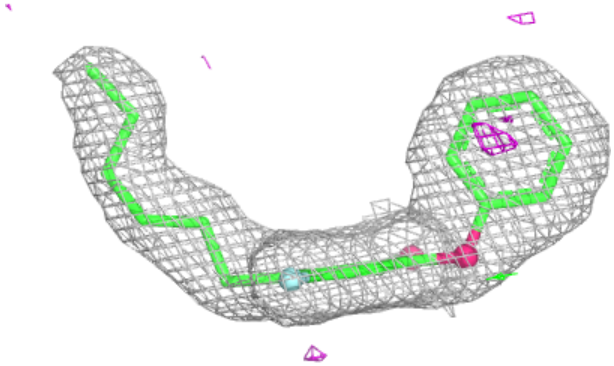
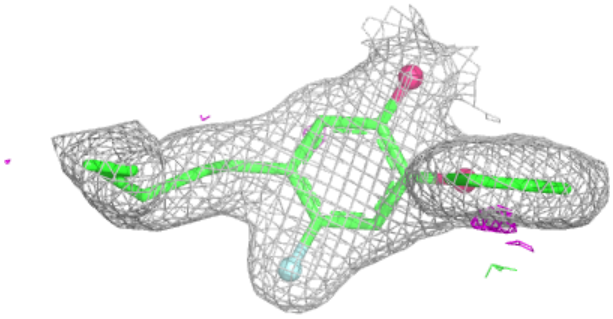
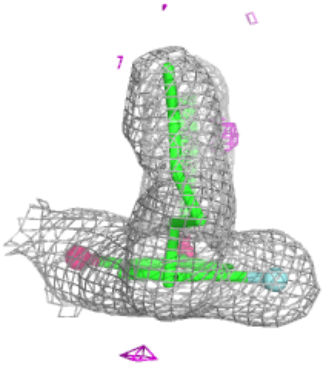
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

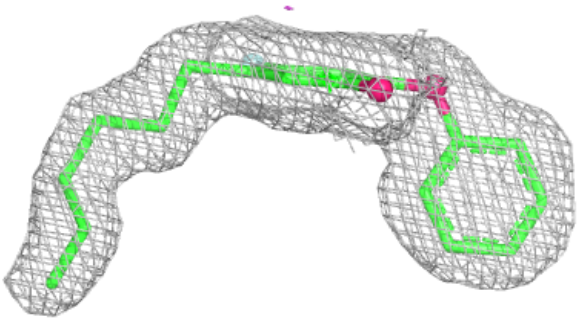


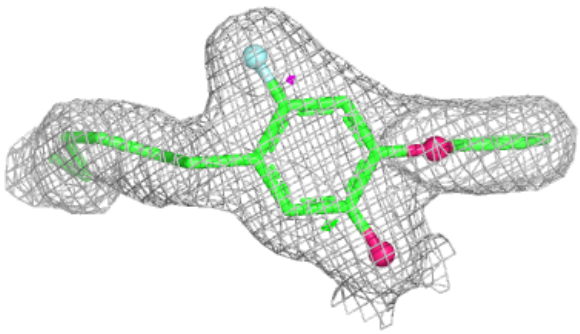


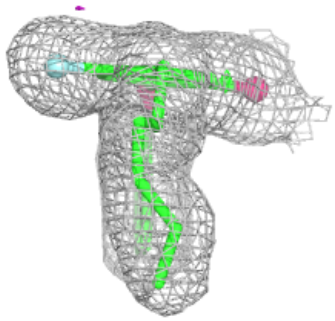


Electron density around W0I E 1258:

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







Electron density around W0I F 1258:

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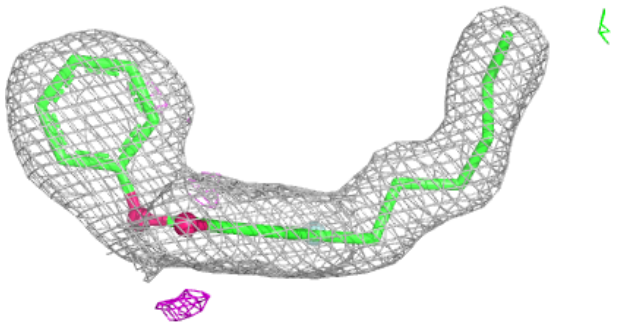
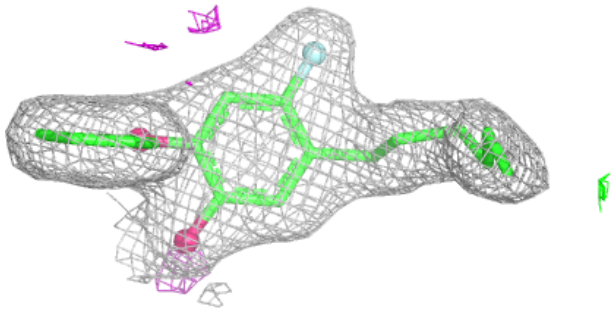
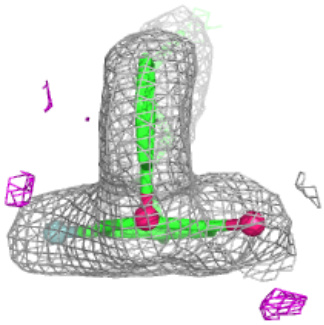
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

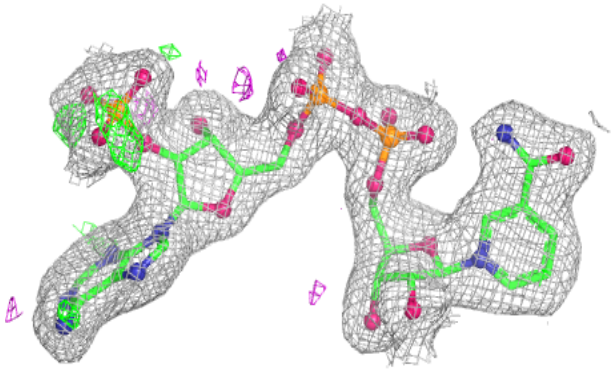


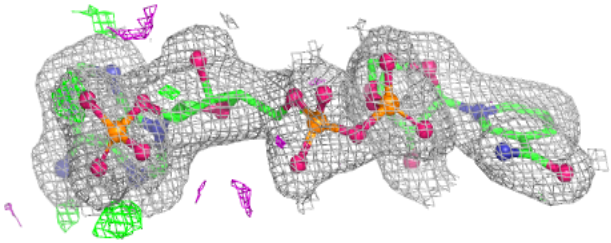


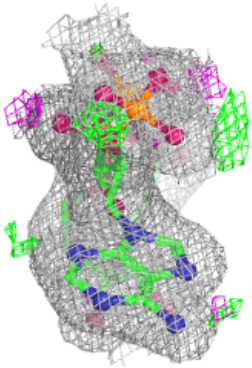


Electron density around NAP C 1257:

$2mF_o$-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 1260:

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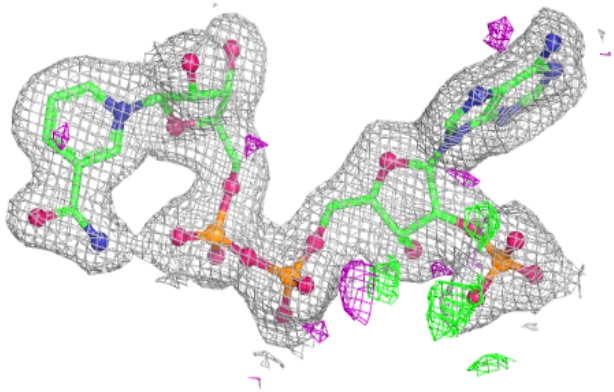
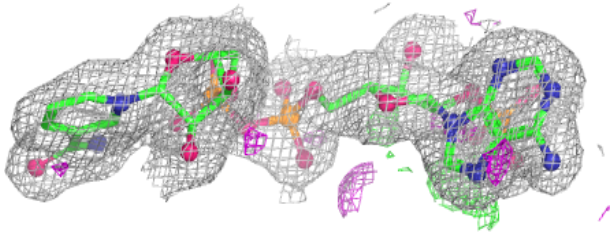
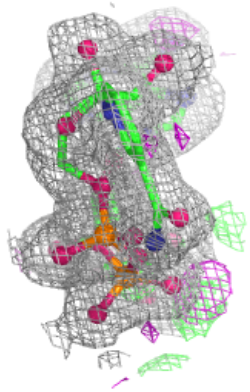
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around NAP E 1257:

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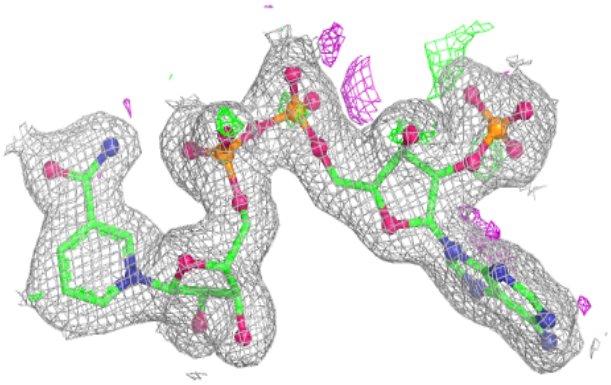
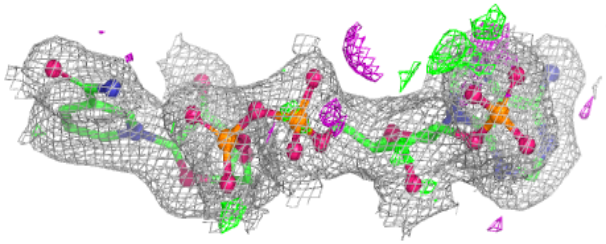
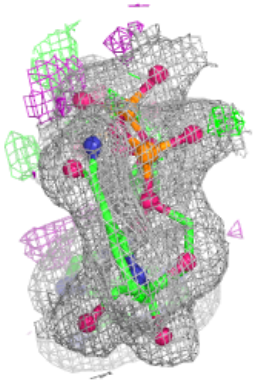
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around NAP F 1257:

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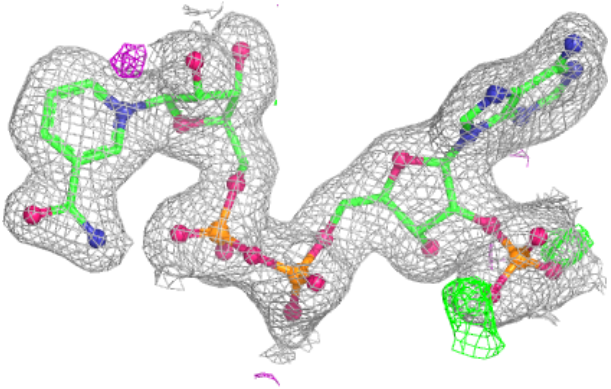
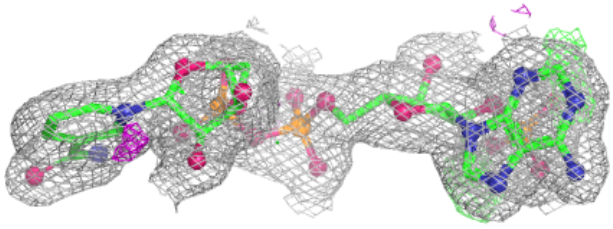
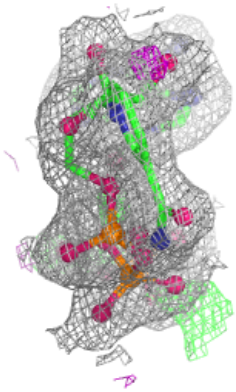
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

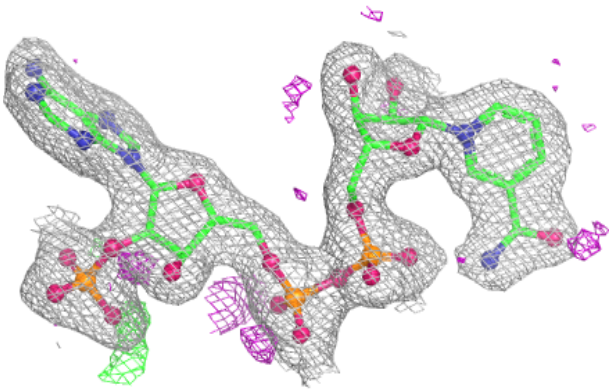


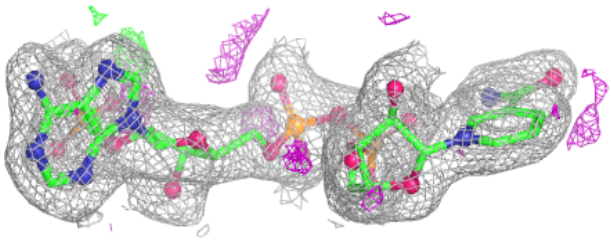


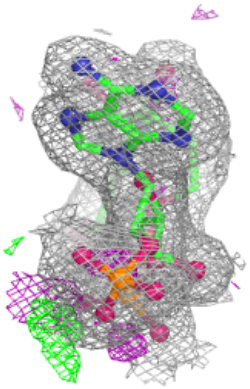


Electron density around NAP G 1257:

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

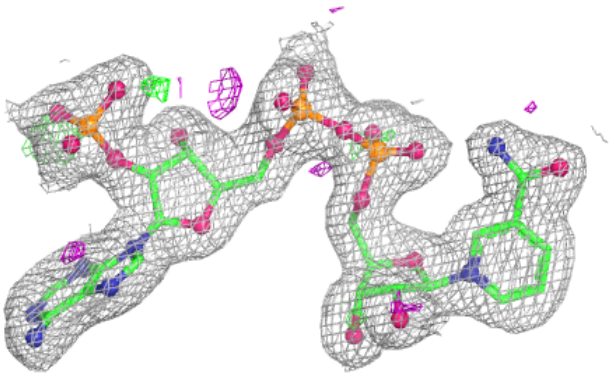


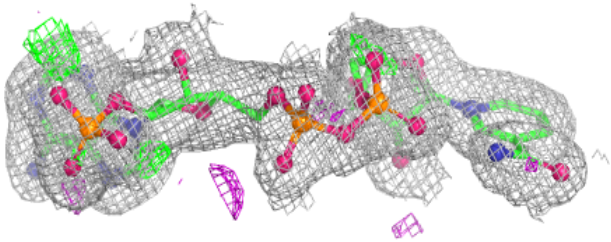


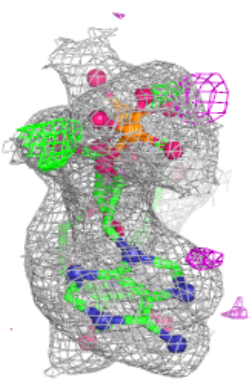


Electron density around NAP B 1257:

$2mF_o$-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.