



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 03:46 PM BST

PDB ID : 4BNH
Title : Crystal structure of S. aureus FabI in complex with NADP and 5-hexyl- 2-phenoxyphenol
Authors : Schiebel, J.; Chang, A.; Bommineni, G.R.; Tonge, P.J.; Kisker, C.
Deposited on : 2013-05-15
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.14.4.dev1
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) : 2.14.4.dev1

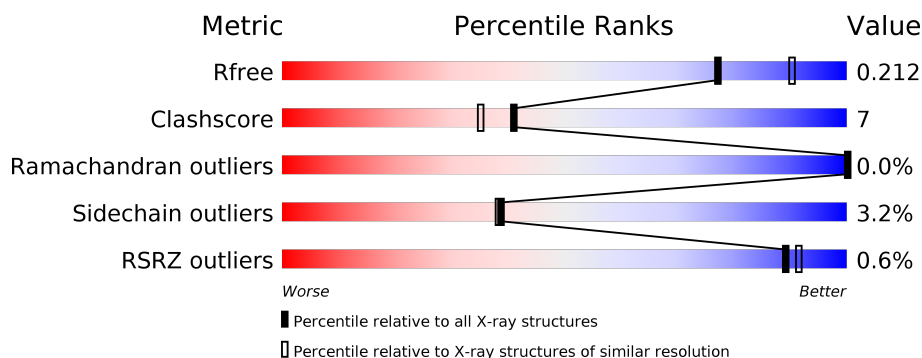
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 $\leq 5\%$. 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	<div> <div style="width: 77%;"></div> <div style="width: 13%;"></div> <div style="width: 10%;"></div> </div>
1	B	282	<div> <div style="width: 79%;"></div> <div style="width: 10%;"></div> <div style="width: 10%;"></div> </div>
1	C	282	<div> <div style="width: 74%;"></div> <div style="width: 16%;"></div> <div style="width: 10%;"></div> </div>
1	D	282	<div> <div style="width: 80%;"></div> <div style="width: 8%;"></div> <div style="width: 10%;"></div> </div>
1	E	282	<div> <div style="width: 72%;"></div> <div style="width: 17%;"></div> <div style="width: 10%;"></div> </div>
1	F	282	<div> <div style="width: 79%;"></div> <div style="width: 11%;"></div> <div style="width: 10%;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	282	<div><div></div><div>78%</div><div>12%</div><div>•</div><div>10%</div></div>
1	H	282	<div>%<div><div></div><div>77%</div><div>12%</div><div>•</div><div>10%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17737 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	254	Total	C	N	O	S	0	13	0
			2052	1289	359	399	5			
1	B	255	Total	C	N	O	S	0	5	0
			1992	1255	344	389	4			
1	C	255	Total	C	N	O	S	0	6	0
			2000	1260	347	389	4			
1	D	254	Total	C	N	O	S	0	5	0
			1987	1251	346	386	4			
1	E	255	Total	C	N	O	S	0	13	0
			2061	1295	363	398	5			
1	F	255	Total	C	N	O	S	0	4	0
			1984	1250	341	389	4			
1	G	255	Total	C	N	O	S	0	6	0
			2000	1260	347	389	4			
1	H	254	Total	C	N	O	S	0	3	0
			1973	1242	343	384	4			

There are 224 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	1	MET	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q7A6D8
B	2	VAL	LEU	engineered mutation	UNP Q7A6D8
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	1	MET	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	TYR	-	expression tag	UNP Q7A6D8
D	-12	ASP	-	expression tag	UNP Q7A6D8
D	-11	ILE	-	expression tag	UNP Q7A6D8
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	1	MET	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	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
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	1	MET	-	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

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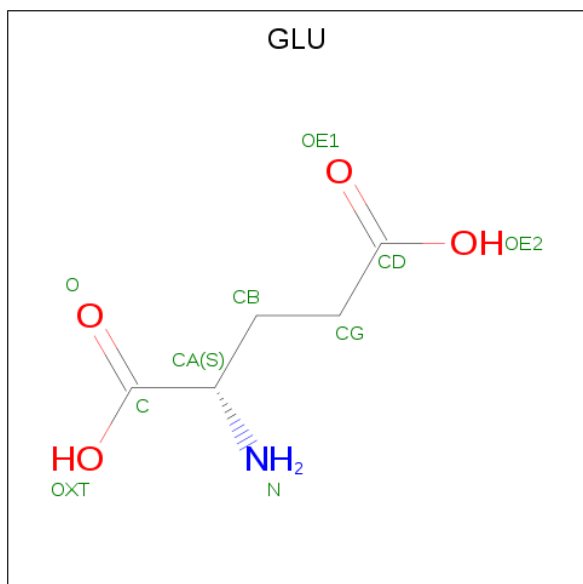
Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	TYR	-	expression tag	UNP Q7A6D8
G	-12	ASP	-	expression tag	UNP Q7A6D8
G	-11	ILE	-	expression tag	UNP Q7A6D8
G	-10	PRO	-	expression tag	UNP Q7A6D8
G	-9	THR	-	expression tag	UNP Q7A6D8
G	-8	THR	-	expression tag	UNP Q7A6D8
G	-7	GLU	-	expression tag	UNP 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	1	MET	-	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

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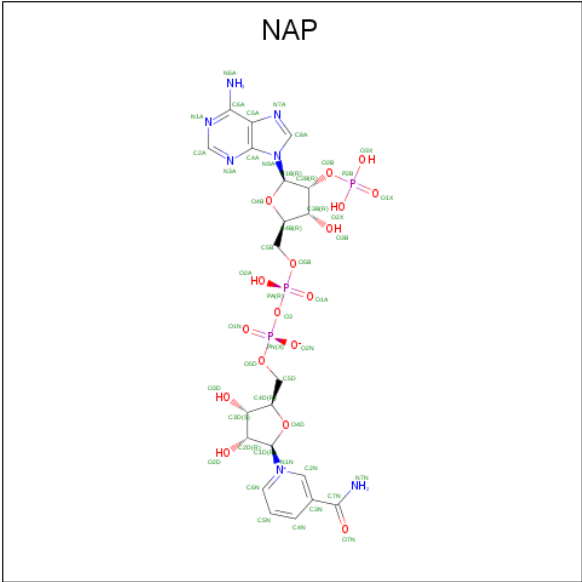
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	expression tag	UNP Q7A6D8
H	2	VAL	LEU	engineered mutation	UNP Q7A6D8

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



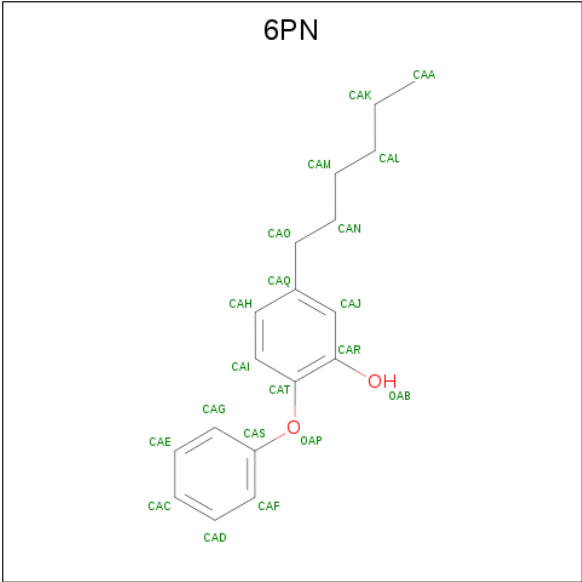
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 5-hexyl-2-phenoxyphenol (three-letter code: 6PN) (formula: C₁₈H₂₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	C	1	Total	C	O	0	0
			20	18	2		
4	D	1	Total	C	O	0	0
			20	18	2		
4	E	1	Total	C	O	0	0
			20	18	2		
4	F	1	Total	C	O	0	0
			20	18	2		
4	G	1	Total	C	O	0	0
			20	18	2		
4	H	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	177	Total	O	0	0
			177	177		
5	B	131	Total	O	0	0
			131	131		
5	C	140	Total	O	0	0
			140	140		
5	D	106	Total	O	0	0
			106	106		

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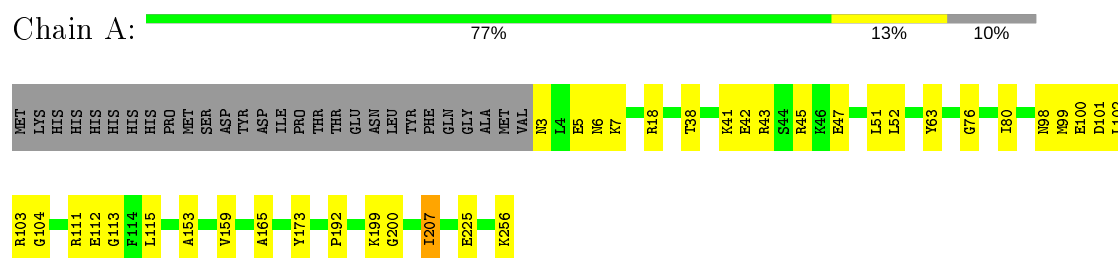
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	156	Total 156	O 156	0	0
5	F	130	Total 130	O 130	0	0
5	G	132	Total 132	O 132	0	0
5	H	102	Total 102	O 102	0	0

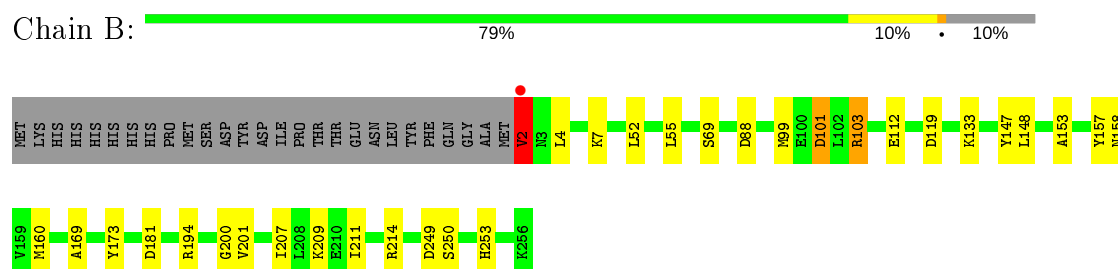
3 Residue-property plots [i](#)

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.

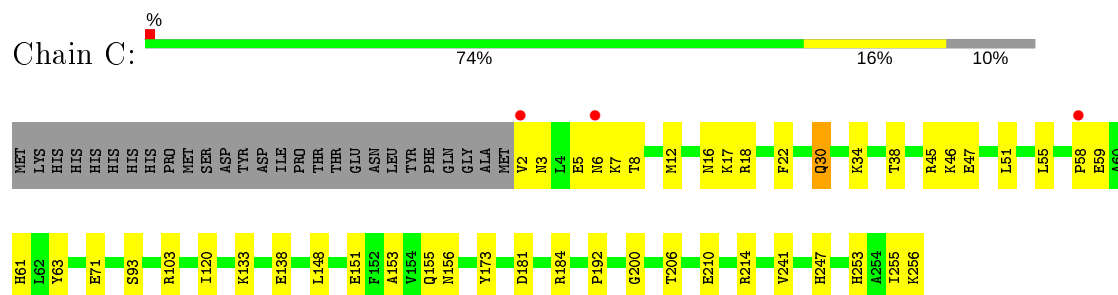
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



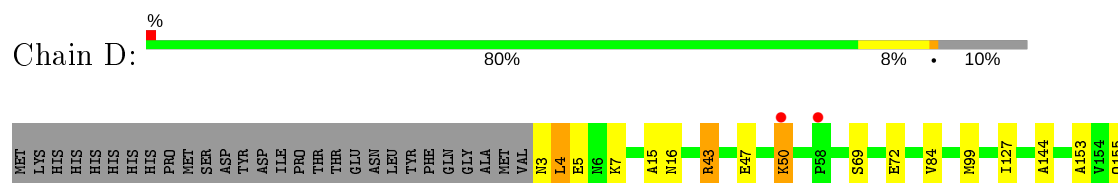
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



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



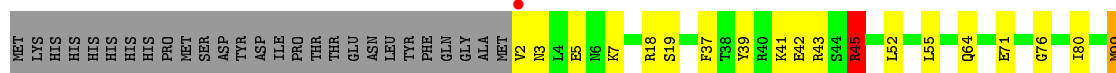
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]





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

Chain E: 72% 17% 10%



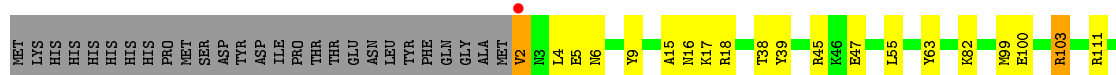
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain F: 79% 11% 10%



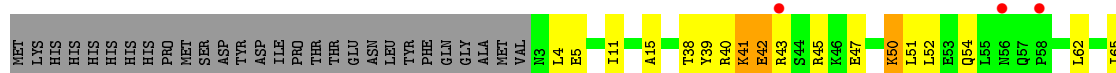
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain G: 78% 12% 10%



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

Chain H: 77% 12% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.46 Å 94.58 Å 94.81 Å 98.00° 112.68° 96.93°	Depositor
Resolution (Å)	33.48 – 2.15 33.48 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (33.48-2.15) 98.0 (33.48-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.16 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.147 , 0.196 0.168 , 0.212	Depositor DCC
R_{free} test set	7553 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17737	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, 6PN

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	0.67	0/2091	0.90	1/2813 (0.0%)
1	B	0.64	0/2028	0.88	3/2732 (0.1%)
1	C	0.59	0/2039	0.82	1/2746 (0.0%)
1	D	0.58	0/2023	0.81	0/2724
1	E	0.65	0/2100	0.87	1/2825 (0.0%)
1	F	0.61	0/2017	0.83	1/2718 (0.0%)
1	G	0.60	0/2039	0.85	2/2746 (0.1%)
1	H	0.58	0/2003	0.84	0/2698
All	All	0.62	0/16340	0.85	9/22002 (0.0%)

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	101	ASP	CB-CG-OD1	6.34	124.01	118.30
1	G	103	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	G	103	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	207	ILE	CG1-CB-CG2	-5.74	98.77	111.40
1	B	103	ARG	NE-CZ-NH1	5.63	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	101	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	12	MET	CG-SD-CE	5.04	108.26	100.20
1	E	45	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	VAL	Peptide
1	E	2	VAL	Peptide

5.2 Too-close contacts

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	2052	0	2071	56	0
1	B	1992	0	2009	27	0
1	C	2000	0	2022	37	0
1	D	1987	0	2007	22	0
1	E	2061	0	2087	65	0
1	F	1984	0	1996	28	0
1	G	2000	0	2022	22	0
1	H	1973	0	1988	29	0
2	A	10	0	5	1	0
2	B	10	0	5	1	0
2	C	20	0	10	3	0
2	D	10	0	5	1	0
2	E	10	0	5	1	0
2	F	10	0	5	0	0
3	A	48	0	25	1	0
3	B	48	0	25	1	0
3	C	48	0	25	2	0
3	D	48	0	25	0	0
3	E	48	0	25	1	0
3	F	48	0	25	2	0
3	G	48	0	25	0	0
3	H	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	21	0	0
4	B	20	0	22	2	0
4	C	20	0	21	0	0
4	D	20	0	21	1	0
4	E	20	0	21	2	0
4	F	20	0	21	1	0
4	G	20	0	21	0	0
4	H	20	0	22	3	0
5	A	177	0	0	4	0
5	B	131	0	0	3	0
5	C	140	0	0	7	0
5	D	106	0	0	2	0
5	E	156	0	0	7	0
5	F	130	0	0	7	0
5	G	132	0	0	2	0
5	H	102	0	0	2	0
All	All	17737	0	16607	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (236) 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:18:ARG:NH2	5:F:2016:HOH:O	1.82	1.11
1:F:214:ARG:HH12	1:H:214[B]:ARG:NH2	1.67	0.91
1:E:101[B]:ASP:OD2	5:E:2076:HOH:O	1.89	0.90
1:A:100[B]:GLU:OE2	1:E:41:LYS:NZ	2.06	0.89
1:A:104[B]:GLY:HA3	1:E:43:ARG:HH22	1.38	0.89
1:F:102:LEU:O	5:F:2064:HOH:O	1.90	0.88
1:E:18[A]:ARG:HH22	1:E:199:LYS:HZ3	1.20	0.87
1:E:18[A]:ARG:NH2	1:E:199:LYS:HZ3	1.73	0.86
1:D:43:ARG:H	1:D:43:ARG:HE	1.20	0.86
1:E:18[A]:ARG:NH2	1:E:199:LYS:NZ	2.24	0.86
1:F:214:ARG:HH12	1:H:214[B]:ARG:HH21	1.25	0.84
1:B:2:VAL:N	1:C:2:VAL:HG12	1.93	0.84
1:A:41:LYS:HE2	1:E:100[B]:GLU:HG3	1.58	0.83
1:D:3:ASN:HD21	1:D:5:GLU:HG3	1.44	0.82
1:C:18[A]:ARG:HD2	5:C:2021:HOH:O	1.79	0.81
1:C:7:LYS:HE3	2:C:1259:GLU:OE2	1.80	0.79
1:C:18[A]:ARG:NH2	5:C:2023:HOH:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLU:CG	1:C:214[B]:ARG:HD2	2.13	0.79
1:A:42[A]:GLU:OE1	1:E:112:GLU:HG2	1.85	0.77
1:C:210:GLU:HG3	1:C:214[B]:ARG:HD2	1.67	0.76
1:C:253:HIS:HD2	5:C:2140:HOH:O	1.67	0.76
1:A:41:LYS:HE2	1:E:100[B]:GLU:CG	2.15	0.75
1:F:148:LEU:HD21	1:H:256:LYS:HG2	1.69	0.75
1:E:42[B]:GLU:OE1	1:E:45:ARG:NH2	2.18	0.73
1:B:99:MET:C	1:B:101:ASP:H	1.95	0.70
1:C:2:VAL:HG13	1:C:2:VAL:O	1.89	0.70
1:E:18[A]:ARG:HH22	1:E:199:LYS:NZ	1.85	0.70
1:A:41:LYS:CE	1:E:100[B]:GLU:HG3	2.21	0.70
1:A:18[A]:ARG:HH22	1:A:199:LYS:HE2	1.57	0.69
1:E:201:VAL:HG11	4:E:1258:6PN:HAKA	1.75	0.69
5:E:2134:HOH:O	1:H:239[B]:SER:O	2.10	0.69
1:F:155:GLN:O	1:F:156:ASN:HB2	1.93	0.69
1:A:42[B]:GLU:OE1	1:A:45:ARG:NH2	2.21	0.68
1:A:101[A]:ASP:HB3	1:A:159:VAL:CG1	2.24	0.68
1:A:256:LYS:HG2	1:C:148:LEU:HD21	1.75	0.67
1:A:99[A]:MET:CE	1:E:99[A]:MET:SD	2.85	0.65
1:A:43:ARG:HG2	1:E:100[A]:GLU:HG3	1.79	0.65
1:E:103[B]:ARG:NH1	1:E:202:GLY:HA2	2.11	0.64
1:B:253:HIS:HD2	5:C:2049:HOH:O	1.80	0.64
1:D:201:VAL:HG11	4:D:1258:6PN:HAKA	1.79	0.64
1:D:210:GLU:HG2	1:D:214[B]:ARG:HD2	1.79	0.64
1:F:214:ARG:NH1	1:H:214[B]:ARG:NH2	2.44	0.63
1:E:3:ASN:HD21	1:E:5:GLU:HB2	1.62	0.63
1:A:101[A]:ASP:O	1:A:102[A]:LEU:HD23	1.99	0.63
5:A:2156:HOH:O	1:D:239[B]:SER:O	2.15	0.63
1:A:101[B]:ASP:HA	1:E:43:ARG:NH1	2.14	0.62
1:A:43:ARG:HH22	1:E:104[B]:GLY:HA3	1.62	0.62
1:H:210:GLU:HG2	1:H:214[B]:ARG:HD3	1.81	0.62
1:B:99:MET:C	1:B:101:ASP:N	2.51	0.62
1:B:103:ARG:NH2	1:B:200:GLY:O	2.33	0.62
1:B:201:VAL:HG11	4:B:1258:6PN:HAK	1.82	0.60
1:A:101[B]:ASP:OD2	5:A:2081:HOH:O	2.17	0.60
1:H:52:LEU:HD11	1:H:62:LEU:HD11	1.82	0.59
1:A:101[A]:ASP:HB3	1:A:159:VAL:HG11	1.85	0.58
1:A:43:ARG:HH22	1:E:104[B]:GLY:CA	2.16	0.58
1:C:5:GLU:O	1:C:6:ASN:HB2	2.03	0.58
1:F:2:VAL:N	1:G:2:VAL:HG12	2.20	0.57
1:E:249:ASP:O	1:E:250:SER:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:ALA:O	1:H:47:GLU:HG2	2.04	0.57
1:B:148:LEU:HD21	1:D:256:LYS:HG2	1.87	0.57
1:A:104[B]:GLY:HA3	1:E:43:ARG:NH2	2.15	0.57
1:G:103:ARG:NH2	1:G:200:GLY:O	2.39	0.56
1:A:5:GLU:O	1:A:6:ASN:HB2	2.06	0.56
1:F:5:GLU:O	1:F:6:ASN:HB2	2.06	0.56
1:A:256:LYS:HG2	1:C:148:LEU:CD2	2.37	0.55
1:C:3:ASN:HD21	1:C:5:GLU:HG3	1.71	0.55
1:E:155:GLN:O	1:E:156:ASN:HB2	2.07	0.55
1:A:103[A]:ARG:NH2	1:A:200:GLY:O	2.40	0.54
5:F:2113:HOH:O	1:G:239[B]:SER:O	2.18	0.54
1:E:18[A]:ARG:NH2	1:E:199:LYS:HZ2	2.04	0.54
1:G:38:THR:HA	1:G:63:TYR:O	2.07	0.53
1:E:155:GLN:HB2	5:E:2104:HOH:O	2.08	0.53
1:A:111:ARG:NH1	1:B:119:ASP:OD1	2.39	0.53
1:A:101[B]:ASP:OD2	1:A:113:GLY:HA3	2.09	0.52
5:A:2097:HOH:O	1:E:42[A]:GLU:OE2	2.19	0.52
1:A:100[B]:GLU:HG3	1:E:41:LYS:HZ3	1.73	0.52
1:H:155:GLN:O	1:H:156:ASN:HB2	2.09	0.52
1:A:100[B]:GLU:CD	1:E:41:LYS:HZ2	2.13	0.52
1:D:213:GLU:HB3	1:D:214[B]:ARG:HG3	1.91	0.52
1:D:155:GLN:O	1:D:156:ASN:HB2	2.10	0.52
1:F:147:TYR:HB2	3:F:1257:NAP:C5N	2.40	0.52
1:F:147:TYR:HB2	3:F:1257:NAP:H5N	1.92	0.52
1:E:76:GLY:O	1:E:80:ILE:HG13	2.10	0.52
1:A:101[A]:ASP:HB3	1:A:159:VAL:HG12	1.91	0.51
1:C:59:GLU:HG3	1:C:61:HIS:CE1	2.45	0.51
2:E:1259:GLU:HB2	1:F:103:ARG:HH21	1.74	0.51
1:G:136:MET:HA	5:G:2067:HOH:O	2.11	0.51
1:C:18[B]:ARG:HH11	1:C:18[B]:ARG:CG	2.23	0.51
1:E:253:HIS:HD2	5:H:2038:HOH:O	1.94	0.51
1:A:207:ILE:HD13	5:A:2144:HOH:O	2.11	0.51
1:F:7:LYS:HA	1:F:88:ASP:OD2	2.10	0.51
1:H:42:GLU:O	1:H:45:ARG:N	2.40	0.51
1:C:103:ARG:HH12	2:C:1260:GLU:N	2.09	0.51
1:B:7:LYS:HA	1:B:88:ASP:OD2	2.11	0.51
1:D:3:ASN:ND2	1:D:5:GLU:HG3	2.20	0.50
1:A:165:ALA:CB	1:B:169:ALA:HB2	2.41	0.50
1:C:71[A]:GLU:HG2	5:C:2058:HOH:O	2.11	0.50
1:F:103:ARG:NH1	1:F:200:GLY:O	2.44	0.50
1:A:100[B]:GLU:CD	1:E:41:LYS:NZ	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LYS:HE2	1:B:181:ASP:OD2	2.12	0.50
1:F:133:LYS:NZ	5:F:2075:HOH:O	2.43	0.50
1:H:43:ARG:O	1:H:47:GLU:HB2	2.11	0.50
1:A:43:ARG:NH1	1:E:101[B]:ASP:HA	2.27	0.49
1:A:99[A]:MET:HE1	1:E:99[A]:MET:SD	2.51	0.49
1:A:100[B]:GLU:HG3	1:E:41:LYS:NZ	2.28	0.49
1:A:41:LYS:HE2	1:E:100[B]:GLU:CD	2.33	0.49
1:H:151:GLU:OE2	5:H:2065:HOH:O	2.19	0.49
1:C:7:LYS:CE	2:C:1259:GLU:OE2	2.56	0.49
1:E:157:TYR:CZ	1:E:160:MET:HG3	2.47	0.48
1:B:214:ARG:HD3	5:B:2108:HOH:O	2.13	0.48
1:C:30:GLN:O	1:C:30:GLN:HG3	2.12	0.48
1:E:39:TYR:CZ	1:E:64:GLN:HB2	2.48	0.48
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.49	0.48
1:C:5:GLU:O	1:C:6:ASN:CB	2.61	0.48
1:F:154:VAL:HG12	4:F:1258:6PN:HAAB	1.94	0.48
1:A:3:ASN:HD21	1:A:5:GLU:HB2	1.79	0.48
1:C:16:ASN:HA	1:C:47:GLU:HG2	1.96	0.48
1:A:112:GLU:HB3	1:E:42[A]:GLU:OE1	2.14	0.47
1:F:41:LYS:HZ3	1:F:41:LYS:HG3	1.61	0.47
1:E:99[B]:MET:HE3	1:E:103[B]:ARG:HE	1.79	0.47
1:E:194[A]:ARG:NH1	1:E:205:ASN:OD1	2.47	0.47
3:H:1257:NAP:O2D	4:H:1258:6PN:OAB	2.32	0.47
1:A:225:GLU:OE2	1:D:239[B]:SER:OG	2.23	0.47
1:G:207:ILE:O	1:G:211:ILE:HG12	2.15	0.47
1:C:18[B]:ARG:HH11	1:C:18[B]:ARG:HG3	1.78	0.47
1:C:103:ARG:NH2	1:C:200:GLY:O	2.47	0.47
1:E:194[B]:ARG:HG3	5:E:2126:HOH:O	2.15	0.47
1:D:50:LYS:HE3	1:D:50:LYS:HB2	1.74	0.47
1:G:5:GLU:O	1:G:6:ASN:HB2	2.15	0.47
1:C:22:PHE:CZ	1:C:51:LEU:HD22	2.49	0.46
1:H:50:LYS:HE3	1:H:50:LYS:HB2	1.55	0.46
1:D:4:LEU:O	1:D:7:LYS:HB2	2.15	0.46
1:H:40:ARG:HB2	3:H:1257:NAP:C2A	2.45	0.46
1:E:173:TYR:CZ	1:F:153:ALA:HA	2.51	0.46
1:B:157:TYR:CZ	1:B:160:MET:HG3	2.50	0.46
1:B:99:MET:O	1:B:101:ASP:N	2.48	0.46
1:A:100[A]:GLU:HB3	1:E:196:LEU:HD21	1.97	0.46
1:C:58:PRO:HD2	5:C:2047:HOH:O	2.16	0.46
1:C:120:ILE:HD13	3:C:1257:NAP:H61A	1.80	0.45
1:A:104[B]:GLY:CA	1:E:43:ARG:HH22	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:LYS:HE3	5:E:2008:HOH:O	2.16	0.45
1:F:224:VAL:HG23	5:F:2116:HOH:O	2.15	0.45
1:G:157:TYR:CZ	1:G:160:MET:HG3	2.51	0.45
1:A:38:THR:HA	1:A:63:TYR:O	2.17	0.45
1:C:8:THR:HA	1:C:34:LYS:O	2.17	0.45
1:E:52:LEU:HA	1:E:52:LEU:HD23	1.80	0.45
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.83	0.45
1:B:249:ASP:O	1:B:250:SER:HB2	2.16	0.45
1:F:18:ARG:HD3	5:F:2017:HOH:O	2.15	0.45
1:G:82:LYS:HE3	1:G:82:LYS:HB2	1.81	0.45
1:A:98:ASN:C	1:A:100[B]:GLU:H	2.20	0.45
1:E:37:PHE:CE2	1:E:52:LEU:HD21	2.52	0.45
1:B:103:ARG:HD3	2:B:1259:GLU:OE1	2.18	0.44
1:A:153:ALA:HA	1:B:173:TYR:CZ	2.52	0.44
1:C:192:PRO:HA	3:C:1257:NAP:O7N	2.18	0.44
1:A:256:LYS:HE3	1:C:148:LEU:HD21	1.98	0.44
1:H:154:VAL:HG12	4:H:1258:6PN:HAAB	2.00	0.44
1:B:158:ASN:HB3	5:B:2062:HOH:O	2.17	0.44
1:B:214:ARG:NH1	1:D:214[B]:ARG:NH1	2.65	0.44
1:F:214:ARG:NH1	1:H:214[B]:ARG:HH21	2.03	0.44
1:D:15:ALA:O	1:D:47:GLU:HG2	2.17	0.44
1:A:43:ARG:HH12	1:E:104[B]:GLY:HA3	1.82	0.44
1:C:18[B]:ARG:CD	5:C:2021:HOH:O	2.64	0.44
1:F:184:ARG:HD2	1:F:241:VAL:O	2.18	0.44
1:H:103:ARG:NH2	1:H:200:GLY:O	2.51	0.44
1:A:7:LYS:HA	1:A:7:LYS:HD3	1.75	0.44
1:A:173:TYR:CZ	1:B:153:ALA:HA	2.53	0.44
1:E:224:VAL:O	1:E:228:LYS:HG3	2.18	0.44
1:A:18[A]:ARG:HH22	1:A:199:LYS:CE	2.28	0.43
1:F:52:LEU:HD23	1:F:52:LEU:HA	1.79	0.43
1:B:214:ARG:HH12	1:D:214[B]:ARG:NH1	2.16	0.43
1:E:100[B]:GLU:HG2	1:E:100[B]:GLU:H	1.37	0.43
1:E:101[A]:ASP:HB3	1:E:159:VAL:CG1	2.49	0.43
1:H:201:VAL:HG11	4:H:1258:6PN:HAKA	2.01	0.43
1:H:51:LEU:O	1:H:54:GLN:HG3	2.18	0.43
1:C:151:GLU:OE2	1:C:247:HIS:NE2	2.52	0.43
1:E:19:SER:HB3	5:E:2013:HOH:O	2.18	0.43
1:C:173:TYR:CZ	1:D:153:ALA:HA	2.53	0.43
1:G:155:GLN:O	1:G:156:ASN:HB2	2.18	0.43
1:A:98:ASN:C	1:A:100[B]:GLU:N	2.70	0.43
1:C:38:THR:HA	1:C:63:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194[B]:ARG:NH2	5:D:2087:HOH:O	2.52	0.43
1:G:39:TYR:CE2	1:G:45:ARG:HB2	2.54	0.43
1:F:255:ILE:O	1:H:256:LYS:HE2	2.19	0.43
1:B:133:LYS:HD3	5:B:2069:HOH:O	2.18	0.42
1:G:18[A]:ARG:HD3	5:G:2112:HOH:O	2.19	0.42
1:H:41:LYS:HD2	3:H:1257:NAP:P2B	2.59	0.42
1:H:215:ALA:O	1:H:218:LYS:HD2	2.18	0.42
1:C:153:ALA:HA	1:D:173:TYR:CZ	2.55	0.42
1:E:52:LEU:HD23	1:E:55:LEU:HD12	2.01	0.42
1:E:71:GLU:H	1:E:71:GLU:CD	2.22	0.42
1:G:111:ARG:NH1	1:H:119:ASP:OD1	2.46	0.42
1:D:16:ASN:HB2	5:D:2016:HOH:O	2.20	0.42
1:A:76:GLY:O	1:A:80:ILE:HG13	2.19	0.42
1:A:192:PRO:HA	3:A:1257:NAP:O7N	2.20	0.42
1:B:207:ILE:HG13	4:B:1258:6PN:HALA	2.01	0.42
1:E:153:ALA:HA	1:F:173:TYR:CZ	2.55	0.42
1:G:100:GLU:CD	1:G:100:GLU:H	2.21	0.42
1:G:15:ALA:O	1:G:16:ASN:HB3	2.19	0.42
1:G:4:LEU:HD13	1:G:9:TYR:HE2	1.84	0.42
1:H:39:TYR:CZ	1:H:45:ARG:HD2	2.55	0.42
1:B:207:ILE:O	1:B:211:ILE:HG12	2.20	0.42
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.72	0.42
1:H:38:THR:HG21	1:H:65:ILE:HD12	2.02	0.42
1:A:101[B]:ASP:HA	1:E:43:ARG:HH12	1.84	0.42
1:D:43:ARG:N	1:D:43:ARG:HE	2.01	0.42
1:B:147:TYR:HB2	3:B:1257:NAP:C5N	2.50	0.41
1:E:148:LEU:HD21	1:G:256:LYS:HD2	2.01	0.41
1:C:255:ILE:O	1:C:255:ILE:HG13	2.20	0.41
1:E:207:ILE:HD11	5:E:2104:HOH:O	2.19	0.41
1:E:207:ILE:O	1:E:211:ILE:HG12	2.21	0.41
1:C:155:GLN:O	1:C:156:ASN:HB2	2.20	0.41
1:C:184:ARG:HD2	1:C:241:VAL:O	2.20	0.41
1:G:2:VAL:HG13	1:G:2:VAL:O	2.20	0.41
1:G:117:ALA:O	1:G:121:SER:HB2	2.20	0.41
1:F:210:GLU:OE2	1:F:214:ARG:NH1	2.53	0.41
1:A:199:LYS:HD2	2:D:1259:GLU:N	2.35	0.41
1:E:101[B]:ASP:OD2	1:E:113:GLY:HA3	2.20	0.41
1:F:5:GLU:O	1:F:6:ASN:CB	2.69	0.41
1:C:133:LYS:HE3	1:C:181:ASP:OD2	2.20	0.41
1:F:18:ARG:CD	5:F:2017:HOH:O	2.69	0.41
1:H:11:ILE:HG21	1:H:11:ILE:HD13	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:HB2	1:B:169:ALA:HB2	2.03	0.41
1:D:69:SER:OG	1:D:72:GLU:HG3	2.21	0.41
1:E:201:VAL:CG1	4:E:1258:6PN:HAKA	2.47	0.41
1:A:99[B]:MET:HB3	1:A:99[B]:MET:HE2	1.85	0.41
2:A:1259:GLU:N	1:E:199:LYS:HE3	2.36	0.41
1:H:143:VAL:HA	1:H:186:ASN:O	2.21	0.41
1:D:144:ALA:O	1:D:187:ALA:HA	2.20	0.41
1:E:99[B]:MET:CE	1:E:103[B]:ARG:HE	2.33	0.40
1:G:196:LEU:HA	1:G:196:LEU:HD12	1.79	0.40
1:A:47:GLU:O	1:A:51:LEU:HG	2.21	0.40
1:E:102[B]:LEU:HD23	1:E:102[B]:LEU:HA	1.75	0.40
1:E:192:PRO:HA	3:E:1257:NAP:O7N	2.21	0.40
1:G:99:MET:O	1:G:100:GLU:C	2.59	0.40
1:H:112:GLU:CD	1:H:112:GLU:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/282 (94%)	254 (96%)	11 (4%)	0	100	100
1	B	258/282 (92%)	246 (95%)	12 (5%)	0	100	100
1	C	259/282 (92%)	246 (95%)	13 (5%)	0	100	100
1	D	257/282 (91%)	247 (96%)	10 (4%)	0	100	100
1	E	266/282 (94%)	250 (94%)	16 (6%)	0	100	100
1	F	257/282 (91%)	243 (95%)	14 (5%)	0	100	100
1	G	259/282 (92%)	249 (96%)	10 (4%)	0	100	100
1	H	255/282 (90%)	244 (96%)	10 (4%)	1 (0%)	34	29
All	All	2076/2256 (92%)	1979 (95%)	96 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	155	GLN

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%)	218 (100%)	1 (0%)	88	92
1	B	213/234 (91%)	206 (97%)	7 (3%)	38	37
1	C	214/234 (92%)	205 (96%)	9 (4%)	30	28
1	D	212/234 (91%)	205 (97%)	7 (3%)	38	37
1	E	220/234 (94%)	212 (96%)	8 (4%)	35	33
1	F	212/234 (91%)	206 (97%)	6 (3%)	43	44
1	G	214/234 (92%)	209 (98%)	5 (2%)	50	53
1	H	210/234 (90%)	203 (97%)	7 (3%)	38	37
All	All	1714/1872 (92%)	1664 (97%)	50 (3%)	39	42

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	B	2	VAL
1	B	4	LEU
1	B	55	LEU
1	B	69	SER
1	B	112	GLU
1	B	194	ARG
1	B	209	LYS
1	C	17	LYS
1	C	30	GLN
1	C	45	ARG
1	C	46	LYS
1	C	55	LEU

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Mol	Chain	Res	Type
1	C	93	SER
1	C	138	GLU
1	C	206	THR
1	C	256	LYS
1	D	4	LEU
1	D	43	ARG
1	D	50	LYS
1	D	84	VAL
1	D	99	MET
1	D	127	ILE
1	D	213	GLU
1	E	45	ARG
1	E	99[A]	MET
1	E	99[B]	MET
1	E	138	GLU
1	E	199	LYS
1	E	208	LEU
1	E	209	LYS
1	E	210	GLU
1	F	2	VAL
1	F	50	LYS
1	F	55	LEU
1	F	138	GLU
1	F	209	LYS
1	F	218	LYS
1	G	2	VAL
1	G	17	LYS
1	G	47	GLU
1	G	55	LEU
1	G	138	GLU
1	H	4	LEU
1	H	5	GLU
1	H	41	LYS
1	H	42	GLU
1	H	50	LYS
1	H	138	GLU
1	H	255	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN

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Mol	Chain	Res	Type
1	A	253	HIS
1	B	253	HIS
1	C	3	ASN
1	C	253	HIS
1	D	3	ASN
1	D	56	ASN
1	D	253	HIS
1	E	3	ASN
1	F	56	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLU	B	1259	-	2,9,9	0.12	0	2,11,11	1.08	0
2	GLU	C	1260	-	2,9,9	0.10	0	2,11,11	1.45	1 (50%)
4	6PN	G	1258	-	21,21,21	0.76	0	26,26,26	1.37	5 (19%)
3	NAP	H	1257	-	45,52,52	1.63	4 (8%)	56,80,80	1.80	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	A	1257	-	45,52,52	1.68	5 (11%)	56,80,80	1.88	8 (14%)
3	NAP	D	1257	-	45,52,52	1.70	6 (13%)	56,80,80	1.66	10 (17%)
3	NAP	B	1257	-	45,52,52	1.63	4 (8%)	56,80,80	1.54	8 (14%)
3	NAP	E	1257	-	45,52,52	1.60	4 (8%)	56,80,80	1.61	8 (14%)
2	GLU	D	1259	-	2,9,9	0.13	0	2,11,11	0.83	0
3	NAP	F	1257	-	45,52,52	1.48	4 (8%)	56,80,80	1.79	8 (14%)
2	GLU	F	1259	-	2,9,9	0.16	0	2,11,11	1.60	0
4	6PN	F	1258	-	21,21,21	0.72	1 (4%)	26,26,26	1.32	5 (19%)
4	6PN	E	1258	-	21,21,21	0.75	0	26,26,26	0.92	2 (7%)
2	GLU	C	1259	-	2,9,9	0.20	0	2,11,11	2.23	1 (50%)
4	6PN	H	1258	-	21,21,21	0.66	0	26,26,26	1.09	1 (3%)
3	NAP	G	1257	-	45,52,52	1.62	5 (11%)	56,80,80	1.60	9 (16%)
4	6PN	B	1258	-	21,21,21	0.82	1 (4%)	26,26,26	1.08	2 (7%)
2	GLU	A	1259	-	2,9,9	0.22	0	2,11,11	1.34	0
3	NAP	C	1257	-	45,52,52	1.59	4 (8%)	56,80,80	1.51	6 (10%)
4	6PN	A	1258	-	21,21,21	0.72	1 (4%)	26,26,26	0.95	2 (7%)
4	6PN	D	1258	-	21,21,21	0.61	0	26,26,26	0.69	0
4	6PN	C	1258	-	21,21,21	0.77	0	26,26,26	1.07	2 (7%)
2	GLU	E	1259	-	2,9,9	0.34	0	2,11,11	1.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	B	1259	-	-	1/3/9/9	-
2	GLU	C	1260	-	-	2/3/9/9	-
4	6PN	G	1258	-	-	2/10/10/10	0/2/2/2
3	NAP	H	1257	-	-	5/31/67/67	0/5/5/5
3	NAP	A	1257	-	-	6/31/67/67	0/5/5/5
3	NAP	D	1257	-	-	5/31/67/67	0/5/5/5
3	NAP	B	1257	-	-	5/31/67/67	0/5/5/5
3	NAP	E	1257	-	-	6/31/67/67	0/5/5/5
2	GLU	D	1259	-	-	3/3/9/9	-
3	NAP	F	1257	-	-	6/31/67/67	0/5/5/5
2	GLU	F	1259	-	-	3/3/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6PN	F	1258	-	-	1/10/10/10	0/2/2/2
4	6PN	E	1258	-	-	3/10/10/10	0/2/2/2
2	GLU	C	1259	-	-	2/3/9/9	-
4	6PN	H	1258	-	-	3/10/10/10	0/2/2/2
3	NAP	G	1257	-	-	6/31/67/67	0/5/5/5
4	6PN	B	1258	-	-	2/10/10/10	0/2/2/2
2	GLU	A	1259	-	-	1/3/9/9	-
3	NAP	C	1257	-	-	6/31/67/67	0/5/5/5
4	6PN	A	1258	-	-	3/10/10/10	0/2/2/2
4	6PN	D	1258	-	-	2/10/10/10	0/2/2/2
4	6PN	C	1258	-	-	0/10/10/10	0/2/2/2
2	GLU	E	1259	-	-	2/3/9/9	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1257	NAP	O7N-C7N	8.24	1.39	1.24
3	D	1257	NAP	O7N-C7N	7.98	1.39	1.24
3	H	1257	NAP	O7N-C7N	7.95	1.39	1.24
3	G	1257	NAP	O7N-C7N	7.90	1.39	1.24
3	C	1257	NAP	O7N-C7N	7.86	1.39	1.24
3	A	1257	NAP	O7N-C7N	7.61	1.38	1.24
3	E	1257	NAP	O7N-C7N	7.15	1.37	1.24
3	F	1257	NAP	O7N-C7N	7.01	1.37	1.24
3	D	1257	NAP	C2A-N3A	4.59	1.39	1.32
3	E	1257	NAP	C2A-N3A	4.19	1.38	1.32
3	A	1257	NAP	C2A-N3A	4.16	1.38	1.32
3	H	1257	NAP	C2A-N3A	4.09	1.38	1.32
3	G	1257	NAP	C2A-N3A	3.73	1.38	1.32
3	B	1257	NAP	C2A-N3A	3.48	1.37	1.32
3	E	1257	NAP	C2A-N1A	3.33	1.40	1.33
3	F	1257	NAP	C2A-N3A	3.13	1.37	1.32
3	F	1257	NAP	P2B-O2B	3.07	1.65	1.59
3	C	1257	NAP	C2A-N3A	3.04	1.37	1.32
3	D	1257	NAP	C2A-N1A	2.95	1.39	1.33
4	B	1258	6PN	CAJ-CAR	2.92	1.43	1.38
3	G	1257	NAP	C2A-N1A	2.85	1.39	1.33
3	B	1257	NAP	P2B-O2B	2.83	1.64	1.59
3	A	1257	NAP	P2B-O2B	2.76	1.64	1.59
3	C	1257	NAP	C2A-N1A	2.71	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1257	NAP	C2A-N1A	2.71	1.38	1.33
3	C	1257	NAP	P2B-O2B	2.67	1.64	1.59
3	D	1257	NAP	C2N-N1N	2.66	1.38	1.35
3	A	1257	NAP	C2N-N1N	2.56	1.38	1.35
4	F	1258	6PN	CAJ-CAR	2.43	1.42	1.38
3	G	1257	NAP	P2B-O2B	2.34	1.63	1.59
3	B	1257	NAP	C2A-N1A	2.28	1.38	1.33
3	A	1257	NAP	C2A-N1A	2.24	1.38	1.33
3	E	1257	NAP	P2B-O2B	2.21	1.63	1.59
4	A	1258	6PN	OAP-CAS	-2.17	1.35	1.39
3	D	1257	NAP	P2B-O2B	2.12	1.63	1.59
3	G	1257	NAP	C2N-N1N	2.11	1.37	1.35
3	F	1257	NAP	C2A-N1A	2.09	1.37	1.33
3	H	1257	NAP	P2B-O2B	2.07	1.63	1.59
3	D	1257	NAP	PA-O2A	-2.00	1.45	1.55

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1257	NAP	C3N-C7N-N7N	6.32	125.34	117.75
3	F	1257	NAP	N3A-C2A-N1A	-6.04	119.23	128.68
3	B	1257	NAP	N3A-C2A-N1A	-5.89	119.47	128.68
3	F	1257	NAP	C3N-C7N-N7N	5.82	124.74	117.75
3	E	1257	NAP	N3A-C2A-N1A	-5.75	119.69	128.68
3	H	1257	NAP	N3A-C2A-N1A	-5.71	119.76	128.68
3	E	1257	NAP	C3N-C7N-N7N	5.37	124.20	117.75
3	A	1257	NAP	N3A-C2A-N1A	-5.29	120.40	128.68
3	H	1257	NAP	O7N-C7N-C3N	-5.25	113.35	119.63
3	G	1257	NAP	C3N-C7N-N7N	5.13	123.90	117.75
3	A	1257	NAP	O7N-C7N-C3N	-5.08	113.55	119.63
3	D	1257	NAP	C3N-C7N-N7N	5.08	123.85	117.75
3	C	1257	NAP	N3A-C2A-N1A	-5.08	120.74	128.68
3	D	1257	NAP	N3A-C2A-N1A	-5.01	120.84	128.68
3	F	1257	NAP	C1B-N9A-C4A	-4.64	118.48	126.64
3	G	1257	NAP	N3A-C2A-N1A	-4.55	121.56	128.68
3	C	1257	NAP	C3N-C7N-N7N	4.48	123.12	117.75
3	H	1257	NAP	O4B-C1B-C2B	-4.41	98.94	106.59
3	A	1257	NAP	O4D-C1D-C2D	-4.36	100.55	106.93
3	B	1257	NAP	C3N-C7N-N7N	4.07	122.64	117.75
3	A	1257	NAP	C6N-N1N-C2N	-4.05	118.28	121.97
3	F	1257	NAP	O7N-C7N-N7N	-3.71	117.30	122.58
3	D	1257	NAP	C1B-N9A-C4A	-3.61	120.30	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1257	NAP	C2N-C3N-C4N	3.51	122.23	118.26
3	G	1257	NAP	O7N-C7N-C3N	-3.34	115.64	119.63
3	F	1257	NAP	O4D-C1D-C2D	-3.33	102.06	106.93
3	H	1257	NAP	C3N-C7N-N7N	3.33	121.75	117.75
3	C	1257	NAP	O7N-C7N-C3N	-3.32	115.65	119.63
3	E	1257	NAP	C2N-C3N-C4N	3.24	121.93	118.26
3	D	1257	NAP	O3X-P2B-O2X	3.21	119.89	107.64
3	H	1257	NAP	O3X-P2B-O2X	3.19	119.83	107.64
2	C	1259	GLU	CB-CG-CD	-3.15	106.82	113.59
4	G	1258	6PN	CAJ-CAR-CAT	3.12	123.01	119.81
3	C	1257	NAP	C3D-C2D-C1D	-3.03	96.41	100.98
3	B	1257	NAP	O4B-C1B-C2B	-2.95	101.47	106.59
3	D	1257	NAP	O5B-C5B-C4B	-2.94	98.87	108.99
3	H	1257	NAP	O3X-P2B-O1X	-2.94	99.19	110.68
3	D	1257	NAP	O7N-C7N-C3N	-2.83	116.25	119.63
3	H	1257	NAP	O4D-C1D-C2D	-2.81	102.82	106.93
4	F	1258	6PN	CAJ-CAR-CAT	2.79	122.67	119.81
4	G	1258	6PN	CAR-CAJ-CAQ	-2.79	117.86	120.83
3	C	1257	NAP	O3X-P2B-O2X	2.77	118.22	107.64
3	D	1257	NAP	O4D-C1D-C2D	-2.65	103.05	106.93
3	E	1257	NAP	O7N-C7N-C3N	-2.64	116.47	119.63
3	F	1257	NAP	O2X-P2B-O1X	2.64	121.00	110.68
3	H	1257	NAP	C2N-C3N-C4N	2.63	121.24	118.26
3	B	1257	NAP	O4D-C1D-C2D	-2.63	103.08	106.93
3	G	1257	NAP	C3N-C2N-N1N	-2.62	117.87	120.43
4	F	1258	6PN	CAI-CAT-CAR	-2.58	116.64	119.86
3	C	1257	NAP	O4B-C1B-C2B	-2.58	102.12	106.59
4	A	1258	6PN	CAN-CAO-CAQ	-2.56	104.03	113.68
3	G	1257	NAP	O4B-C1B-C2B	-2.56	102.15	106.59
3	H	1257	NAP	C4A-C5A-N7A	-2.53	106.76	109.40
3	F	1257	NAP	O2N-PN-O1N	2.53	124.74	112.24
4	C	1258	6PN	OAP-CAT-CAR	2.52	120.94	116.22
4	G	1258	6PN	CAN-CAO-CAQ	-2.52	104.21	113.68
3	E	1257	NAP	O4D-C1D-C2D	-2.48	103.31	106.93
3	H	1257	NAP	C1B-N9A-C4A	-2.43	122.37	126.64
4	E	1258	6PN	CAN-CAO-CAQ	-2.43	104.54	113.68
3	E	1257	NAP	O7N-C7N-N7N	-2.41	119.16	122.58
4	B	1258	6PN	OAP-CAT-CAR	2.38	120.66	116.22
3	B	1257	NAP	C2N-C3N-C4N	2.36	120.93	118.26
3	B	1257	NAP	O7N-C7N-C3N	-2.35	116.82	119.63
4	E	1258	6PN	CAI-CAH-CAQ	-2.34	117.80	121.03
3	H	1257	NAP	C3N-C2N-N1N	-2.34	118.14	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1258	6PN	OAP-CAT-CAR	2.33	120.58	116.22
3	A	1257	NAP	C2N-C3N-C4N	2.30	120.86	118.26
3	D	1257	NAP	C6N-N1N-C2N	-2.28	119.90	121.97
3	A	1257	NAP	C4A-C5A-N7A	-2.27	107.03	109.40
3	E	1257	NAP	C3N-C2N-N1N	-2.27	118.21	120.43
3	A	1257	NAP	C5N-C4N-C3N	-2.26	117.67	120.34
4	G	1258	6PN	OAB-CAR-CAT	-2.25	114.84	120.09
4	A	1258	6PN	OAP-CAT-CAR	2.24	120.42	116.22
3	D	1257	NAP	O4B-C4B-C3B	2.21	109.49	105.11
3	B	1257	NAP	O2A-PA-O1A	2.20	123.12	112.24
3	F	1257	NAP	C5N-C4N-C3N	2.20	122.94	120.34
4	F	1258	6PN	OAB-CAR-CAT	-2.18	115.01	120.09
3	G	1257	NAP	O2A-PA-O1A	2.17	122.97	112.24
3	E	1257	NAP	O4B-C4B-C3B	2.14	109.34	105.11
3	G	1257	NAP	C3D-C2D-C1D	-2.14	97.76	100.98
4	H	1258	6PN	CAN-CAO-CAQ	-2.09	105.82	113.68
4	F	1258	6PN	CAR-CAJ-CAQ	-2.08	118.62	120.83
4	B	1258	6PN	CAI-CAT-CAR	-2.05	117.30	119.86
4	F	1258	6PN	OAP-CAT-CAR	2.05	120.05	116.22
4	C	1258	6PN	CAN-CAO-CAQ	-2.04	105.98	113.68
2	C	1260	GLU	CG-CB-CA	-2.04	109.08	113.84
3	G	1257	NAP	O5B-C5B-C4B	-2.03	101.99	108.99
3	H	1257	NAP	O5B-C5B-C4B	-2.02	102.03	108.99
3	B	1257	NAP	O3B-C3B-C2B	-2.01	105.44	111.17
3	D	1257	NAP	C2N-C3N-C4N	2.01	120.54	118.26

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1260	GLU	N-CA-CB-CG
2	C	1260	GLU	C-CA-CB-CG
3	H	1257	NAP	C5D-O5D-PN-O1N
3	H	1257	NAP	C5D-O5D-PN-O2N
3	A	1257	NAP	C5D-O5D-PN-O1N
3	A	1257	NAP	C5D-O5D-PN-O2N
3	A	1257	NAP	O4D-C1D-N1N-C2N
3	D	1257	NAP	C5D-O5D-PN-O1N
3	D	1257	NAP	C5D-O5D-PN-O2N
3	B	1257	NAP	PN-O3-PA-O5B
3	B	1257	NAP	C5D-O5D-PN-O3
3	B	1257	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
3	B	1257	NAP	O4D-C1D-N1N-C2N
3	E	1257	NAP	C5D-O5D-PN-O1N
3	E	1257	NAP	C5D-O5D-PN-O2N
3	E	1257	NAP	O4D-C1D-N1N-C2N
2	D	1259	GLU	C-CA-CB-CG
3	F	1257	NAP	C5D-O5D-PN-O1N
3	F	1257	NAP	C5D-O5D-PN-O2N
3	F	1257	NAP	O4D-C1D-N1N-C2N
2	F	1259	GLU	C-CA-CB-CG
2	F	1259	GLU	CA-CB-CG-CD
2	C	1259	GLU	N-CA-CB-CG
2	C	1259	GLU	C-CA-CB-CG
3	G	1257	NAP	PN-O3-PA-O5B
3	G	1257	NAP	C5D-O5D-PN-O3
3	G	1257	NAP	C5D-O5D-PN-O1N
3	G	1257	NAP	C5D-O5D-PN-O2N
3	G	1257	NAP	O4D-C1D-N1N-C2N
3	C	1257	NAP	C5D-O5D-PN-O1N
3	C	1257	NAP	C5D-O5D-PN-O2N
3	C	1257	NAP	O4D-C1D-N1N-C2N
2	E	1259	GLU	C-CA-CB-CG
2	E	1259	GLU	CA-CB-CG-CD
4	B	1258	6PN	CAK-CAL-CAM-CAN
2	D	1259	GLU	CA-CB-CG-CD
4	E	1258	6PN	CAM-CAN-CAO-CAQ
4	G	1258	6PN	CAK-CAL-CAM-CAN
4	H	1258	6PN	CAM-CAN-CAO-CAQ
4	A	1258	6PN	CAK-CAL-CAM-CAN
4	F	1258	6PN	CAL-CAM-CAN-CAO
4	E	1258	6PN	CAK-CAL-CAM-CAN
4	H	1258	6PN	CAK-CAL-CAM-CAN
4	A	1258	6PN	CAL-CAM-CAN-CAO
4	H	1258	6PN	CAL-CAM-CAN-CAO
4	G	1258	6PN	CAL-CAM-CAN-CAO
3	H	1257	NAP	PN-O3-PA-O5B
3	A	1257	NAP	PN-O3-PA-O5B
3	E	1257	NAP	PN-O3-PA-O5B
2	B	1259	GLU	CA-CB-CG-CD
2	A	1259	GLU	CA-CB-CG-CD
4	D	1258	6PN	CAM-CAN-CAO-CAQ
3	A	1257	NAP	C5D-O5D-PN-O3
3	C	1257	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	D	1257	NAP	O4B-C4B-C5B-O5B
4	A	1258	6PN	CAM-CAN-CAO-CAQ
2	D	1259	GLU	N-CA-CB-CG
4	D	1258	6PN	CAL-CAM-CAN-CAO
4	E	1258	6PN	CAL-CAM-CAN-CAO
4	B	1258	6PN	CAL-CAM-CAN-CAO
3	B	1257	NAP	O4B-C4B-C5B-O5B
3	H	1257	NAP	C5D-O5D-PN-O3
3	D	1257	NAP	C2B-O2B-P2B-O3X
3	D	1257	NAP	C5D-O5D-PN-O3
3	E	1257	NAP	C5D-O5D-PN-O3
3	F	1257	NAP	C5D-O5D-PN-O3
3	A	1257	NAP	O4B-C4B-C5B-O5B
3	E	1257	NAP	O4B-C4B-C5B-O5B
3	F	1257	NAP	O4B-C4B-C5B-O5B
3	C	1257	NAP	O4B-C4B-C5B-O5B
3	F	1257	NAP	PA-O3-PN-O2N
3	C	1257	NAP	PA-O3-PN-O2N
3	H	1257	NAP	O4B-C4B-C5B-O5B
3	G	1257	NAP	O4B-C4B-C5B-O5B
2	F	1259	GLU	N-CA-CB-CG

There are no ring outliers.

17 monomers are involved in 25 short contacts:

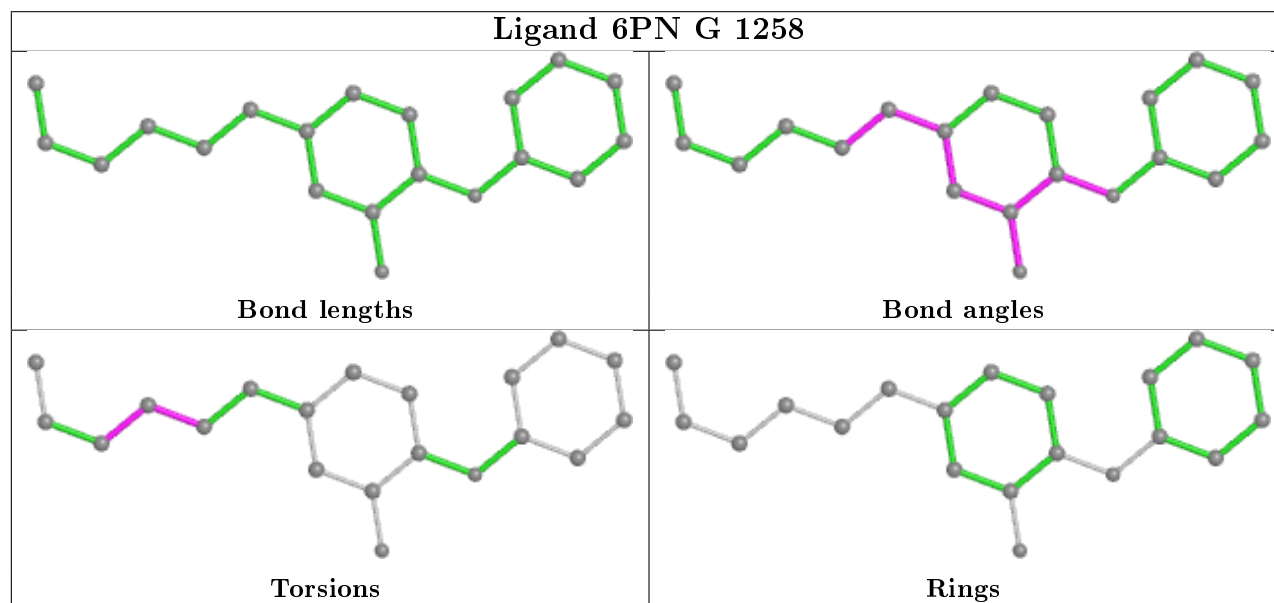
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1259	GLU	1	0
2	C	1260	GLU	1	0
3	H	1257	NAP	3	0
3	A	1257	NAP	1	0
3	B	1257	NAP	1	0
3	E	1257	NAP	1	0
2	D	1259	GLU	1	0
3	F	1257	NAP	2	0
4	F	1258	6PN	1	0
4	E	1258	6PN	2	0
2	C	1259	GLU	2	0
4	H	1258	6PN	3	0
4	B	1258	6PN	2	0
2	A	1259	GLU	1	0
3	C	1257	NAP	2	0
4	D	1258	6PN	1	0

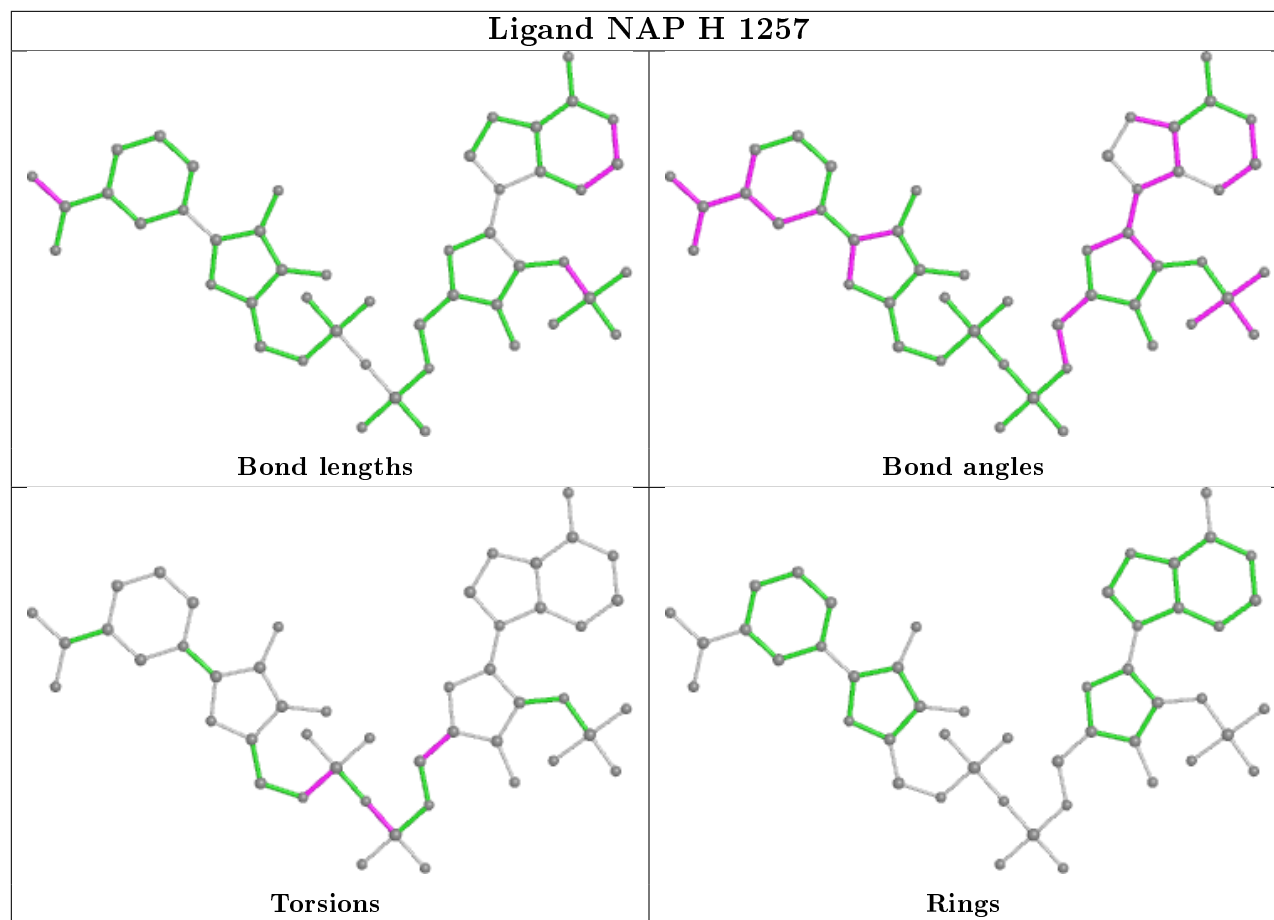
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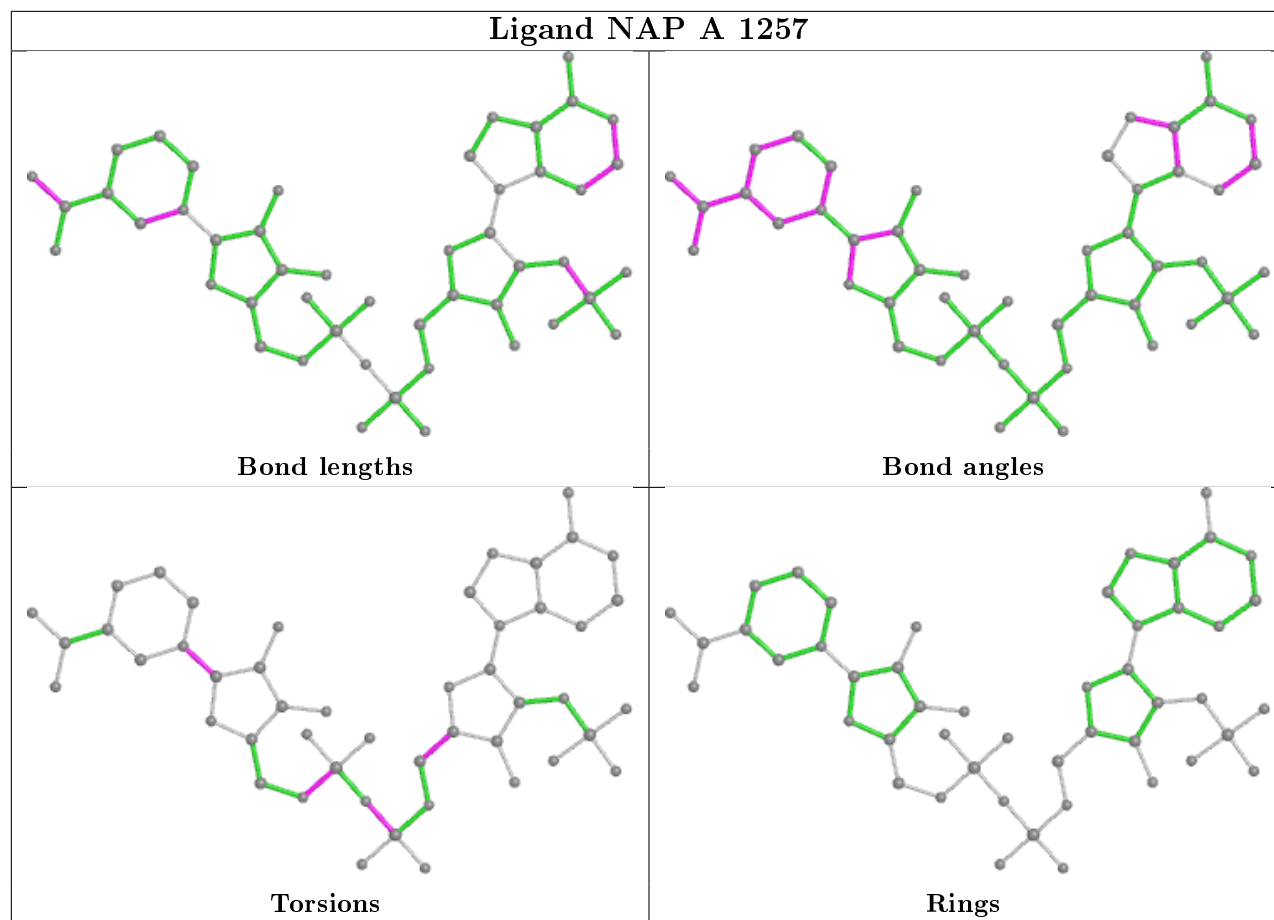
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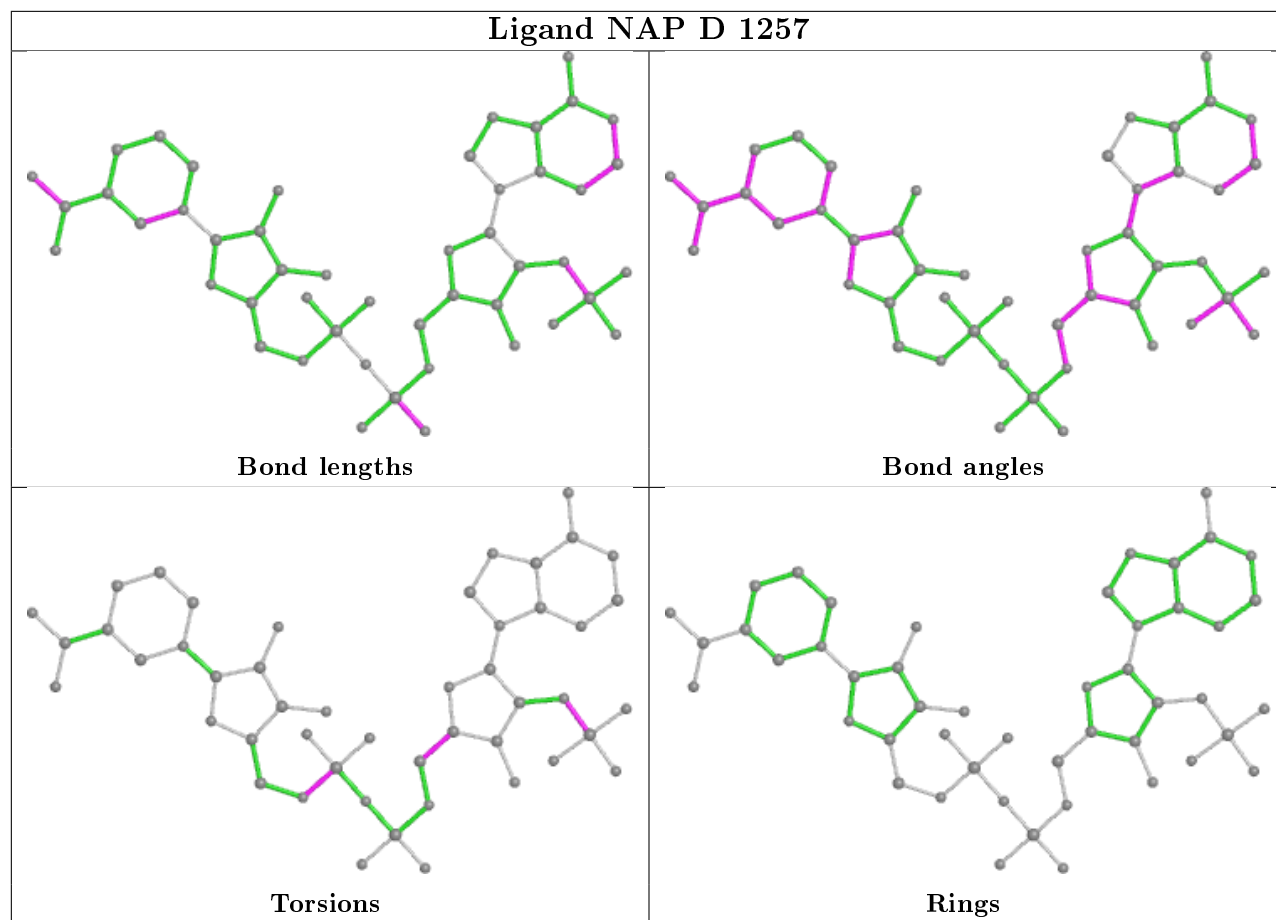
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1259	GLU	1	0

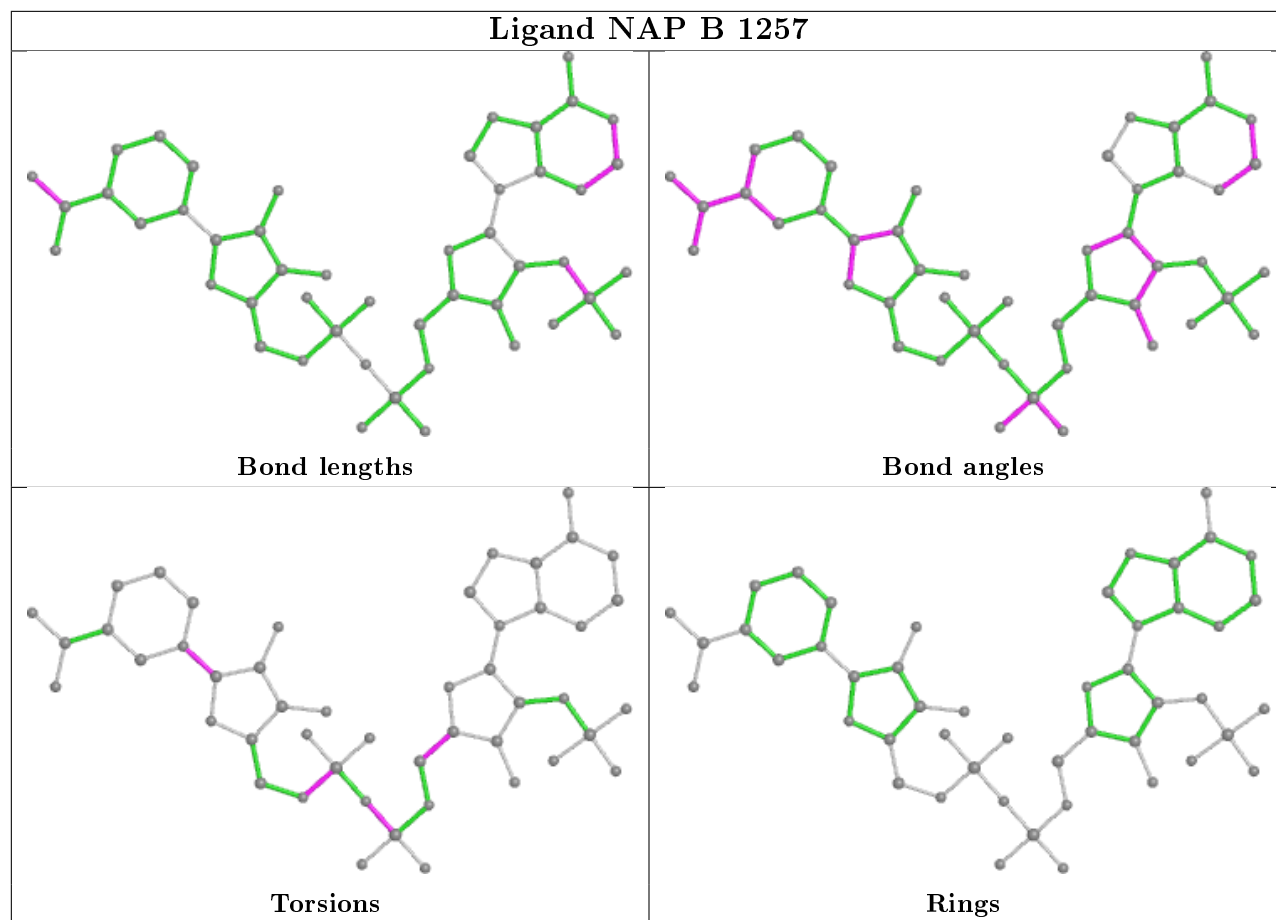
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

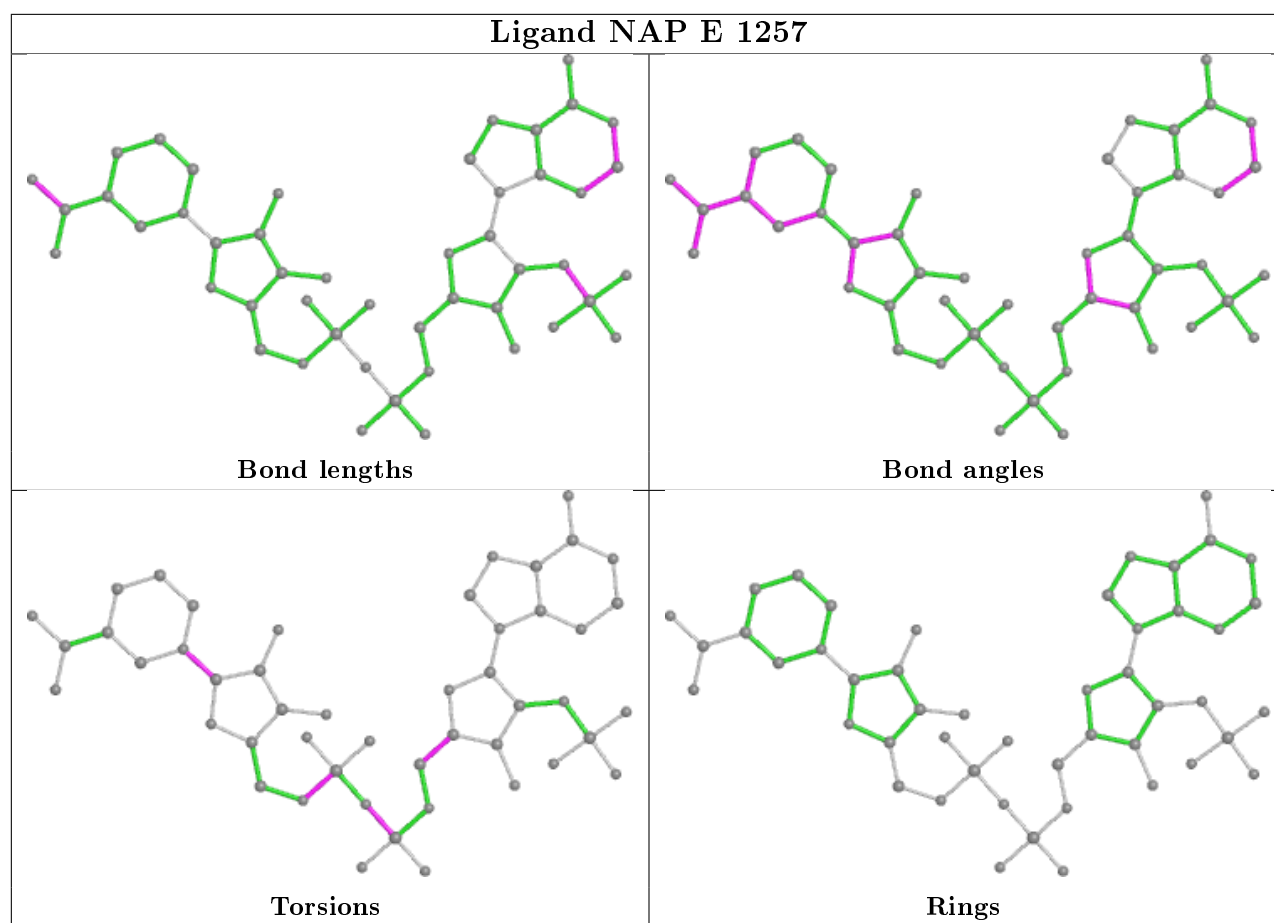




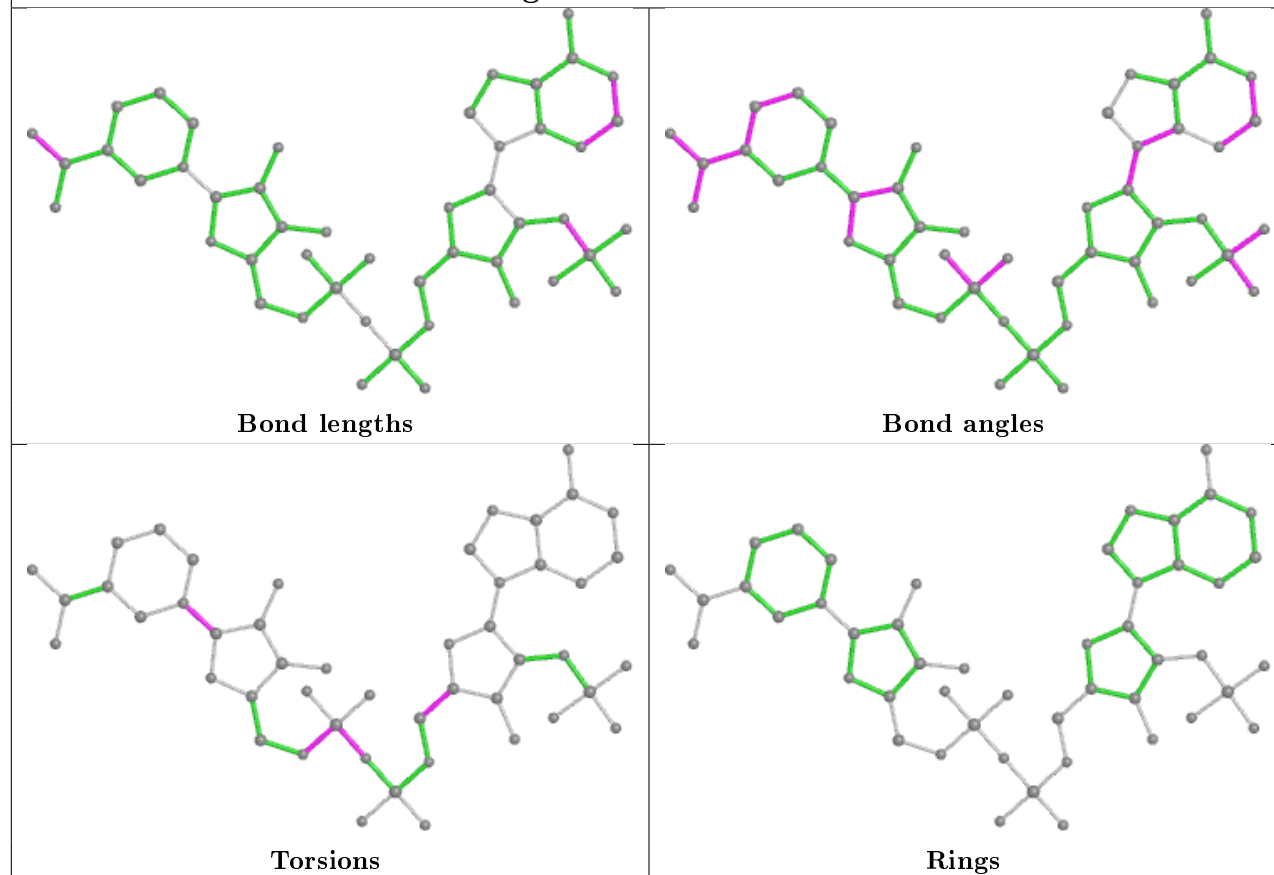




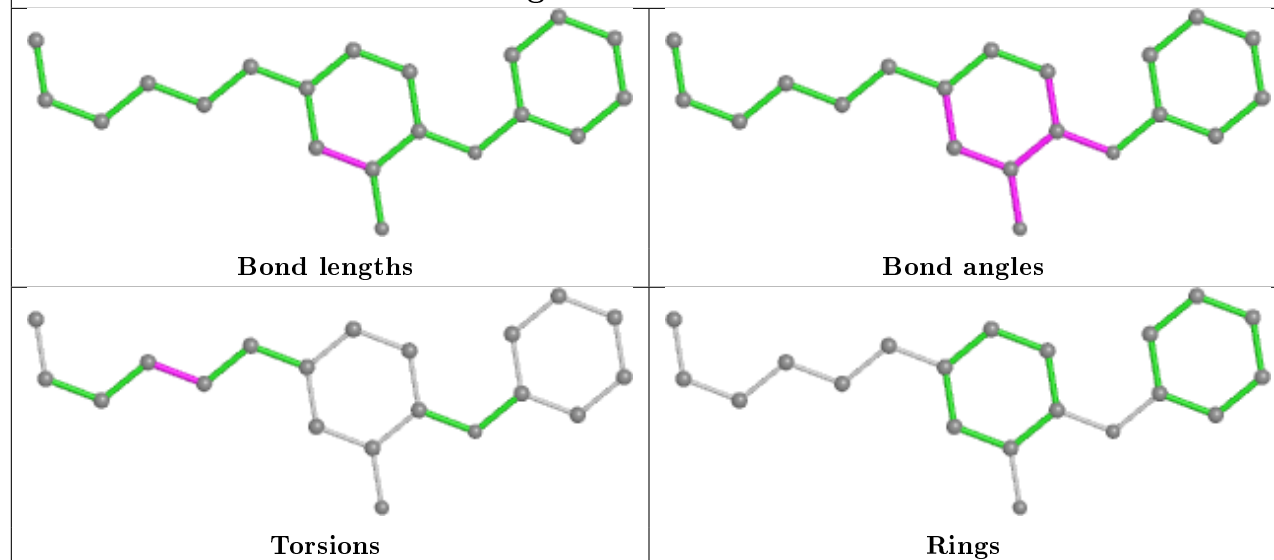


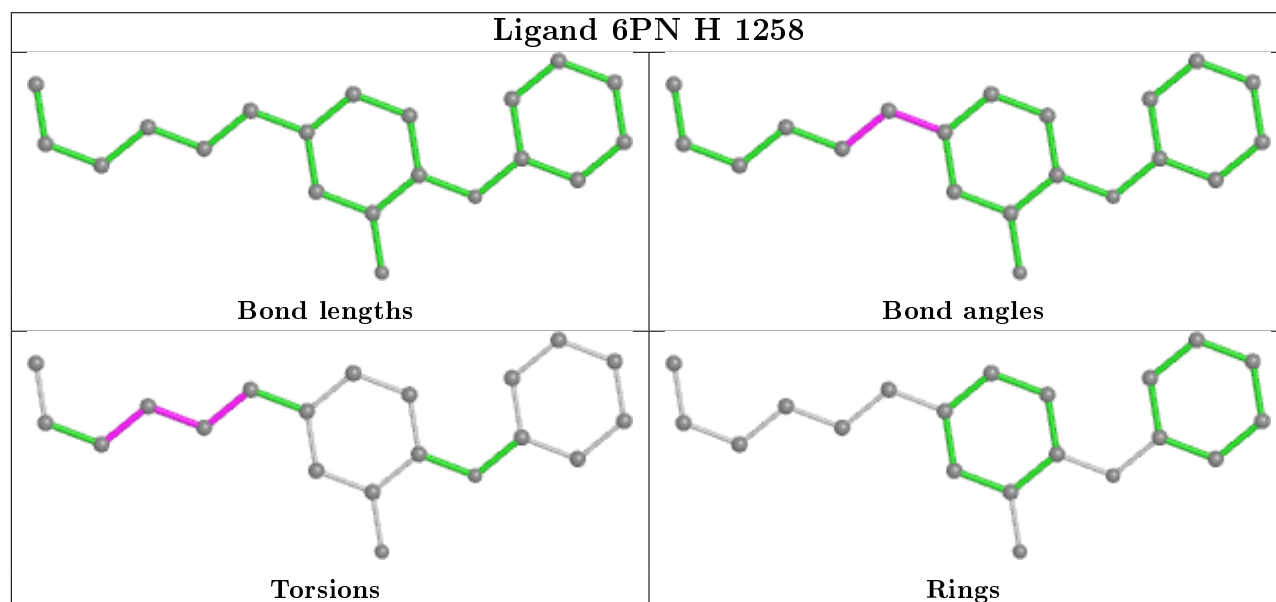
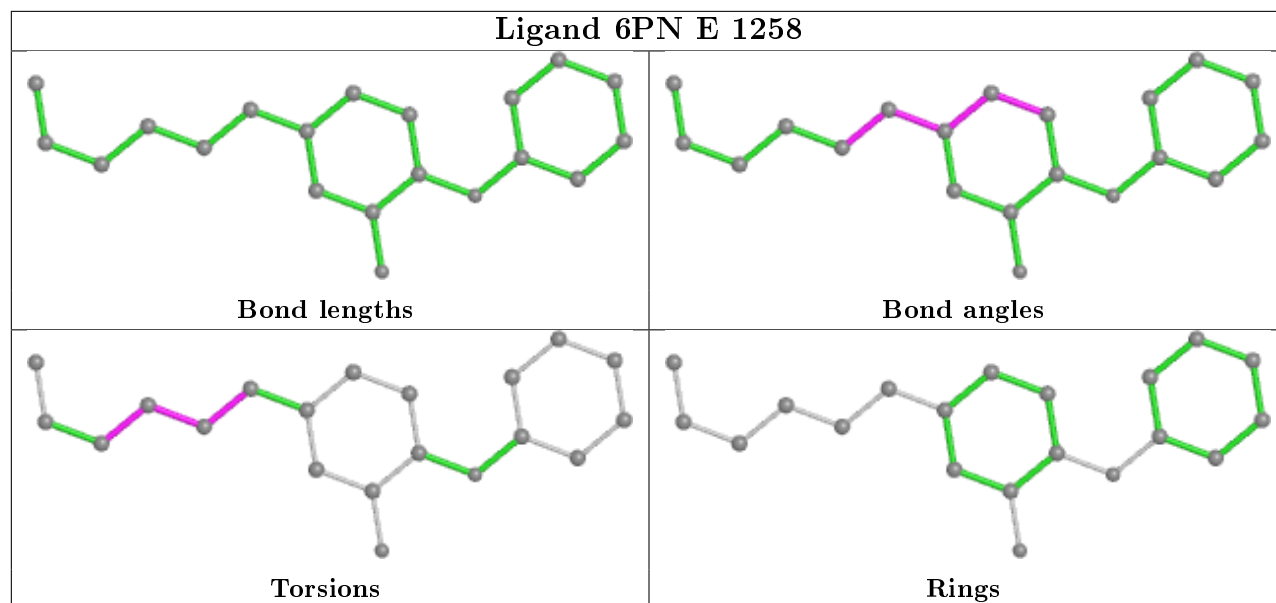


Ligand NAP F 1257

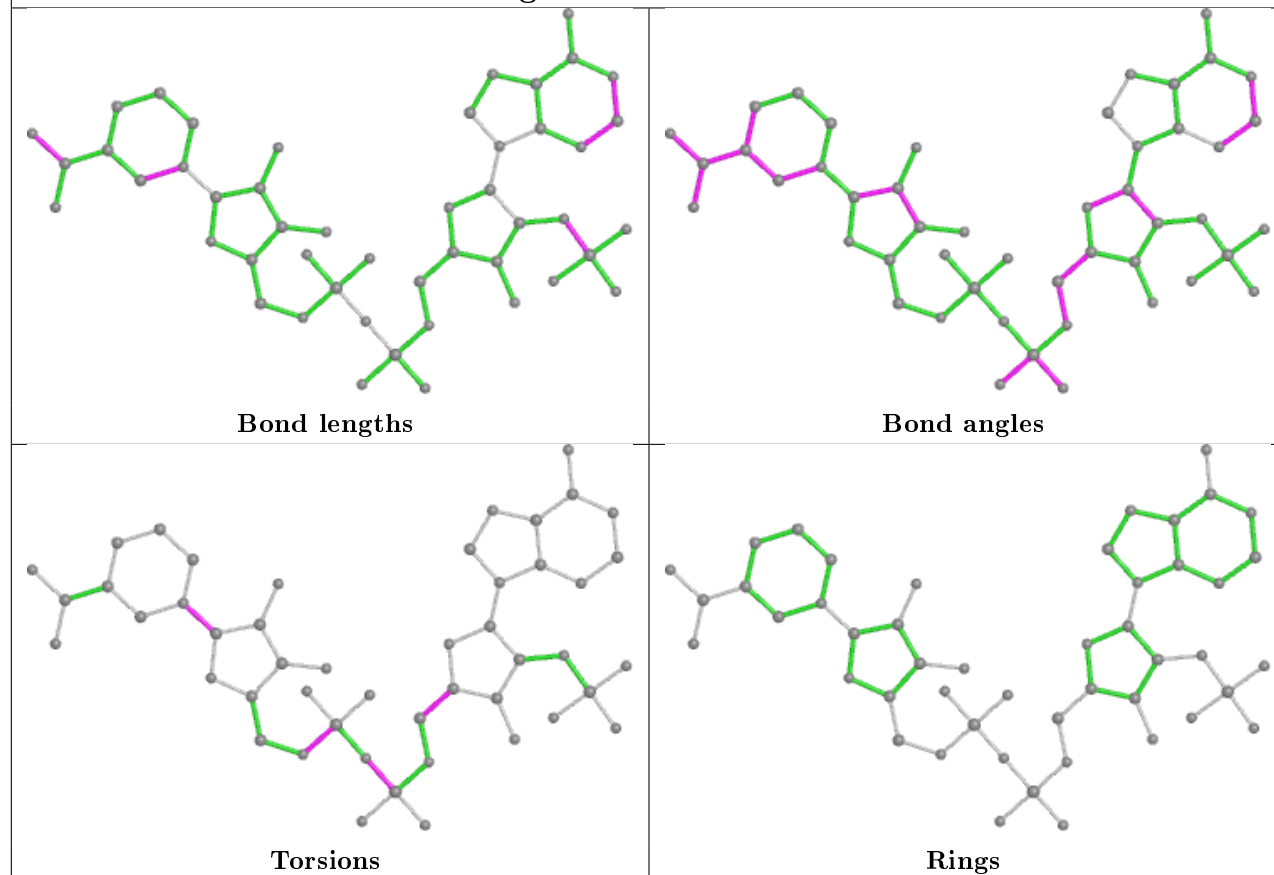


Ligand 6PN F 1258

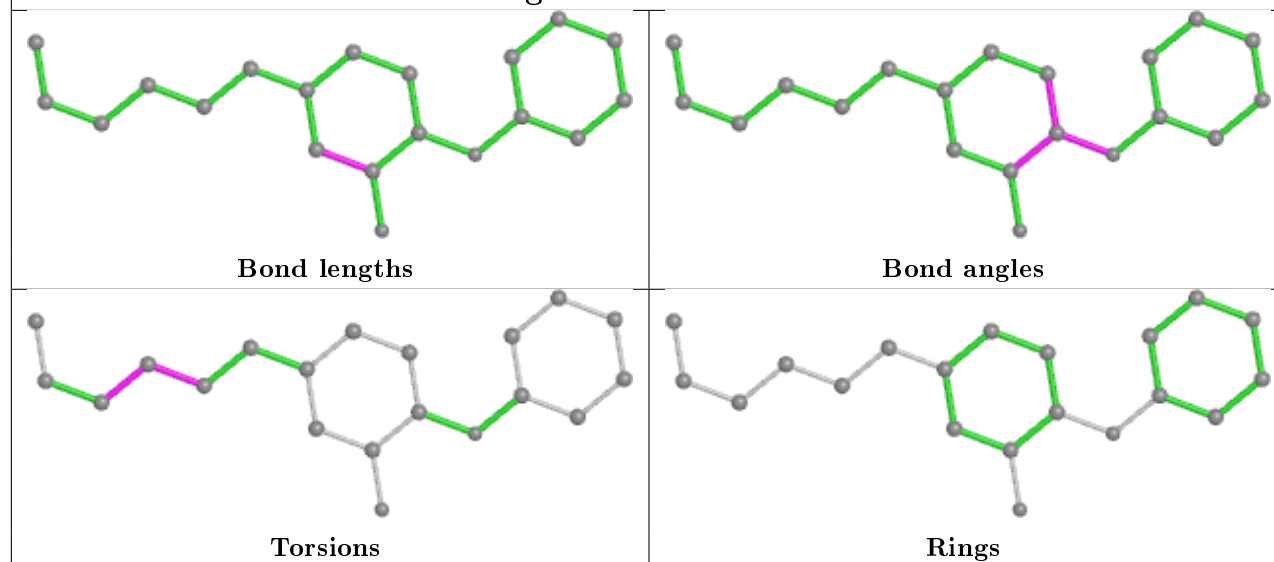




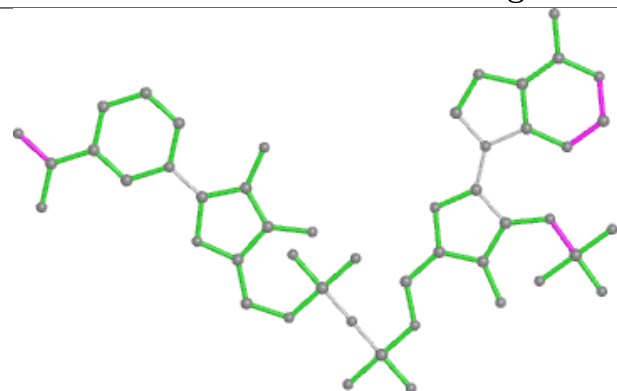
Ligand NAP G 1257



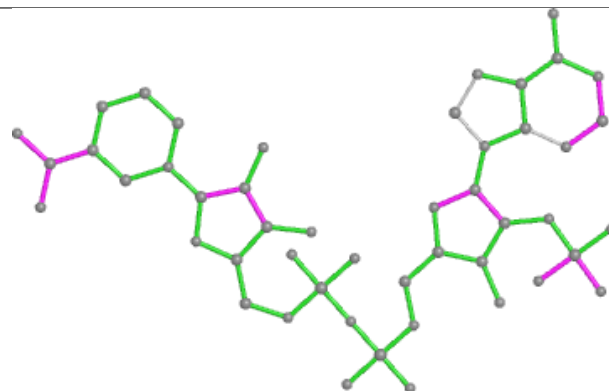
Ligand 6PN B 1258



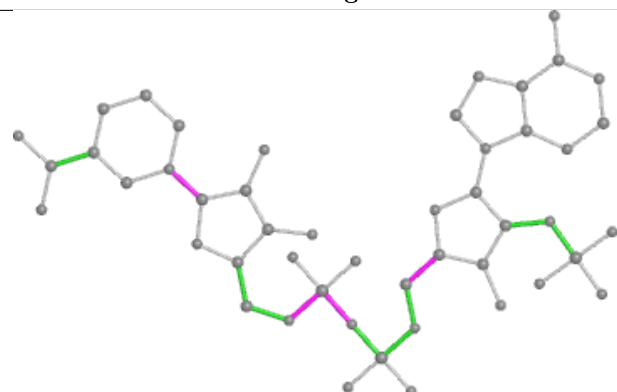
Ligand NAP C 1257



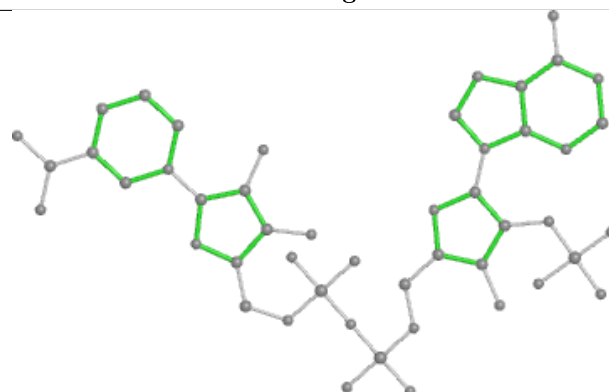
Bond lengths



Bond angles

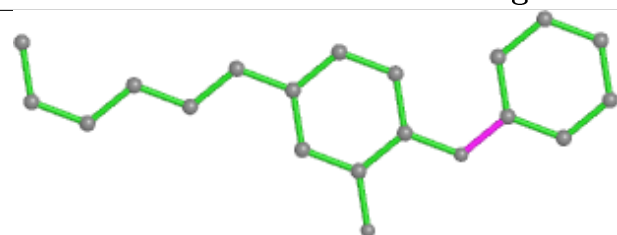


Torsions

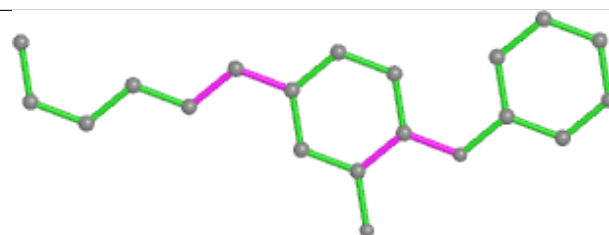


Rings

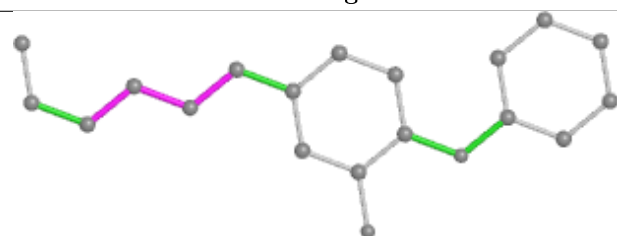
Ligand 6PN A 1258



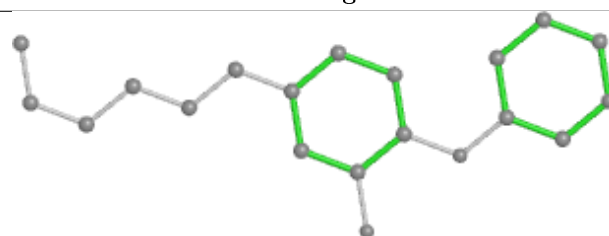
Bond lengths



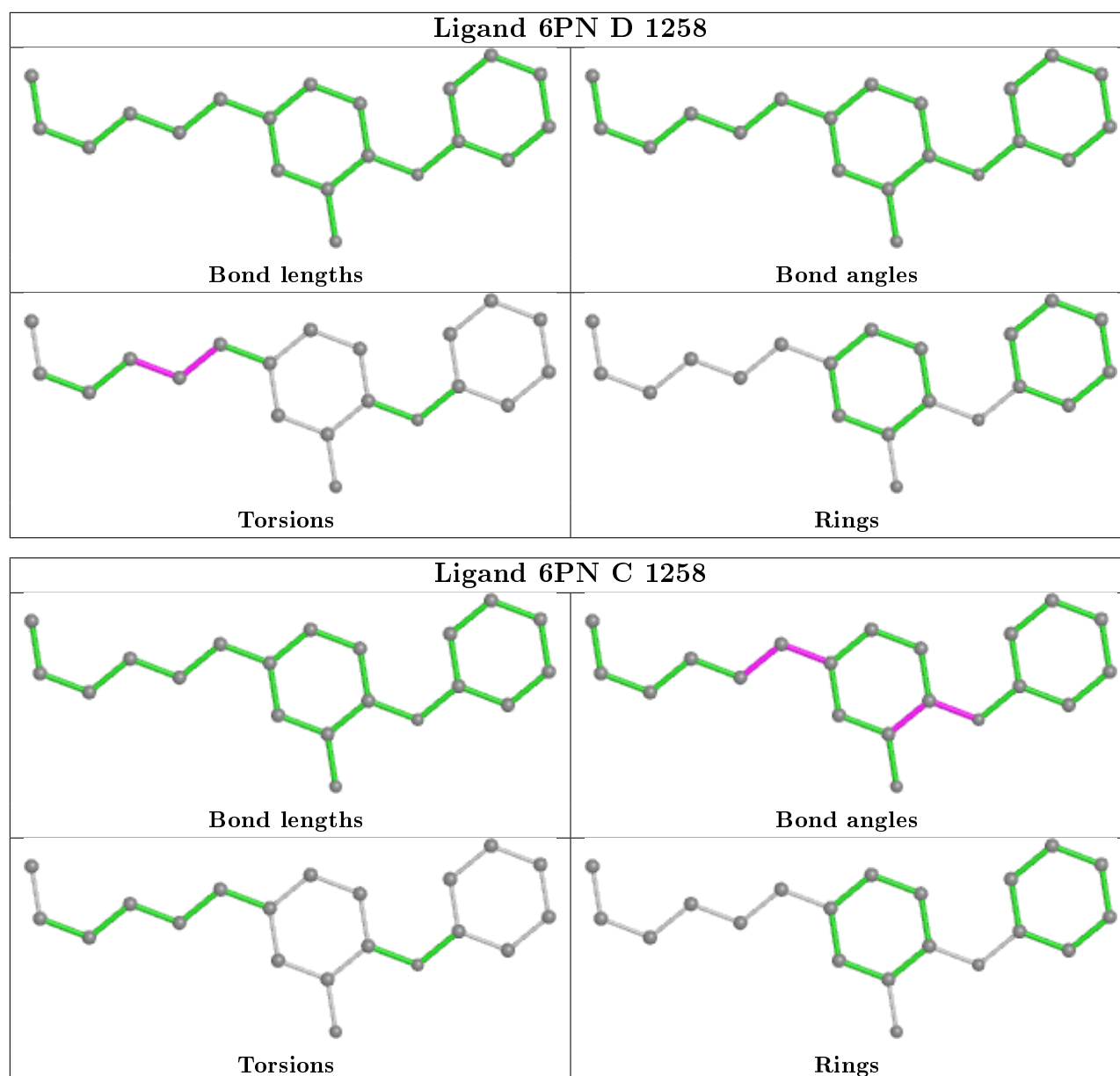
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	254/282 (90%)	-0.43	0 100 100	17, 27, 51, 66	0
1	B	255/282 (90%)	-0.53	1 (0%) 92 94	16, 30, 57, 66	0
1	C	255/282 (90%)	-0.38	3 (1%) 79 83	17, 32, 57, 70	0
1	D	254/282 (90%)	-0.35	2 (0%) 86 89	20, 36, 68, 80	0
1	E	255/282 (90%)	-0.48	1 (0%) 92 94	17, 28, 51, 71	0
1	F	255/282 (90%)	-0.43	1 (0%) 92 94	17, 31, 60, 70	0
1	G	255/282 (90%)	-0.45	1 (0%) 92 94	19, 33, 58, 75	0
1	H	254/282 (90%)	-0.32	3 (1%) 79 83	18, 35, 67, 102	0
All	All	2037/2256 (90%)	-0.42	12 (0%) 89 91	16, 31, 60, 102	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	VAL	3.5
1	D	58	PRO	2.9
1	F	2	VAL	2.7
1	G	2	VAL	2.6
1	E	2	VAL	2.5
1	C	6	ASN	2.4
1	H	43	ARG	2.3
1	H	56	ASN	2.3
1	C	58	PRO	2.3
1	B	2	VAL	2.3
1	H	58	PRO	2.2
1	D	50	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

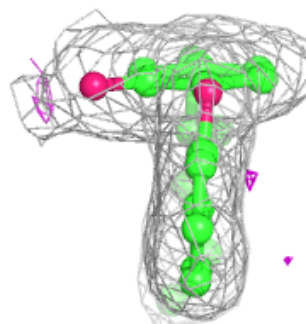
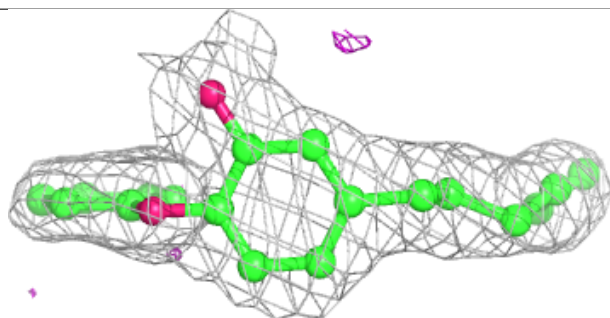
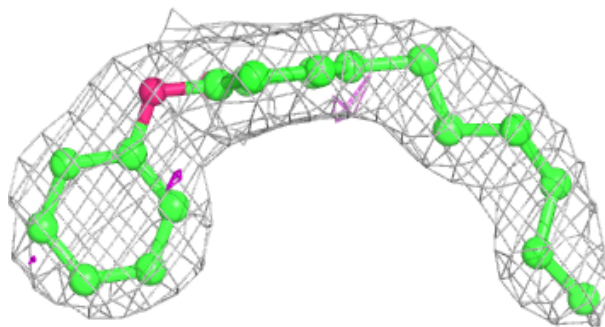
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLU	E	1259	10/10	0.62	0.22	91,92,98,98	0
2	GLU	C	1259	10/10	0.74	0.34	86,88,95,96	0
2	GLU	F	1259	10/10	0.74	0.15	97,98,102,103	0
2	GLU	D	1259	10/10	0.78	0.18	93,94,96,98	0
2	GLU	B	1259	10/10	0.78	0.15	88,89,94,94	0
2	GLU	A	1259	10/10	0.80	0.19	85,88,95,97	0
2	GLU	C	1260	10/10	0.80	0.14	88,88,94,94	0
4	6PN	D	1258	20/20	0.96	0.12	32,39,41,43	0
3	NAP	D	1257	48/48	0.97	0.09	26,34,47,52	0
4	6PN	H	1258	20/20	0.97	0.10	28,35,43,46	0
4	6PN	G	1258	20/20	0.97	0.09	23,29,38,38	0
3	NAP	H	1257	48/48	0.97	0.09	23,32,44,50	0
4	6PN	C	1258	20/20	0.97	0.10	23,30,34,38	0
4	6PN	F	1258	20/20	0.97	0.10	24,27,39,39	0
3	NAP	C	1257	48/48	0.98	0.12	20,28,35,41	0
4	6PN	A	1258	20/20	0.98	0.10	20,24,36,36	0
4	6PN	E	1258	20/20	0.98	0.09	20,27,33,38	0
4	6PN	B	1258	20/20	0.98	0.08	22,26,39,40	0
3	NAP	A	1257	48/48	0.98	0.09	17,25,29,39	0
3	NAP	G	1257	48/48	0.99	0.09	20,28,32,36	0
3	NAP	F	1257	48/48	0.99	0.09	22,28,33,36	0
3	NAP	E	1257	48/48	0.99	0.09	14,24,29,31	0
3	NAP	B	1257	48/48	0.99	0.08	18,27,32,35	0

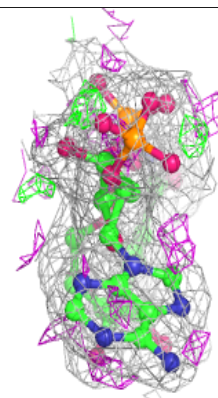
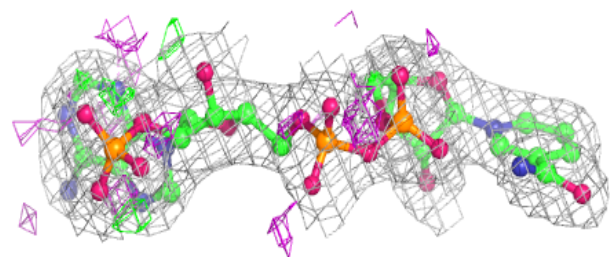
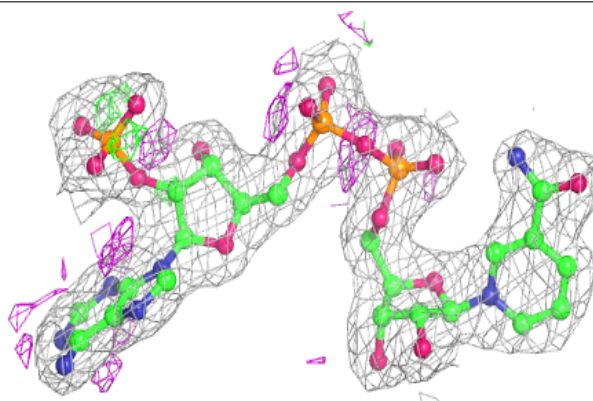
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6PN 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)

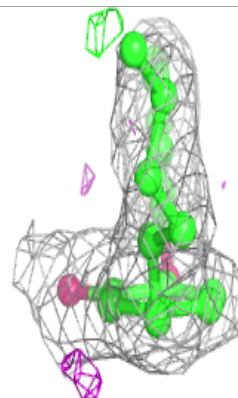
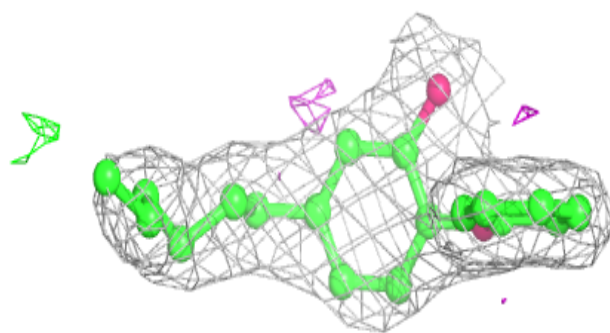
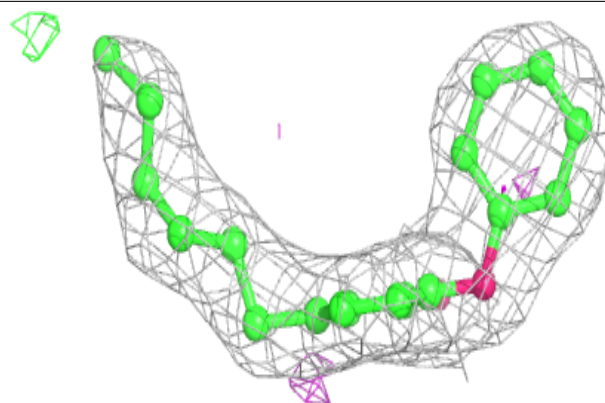
**Electron density around NAP D 1257:**

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

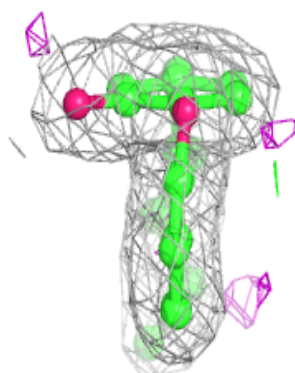
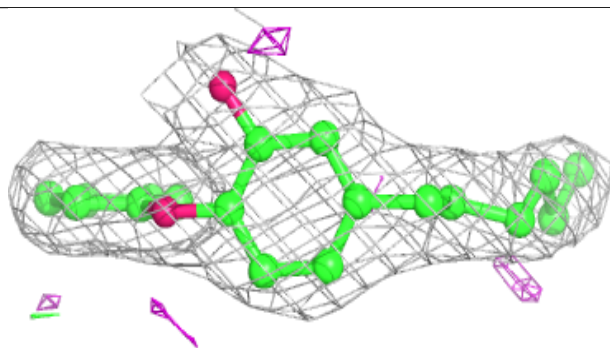
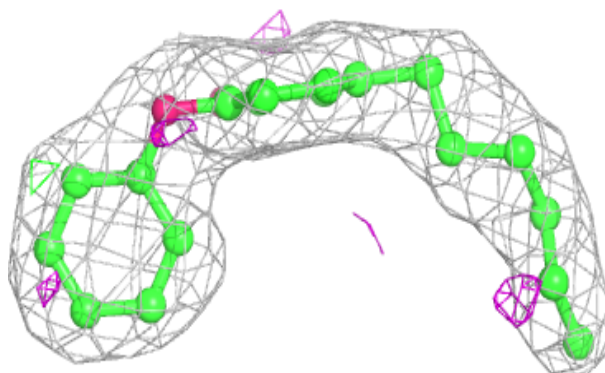


Electron density around 6PN H 1258:

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

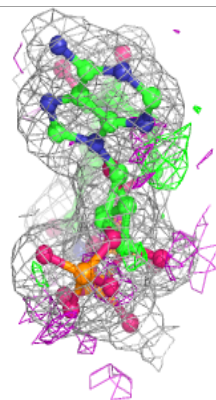
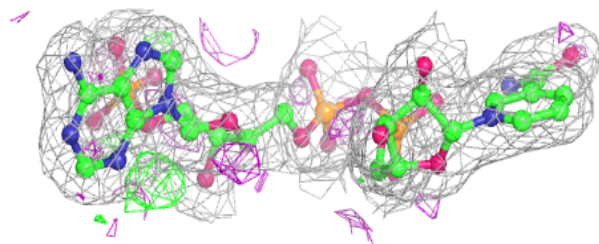
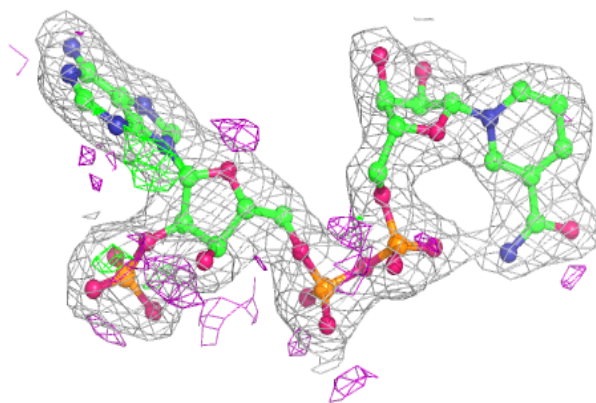
**Electron density around 6PN G 1258:**

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

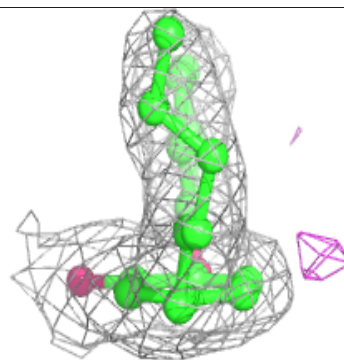
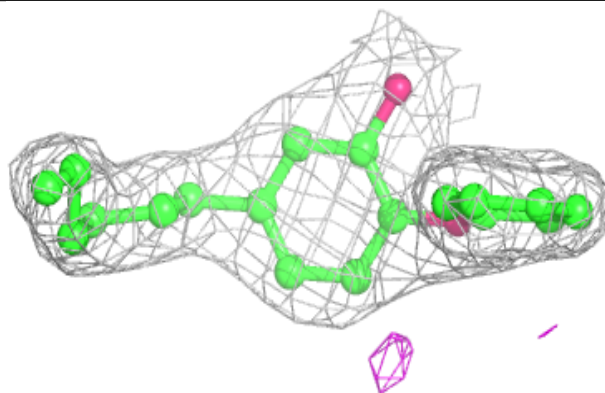
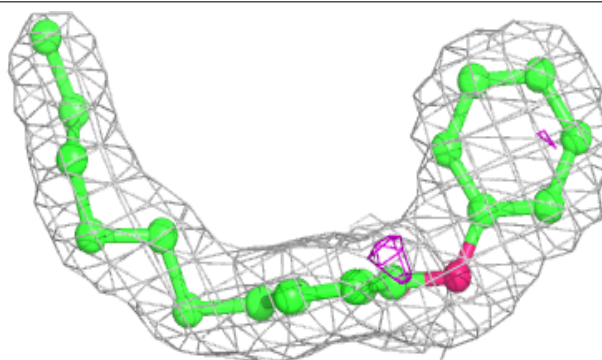


Electron density around NAP H 1257:

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

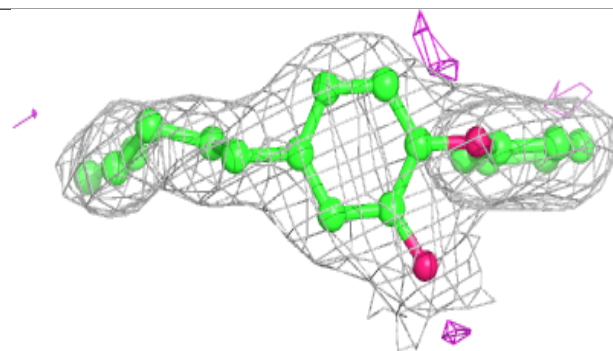
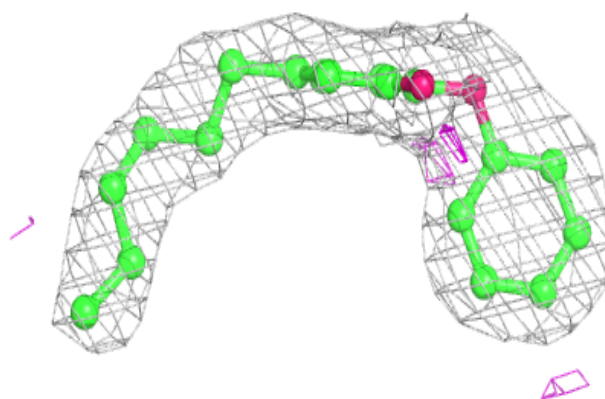
**Electron density around 6PN C 1258:**

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

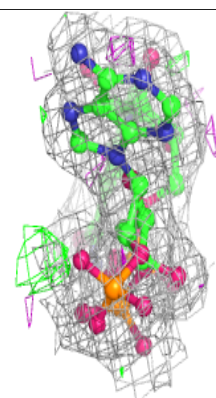
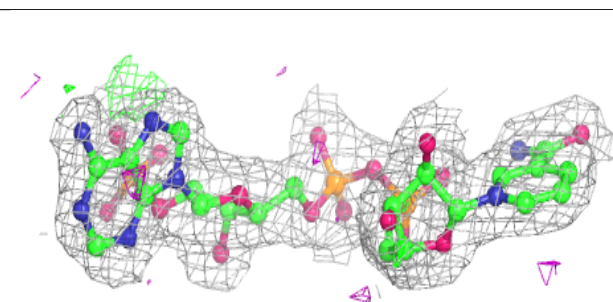
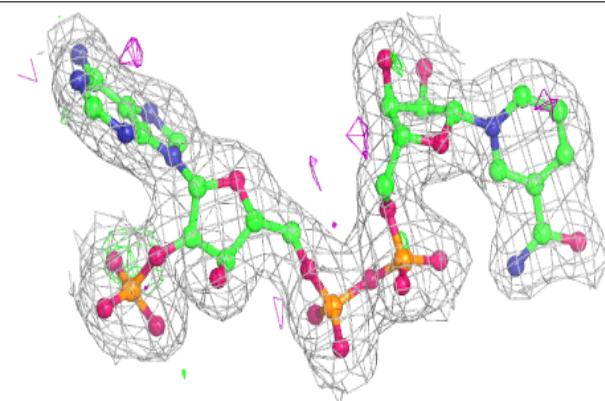


Electron density around 6PN F 1258:

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

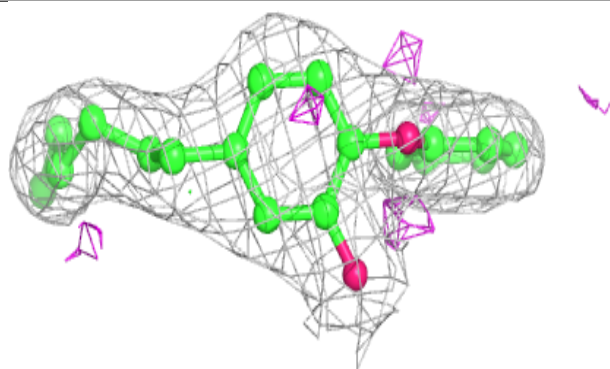
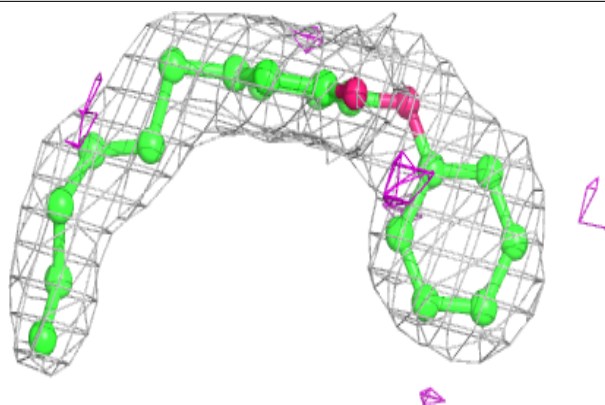
**Electron density around NAP C 1257:**

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

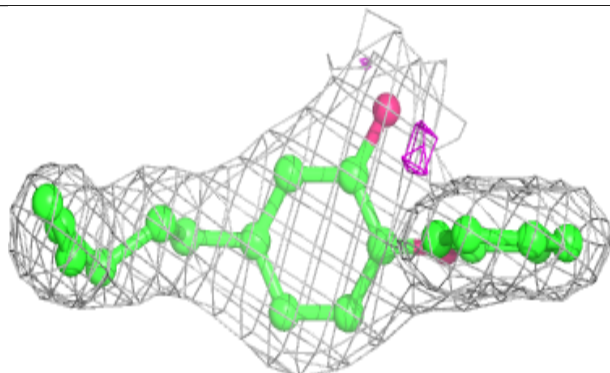
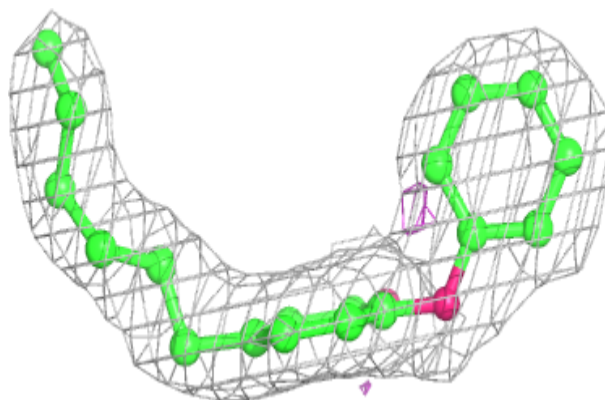


Electron density around 6PN A 1258:

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

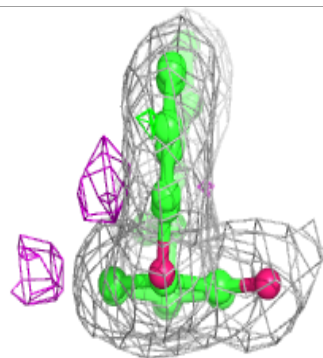
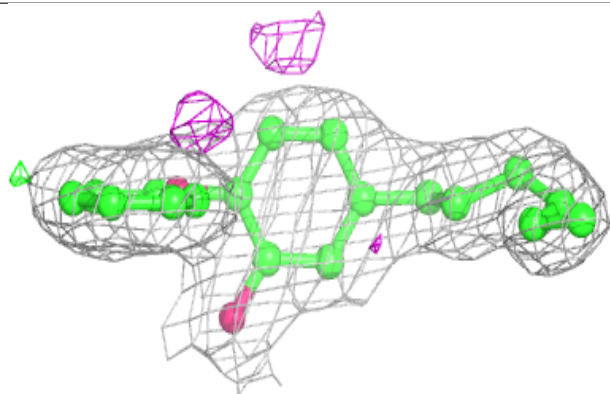
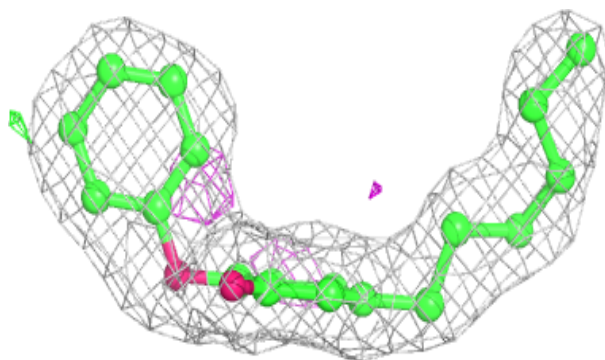
**Electron density around 6PN E 1258:**

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

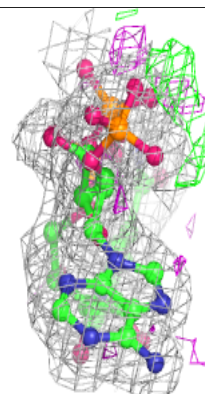
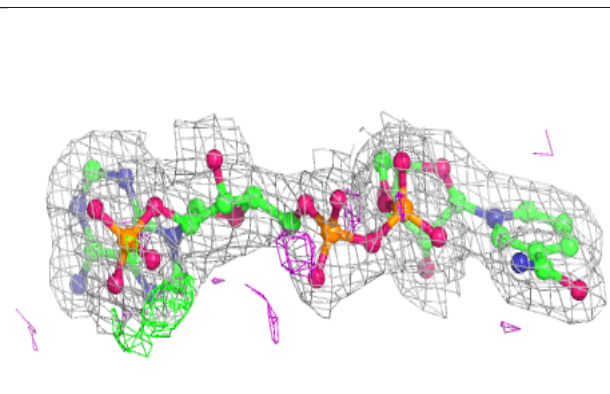
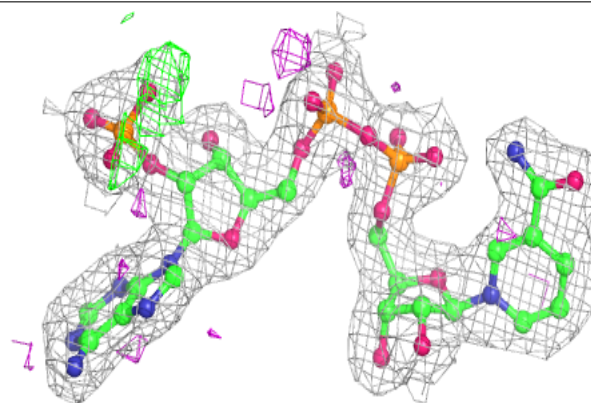


Electron density around 6PN B 1258:

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

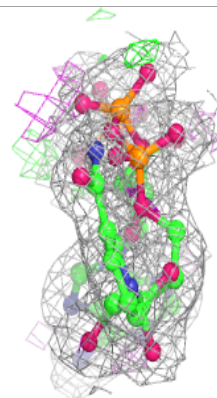
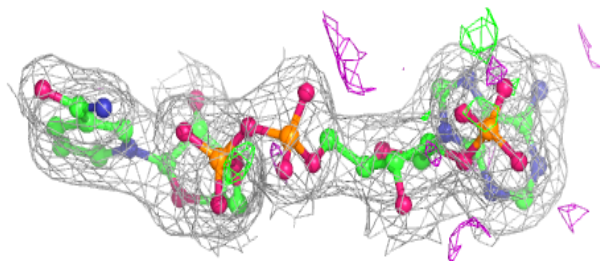
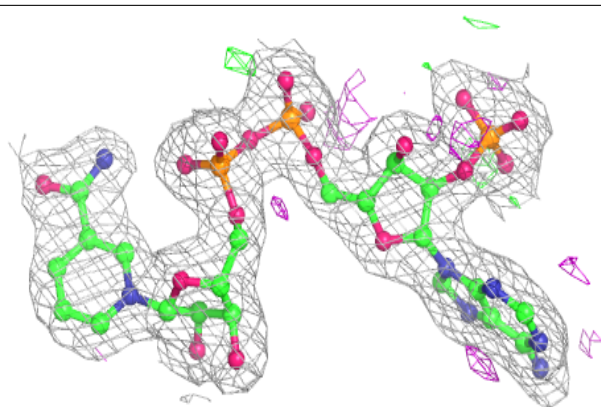
**Electron density around NAP A 1257:**

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

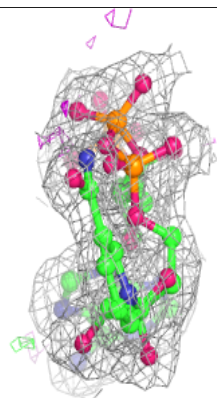
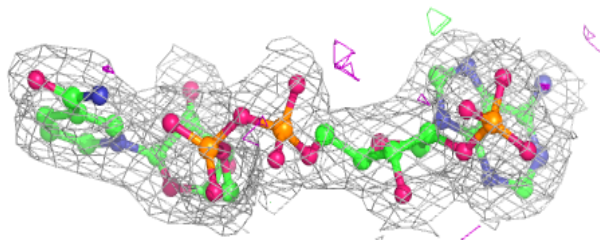
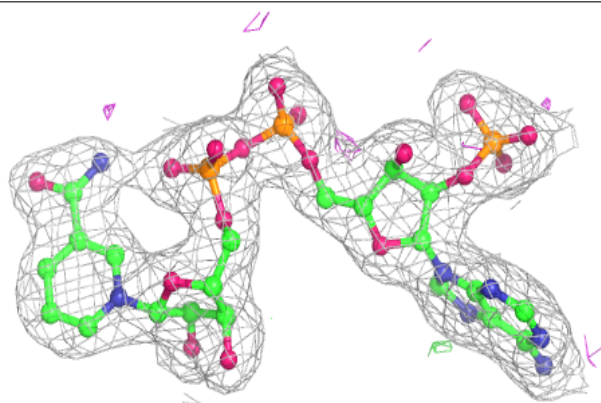


Electron density around NAP G 1257:

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

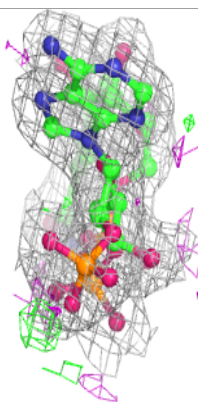
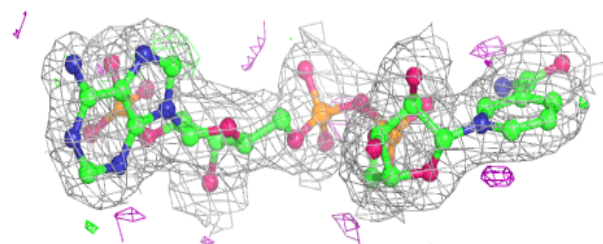
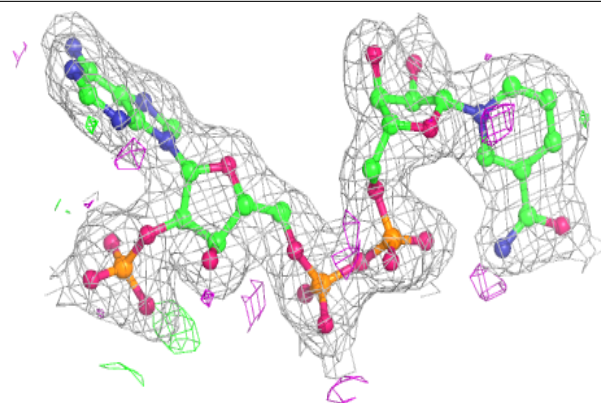
**Electron density around NAP F 1257:**

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

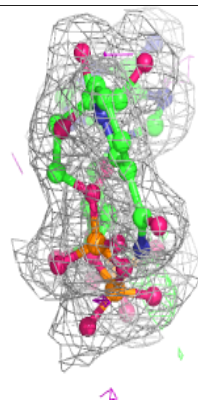
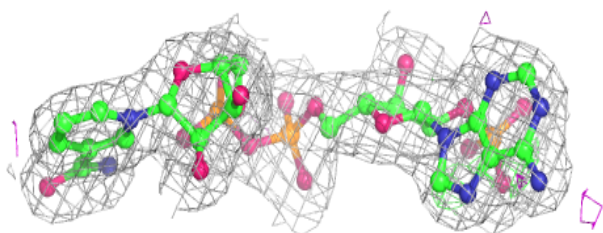
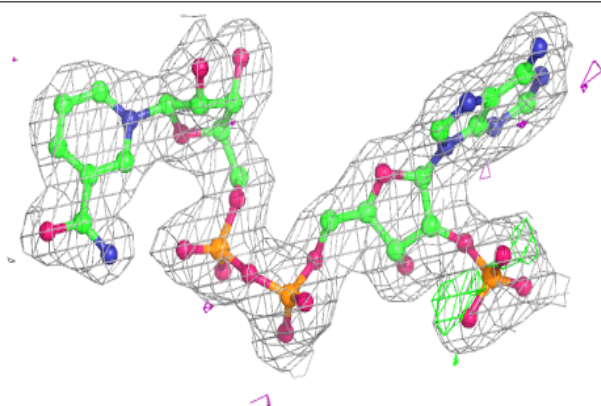


Electron density around NAP E 1257:

$2mF_o-DF_c$ (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

There are no such residues in this entry.