



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 01:32 pm GMT

PDB ID : 4D45  
Title : Crystal structure of *S. aureus* FabI in complex with NADP and 5-bromo- 2-(4-chloro-2-hydroxyphenoxy)benzotrile  
Authors : Tareilus, M.; Schiebel, J.; Chang, A.; Tonge, P.J.; Sotriffer, C.A.; Kisker, C.  
Deposited on : 2014-10-26  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

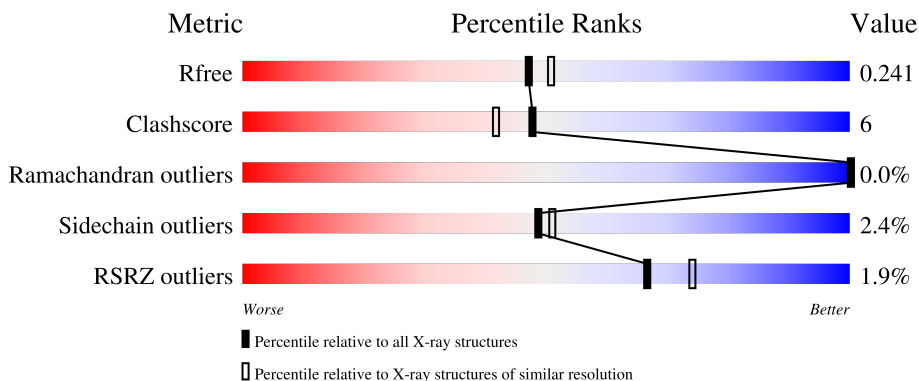
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">80% 9% • 10%</p>
1	B	282	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">76% 13% • 10%</p>
1	C	282	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">77% 12% • 10%</p>
1	D	282	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">75% 14% • 10%</p>
1	E	282	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">79% 11% 10%</p>

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Mol	Chain	Length	Quality of chain
1	F	282	 % 76% 13% 10%
1	G	282	 % 76% 13% 10%
1	H	282	 4% 77% 11% 10%

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	B	1259	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17357 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	4	0
			1977	1245	340	388	4			
1	B	254	Total	C	N	O	S	0	1	0
			1961	1236	338	383	4			
1	C	254	Total	C	N	O	S	0	3	0
			1973	1244	339	386	4			
1	D	254	Total	C	N	O	S	0	3	0
			1971	1241	340	386	4			
1	E	254	Total	C	N	O	S	0	1	0
			1961	1236	338	383	4			
1	F	254	Total	C	N	O	S	0	1	0
			1961	1236	338	383	4			
1	G	254	Total	C	N	O	S	0	4	0
			1977	1246	341	386	4			
1	H	254	Total	C	N	O	S	0	3	0
			1972	1244	340	384	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
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
C	-25	MET	-	expression tag	UNP Q7A6D8
C	-24	LYS	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	-	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

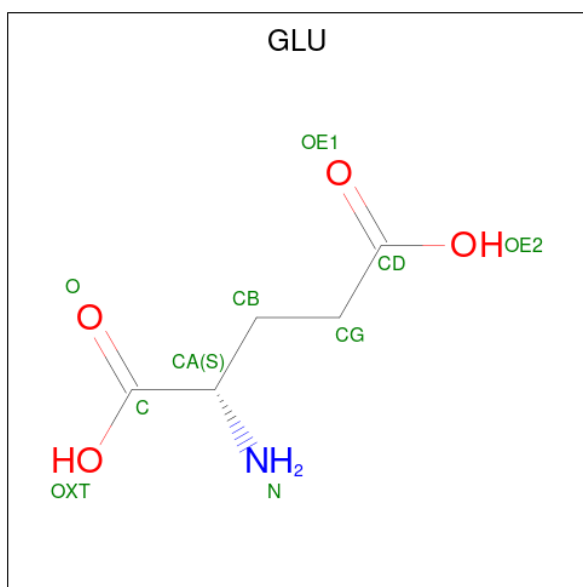
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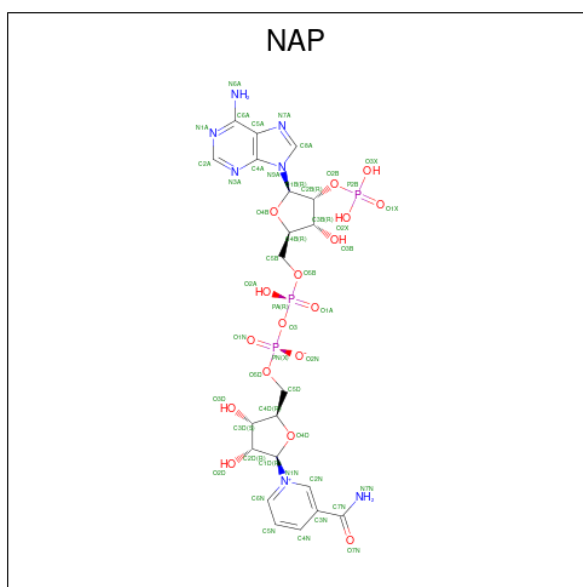
Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q7A6D8
G	0	ALA	-	expression tag	UNP Q7A6D8
H	-25	MET	-	expression tag	UNP Q7A6D8
H	-24	LYS	-	expression tag	UNP Q7A6D8
H	-23	HIS	-	expression tag	UNP Q7A6D8
H	-22	HIS	-	expression tag	UNP Q7A6D8
H	-21	HIS	-	expression tag	UNP 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
A	2	VAL	LEU	engineered mutation	UNP Q7A6D8
B	2	VAL	LEU	engineered mutation	UNP Q7A6D8
C	2	VAL	LEU	engineered mutation	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8
E	2	VAL	LEU	engineered mutation	UNP Q7A6D8
F	2	VAL	LEU	engineered mutation	UNP Q7A6D8
G	2	VAL	LEU	engineered mutation	UNP Q7A6D8
H	2	VAL	LEU	engineered mutation	UNP Q7A6D8

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



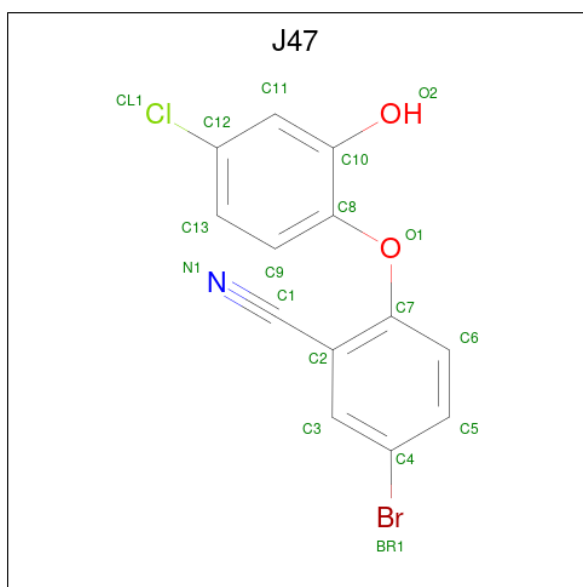
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 10	5	1	4	0	0
2	B	1	Total 10	5	1	4	0	0
2	C	1	Total 10	5	1	4	0	0
2	E	1	Total 10	5	1	4	0	0
2	F	1	Total 10	5	1	4	0	0
2	G	1	Total 10	5	1	4	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 4 is 5-bromo-2-(4-chloro-2-hydroxyphenoxy)benzonitrile (three-letter code: J47) (formula:  $C_{13}H_7BrClNO_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	Cl	N			O
4	A	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0
4	B	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0
4	C	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0
4	D	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0
4	E	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0
4	F	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0
4	G	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0
4	H	1	Total 18	Br 1	C 13	Cl 1	N 1	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total 143	O 143	0	0
5	B	154	Total 154	O 154	0	0
5	C	158	Total 158	O 158	0	0
5	D	93	Total 93	O 93	0	0

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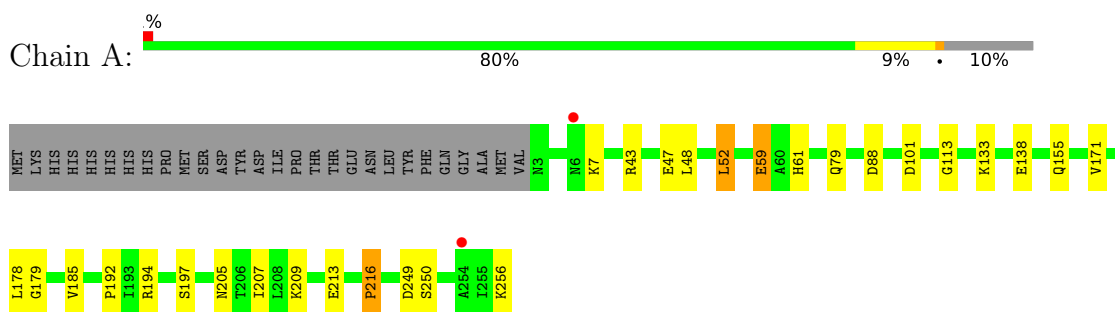
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	E	106	Total 106	O 106	0	0
5	F	124	Total 124	O 124	0	0
5	G	137	Total 137	O 137	0	0
5	H	101	Total 101	O 101	0	0

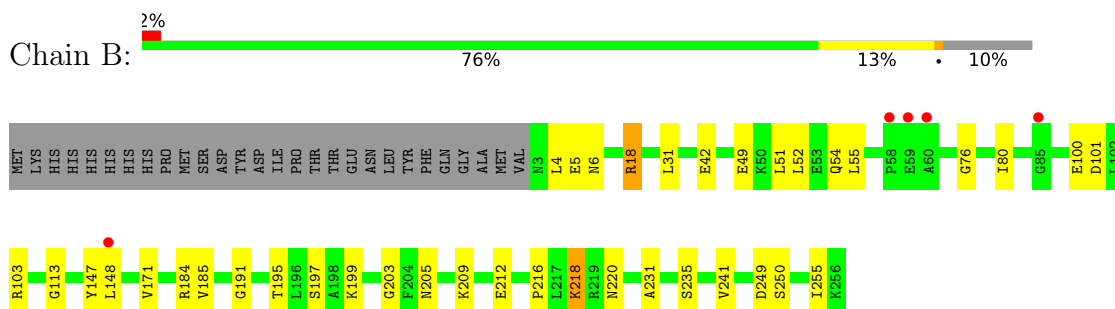
### 3 Residue-property plots [i](#)

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.

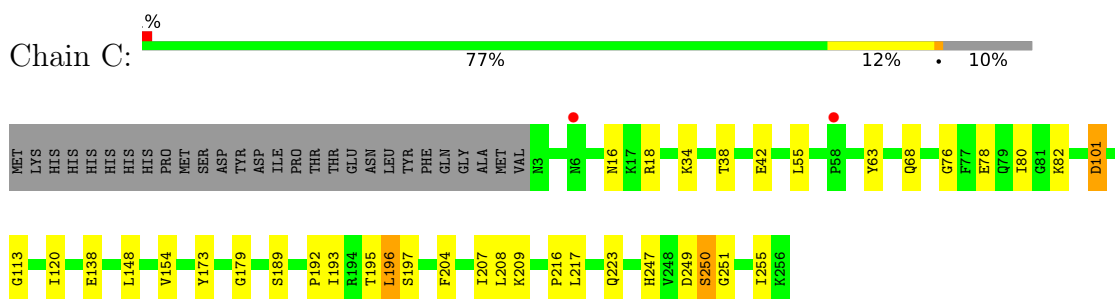
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



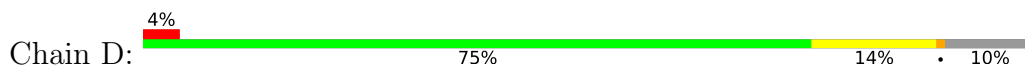
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

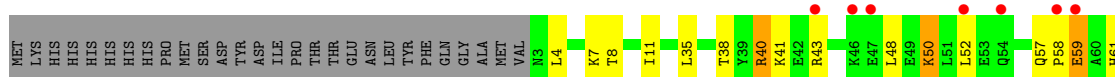


- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

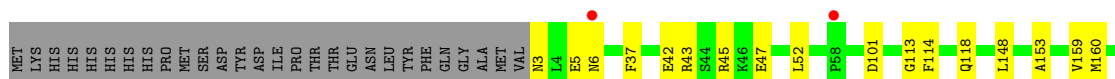
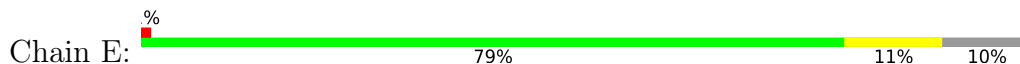


- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

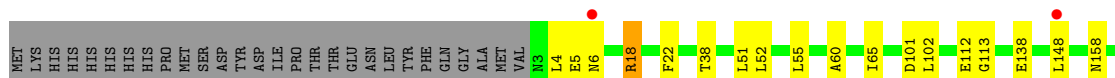
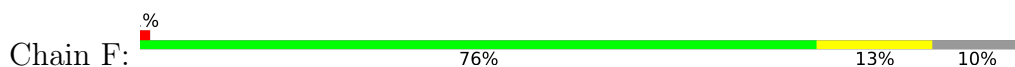




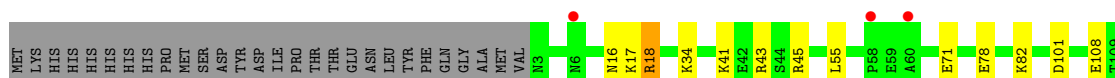
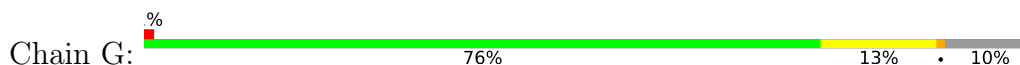
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



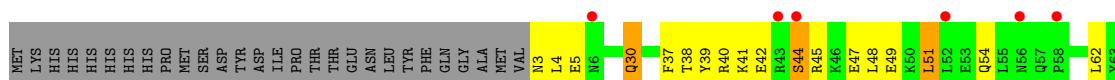
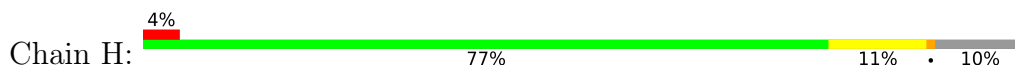
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.08Å 95.17Å 95.20Å 98.43° 97.53° 111.47°	Depositor
Resolution (Å)	46.58 – 2.15 46.58 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.2 (46.58-2.15) 98.2 (46.58-2.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.174 , 0.227 0.193 , 0.241	Depositor DCC
$R_{free}$ test set	7676 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtrriage
Anisotropy	0.625	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, J47

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	0.58	0/2010	0.76	0/2708
1	B	0.60	0/1991	0.82	1/2683 (0.0%)
1	C	0.60	0/2009	0.79	2/2707 (0.1%)
1	D	0.51	0/2001	0.72	0/2696
1	E	0.58	0/1991	0.75	0/2683
1	F	0.63	0/1991	0.83	0/2683
1	G	0.58	0/2010	0.80	1/2707 (0.0%)
1	H	0.54	0/2008	0.75	1/2705 (0.0%)
All	All	0.58	0/16011	0.78	5/21572 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	B	18	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	H	239	SER	C-N-CA	-5.81	110.11	122.30
1	C	101	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	214	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	1977	0	1987	16	0
1	B	1961	0	1974	30	0
1	C	1973	0	1988	25	0
1	D	1971	0	1981	28	0
1	E	1961	0	1974	23	0
1	F	1961	0	1974	25	0
1	G	1977	0	1994	37	0
1	H	1972	0	1993	26	0
2	A	10	0	5	2	0
2	B	10	0	5	5	0
2	C	10	0	5	0	0
2	E	10	0	5	0	0
2	F	10	0	5	1	0
2	G	10	0	5	2	0
3	A	48	0	25	0	0
3	B	48	0	25	3	0
3	C	48	0	25	0	0
3	D	48	0	25	1	0
3	E	48	0	25	0	0
3	F	48	0	25	1	0
3	G	48	0	25	2	0
3	H	48	0	25	2	0
4	A	18	0	6	1	0
4	B	18	0	6	2	0
4	C	18	0	6	1	0
4	D	18	0	6	1	0
4	E	18	0	6	1	0
4	F	18	0	6	3	0
4	G	18	0	6	2	0
4	H	18	0	7	0	0
5	A	143	0	0	1	0
5	B	154	0	0	8	0
5	C	158	0	0	4	0
5	D	93	0	0	1	0
5	E	106	0	0	1	0
5	F	124	0	0	5	0
5	G	137	0	0	10	0
5	H	101	0	0	0	0
All	All	17357	0	16144	199	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 6.

All (199) 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:E:256:LYS:HG2	1:G:148:LEU:HD21	1.43	1.00
1:G:16:ASN:HD21	1:G:196:LEU:HD23	1.32	0.94
2:G:1259:GLU:O	2:G:1259:GLU:HG2	1.73	0.88
1:G:16:ASN:ND2	1:G:196:LEU:HD23	1.93	0.84
1:F:236:ASP:HB2	5:F:2114:HOH:O	1.79	0.81
1:C:154:VAL:HG11	5:C:2108:HOH:O	1.80	0.80
1:E:148:LEU:HD21	1:G:256:LYS:HD2	1.61	0.80
2:B:1259:GLU:HG2	2:B:1259:GLU:O	1.82	0.78
1:C:42[B]:GLU:OE2	5:C:2045:HOH:O	2.03	0.76
2:B:1259:GLU:O	2:B:1259:GLU:CG	2.32	0.75
1:H:45:ARG:O	1:H:49:GLU:HG3	1.86	0.75
1:B:191:GLY:HA3	5:B:2153:HOH:O	1.89	0.72
1:G:192:PRO:HG3	1:G:207:ILE:HG22	1.73	0.69
1:D:210:GLU:HG3	1:D:214:ARG:HD2	1.76	0.68
5:B:2036:HOH:O	1:G:108:GLU:OE1	2.11	0.67
1:H:44:SER:O	1:H:48:LEU:HB2	1.94	0.67
1:F:255:ILE:O	1:H:256:LYS:HE2	1.95	0.67
1:G:71:GLU:HG2	5:G:2052:HOH:O	1.94	0.65
1:F:216:PRO:HG2	1:F:251:GLY:HA3	1.77	0.65
1:G:18:ARG:NH2	5:G:2022:HOH:O	2.31	0.64
1:F:5:GLU:O	1:F:6:ASN:HB2	1.97	0.64
1:D:8:THR:HG21	1:D:84:VAL:HG11	1.81	0.63
1:G:17[A]:LYS:HZ2	1:G:18:ARG:HD2	1.62	0.62
1:C:101:ASP:OD2	1:C:113:GLY:HA3	2.00	0.61
2:A:1259:GLU:HG2	2:A:1259:GLU:O	2.00	0.61
1:G:17[A]:LYS:NZ	1:G:18:ARG:HH11	1.98	0.61
1:B:101:ASP:OD1	1:G:43:ARG:HD3	2.01	0.60
1:F:101:ASP:OD2	1:F:113:GLY:HA3	2.01	0.60
1:C:197:SER:HB3	4:C:1258:J47:C2	2.32	0.59
1:E:42[B]:GLU:OE1	1:E:45:ARG:NH1	2.35	0.59
1:C:192:PRO:HG3	1:C:207:ILE:HG22	1.83	0.59
1:C:217:LEU:HD12	1:C:250:SER:HA	1.84	0.59
1:B:184:ARG:HD2	1:B:241:VAL:O	2.02	0.59
1:E:256:LYS:HG2	1:G:148:LEU:CD2	2.26	0.58
1:A:192:PRO:HG3	1:A:207:ILE:HG22	1.85	0.58
1:B:205:ASN:HB2	5:B:2123:HOH:O	2.02	0.58
1:H:100:GLU:CG	1:H:101:ASP:N	2.66	0.58
1:G:17[A]:LYS:HZ1	1:G:18:ARG:NH1	2.00	0.58
1:D:76:GLY:O	1:D:80:ILE:HG13	2.03	0.58
1:B:255:ILE:O	1:D:256:LYS:HE2	2.05	0.56
1:G:253:HIS:HD2	5:G:2134:HOH:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:HG2	1:A:61:HIS:CE1	2.41	0.56
1:E:118:GLN:HE22	1:E:166:SER:CB	2.18	0.55
1:F:18:ARG:NH2	1:F:194:ARG:HH11	2.03	0.55
1:B:42[B]:GLU:HG3	1:G:110:SER:HB2	1.87	0.55
1:F:52:LEU:HD13	1:F:60:ALA:HB2	1.89	0.55
1:C:189:SER:HB3	1:C:247:HIS:HA	1.89	0.54
1:B:199:LYS:HE2	2:G:1259:GLU:O	2.07	0.53
1:D:7:LYS:HA	1:D:88:ASP:OD2	2.09	0.53
1:F:5:GLU:O	1:F:6:ASN:CB	2.57	0.53
1:C:16:ASN:ND2	1:C:196:LEU:HD13	2.23	0.52
1:E:216:PRO:O	1:H:179:GLY:HA3	2.09	0.52
1:B:5:GLU:O	1:B:6:ASN:HB2	2.10	0.52
1:G:249:ASP:O	1:G:250:SER:HB2	2.09	0.52
1:D:203:GLY:O	1:D:207:ILE:HG13	2.10	0.51
1:B:147:TYR:HB2	3:B:1257:NAP:C5N	2.41	0.51
1:C:204:PHE:CE2	1:C:208:LEU:HD11	2.45	0.51
1:D:48:LEU:O	1:D:52:LEU:HG	2.11	0.51
1:H:192:PRO:HG3	1:H:207:ILE:HG22	1.92	0.51
1:G:18:ARG:O	1:G:195:THR:HG22	2.10	0.51
1:A:249:ASP:O	1:A:250:SER:HB2	2.11	0.51
1:G:191:GLY:HA3	5:G:2135:HOH:O	2.10	0.51
1:C:216:PRO:HG2	1:C:251:GLY:HA3	1.92	0.51
1:B:101:ASP:OD2	1:B:113:GLY:HA3	2.10	0.51
1:D:196:LEU:HD23	5:D:2076:HOH:O	2.11	0.51
1:H:40:ARG:HD3	3:H:1257:NAP:C5A	2.40	0.51
1:H:255:ILE:C	1:H:255:ILE:HD12	2.31	0.51
1:B:147:TYR:HB2	3:B:1257:NAP:H5N	1.92	0.51
1:C:216:PRO:HD3	1:C:255:ILE:HG21	1.93	0.50
1:G:17[A]:LYS:NZ	1:G:18:ARG:NH1	2.58	0.50
1:B:49:GLU:HA	1:B:52:LEU:HD12	1.93	0.50
1:B:103:ARG:HH12	2:B:1259:GLU:C	2.15	0.50
1:C:16:ASN:HD21	1:C:196:LEU:HD13	1.77	0.50
1:E:101:ASP:OD2	1:E:113:GLY:HA3	2.12	0.50
1:D:40:ARG:HD3	3:D:1257:NAP:C6A	2.41	0.50
5:E:2088:HOH:O	1:G:256:LYS:HE2	2.11	0.50
1:E:43:ARG:NH1	1:E:47:GLU:HG2	2.27	0.50
1:H:40:ARG:HD3	3:H:1257:NAP:C6A	2.42	0.50
1:B:54:GLN:HG3	5:B:2039:HOH:O	2.12	0.49
1:B:171:VAL:HG13	1:B:185:VAL:HG12	1.94	0.49
1:H:205[B]:ASN:ND2	1:H:205[B]:ASN:H	2.11	0.49
1:F:38:THR:HG21	1:F:65:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:HG2	1:C:148:LEU:HD21	1.94	0.49
1:A:179:GLY:HA3	1:D:216:PRO:O	2.12	0.49
1:E:42[B]:GLU:OE1	1:E:42[B]:GLU:HA	2.13	0.49
1:C:34:LYS:HD3	5:C:2055:HOH:O	2.13	0.49
1:G:154:VAL:HG12	5:G:2093:HOH:O	2.12	0.49
1:A:155:GLN:NE2	5:A:2095:HOH:O	2.30	0.48
1:B:249:ASP:O	1:B:250:SER:HB2	2.13	0.48
1:F:205:ASN:HB2	5:F:2096:HOH:O	2.13	0.48
1:G:34:LYS:HD2	5:G:2045:HOH:O	2.13	0.48
5:F:2103:HOH:O	1:H:155:GLN:NE2	2.46	0.48
1:G:212:GLU:OE1	5:G:2118:HOH:O	2.20	0.47
1:A:171:VAL:HG13	1:A:185:VAL:HG12	1.97	0.47
1:A:209:LYS:HE2	1:A:213:GLU:OE2	2.15	0.47
1:B:231:ALA:O	1:B:235:SER:HB3	2.13	0.47
1:H:3:ASN:HD21	1:H:5:GLU:HG3	1.78	0.47
1:H:51:LEU:O	1:H:54:GLN:HB2	2.14	0.47
1:H:51:LEU:HD23	1:H:51:LEU:N	2.28	0.47
2:B:1259:GLU:HB2	5:B:2154:HOH:O	2.15	0.46
1:D:59:GLU:HG3	1:D:61:HIS:NE2	2.30	0.46
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.50	0.46
1:B:216:PRO:HA	5:B:2130:HOH:O	2.15	0.46
3:F:1257:NAP:H3D	4:F:1258:J47:N1	2.30	0.46
1:G:212:GLU:HG3	1:G:220:ASN:ND2	2.31	0.46
1:G:45:ARG:CD	5:G:2035:HOH:O	2.64	0.46
1:G:155:GLN:O	1:G:156:ASN:HB2	2.16	0.46
1:C:18:ARG:O	1:C:195:THR:HG22	2.16	0.45
1:C:78:GLU:O	1:C:82:LYS:HG3	2.16	0.45
1:F:102:LEU:HD11	4:F:1258:J47:BR1	2.71	0.45
1:F:158:ASN:HB3	5:F:2057:HOH:O	2.15	0.45
1:A:197:SER:HB3	4:A:1258:J47:C2	2.46	0.45
1:H:37:PHE:HB2	1:H:62:LEU:HD23	1.97	0.45
1:E:160:MET:O	1:E:164:LYS:HG2	2.15	0.45
1:E:244:GLU:HG3	1:E:245:ASN:N	2.32	0.45
1:E:209:LYS:O	1:E:213:GLU:HG3	2.17	0.45
1:D:193:ILE:HG21	1:D:223:GLN:HG3	1.99	0.45
1:D:38:THR:HG21	1:D:65:ILE:HD12	1.98	0.45
1:F:148:LEU:HD21	1:H:256:LYS:HG2	1.98	0.45
1:F:52:LEU:HD13	1:F:60:ALA:CB	2.46	0.45
1:F:217:LEU:O	1:F:218:LYS:HB2	2.17	0.45
1:B:18:ARG:O	1:B:195:THR:HG22	2.17	0.44
1:C:76:GLY:O	1:C:80:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1259:GLU:O	2:A:1259:GLU:CG	2.65	0.44
1:E:197:SER:HB3	4:E:1258:J47:C2	2.47	0.44
1:F:18:ARG:O	1:F:195:THR:HG22	2.17	0.44
1:H:39:TYR:HB2	1:H:44:SER:HB3	1.98	0.44
1:B:100:GLU:OE2	1:G:41:LYS:HE3	2.17	0.44
1:H:209[B]:LYS:HB2	1:H:209[B]:LYS:HE2	1.71	0.44
3:B:1257:NAP:H3D	4:B:1258:J47:N1	2.32	0.44
1:A:216:PRO:O	1:D:179:GLY:HA3	2.18	0.44
1:F:224:VAL:O	1:F:228:LYS:HG3	2.18	0.44
1:A:194:ARG:HH22	1:A:205:ASN:CG	2.20	0.44
1:A:101:ASP:OD2	1:A:113:GLY:HA3	2.18	0.43
1:C:38:THR:HA	1:C:63:TYR:O	2.17	0.43
1:D:11:ILE:HD11	1:D:35:LEU:HD22	2.01	0.43
1:E:209:LYS:HB3	1:E:209:LYS:HE3	1.77	0.43
1:B:197:SER:HB3	4:B:1258:J47:C2	2.48	0.43
1:D:11:ILE:CD1	1:D:35:LEU:HD22	2.48	0.43
1:B:216:PRO:O	1:C:179:GLY:HA3	2.18	0.43
1:C:154:VAL:CG1	5:C:2108:HOH:O	2.51	0.43
1:F:233:LEU:HD21	1:F:246:ILE:HD12	2.01	0.43
1:F:212:GLU:HG3	1:F:220:ASN:ND2	2.33	0.43
1:D:114:PHE:HA	1:D:159:VAL:HG21	2.00	0.43
1:E:249:ASP:O	1:E:250:SER:HB2	2.19	0.43
1:E:153:ALA:HA	1:F:173:TYR:CZ	2.54	0.43
1:F:197:SER:HB3	4:F:1258:J47:C2	2.48	0.43
1:G:197:SER:HB3	4:G:1258:J47:C2	2.49	0.43
1:D:192:PRO:HG3	1:D:207:ILE:HG22	2.01	0.43
1:H:38:THR:HG21	1:H:65:ILE:HD12	2.01	0.43
1:A:48:LEU:O	1:A:52:LEU:HD23	2.19	0.43
1:C:193:ILE:HG21	1:C:223:GLN:HG3	2.00	0.43
1:C:68:GLN:HG3	1:C:120:ILE:HG12	2.00	0.42
1:D:84:VAL:O	1:D:84:VAL:CG1	2.67	0.42
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.87	0.42
1:B:76:GLY:O	1:B:80:ILE:HG13	2.19	0.42
1:C:249:ASP:O	1:C:250:SER:HB2	2.19	0.42
1:E:179:GLY:HA3	1:H:216:PRO:O	2.20	0.42
1:G:216:PRO:HG2	1:G:251:GLY:HA3	2.02	0.42
1:A:133:LYS:HD2	1:A:178:LEU:HD22	2.01	0.42
1:G:45:ARG:HD2	5:G:2035:HOH:O	2.20	0.42
1:H:30:GLN:O	1:H:30:GLN:HG3	2.20	0.42
1:F:178:LEU:O	1:F:181:ASP:HB2	2.19	0.42
1:G:198:ALA:C	1:G:200:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LEU:O	1:D:218:LYS:HB2	2.19	0.42
1:B:51:LEU:O	1:B:54:GLN:HB2	2.20	0.42
1:C:63:TYR:CD1	1:C:63:TYR:N	2.87	0.42
1:C:173:TYR:CZ	1:D:153:ALA:HA	2.55	0.42
1:E:148:LEU:HD21	1:G:256:LYS:CD	2.42	0.42
1:B:241:VAL:HA	5:B:2147:HOH:O	2.20	0.42
1:D:197:SER:HB3	4:D:1258:J47:C2	2.50	0.42
1:A:7:LYS:HA	1:A:88:ASP:OD2	2.20	0.41
1:D:50:LYS:HB2	1:D:50:LYS:HE3	1.78	0.41
1:F:191:GLY:HA3	5:F:2120:HOH:O	2.20	0.41
1:G:147:TYR:HB2	3:G:1257:NAP:C5N	2.50	0.41
1:G:78:GLU:O	1:G:82:LYS:HG3	2.20	0.41
1:H:125:LEU:O	1:H:125:LEU:HG	2.20	0.41
1:B:148:LEU:HD21	1:D:256:LYS:HG2	2.01	0.41
1:A:43:ARG:NH1	1:A:47:GLU:HG2	2.35	0.41
1:B:218:LYS:HD2	5:B:2130:HOH:O	2.20	0.41
1:D:57:GLN:HA	1:D:58:PRO:HD3	1.97	0.41
1:E:5:GLU:O	1:E:6:ASN:HB2	2.21	0.41
1:F:22:PHE:CE1	1:F:51:LEU:HB3	2.55	0.41
1:E:165:ALA:CB	1:F:169:ALA:HB2	2.51	0.41
1:H:184:ARG:HD2	1:H:241:VAL:O	2.20	0.41
1:E:37:PHE:CE2	1:E:52:LEU:HD11	2.56	0.41
1:G:207:ILE:O	1:G:211:ILE:HG12	2.21	0.41
1:B:212:GLU:HG3	1:B:220:ASN:ND2	2.36	0.41
1:D:84:VAL:O	1:D:84:VAL:HG12	2.21	0.41
1:E:114:PHE:HA	1:E:159:VAL:HG21	2.03	0.41
2:F:1259:GLU:O	2:F:1259:GLU:HG2	2.19	0.41
1:B:203:GLY:H	2:B:1259:GLU:N	2.19	0.40
1:E:3:ASN:ND2	1:E:3:ASN:C	2.73	0.40
1:H:3:ASN:ND2	1:H:5:GLU:HG3	2.36	0.40
1:D:41:LYS:HE3	1:D:43:ARG:HH12	1.87	0.40
1:D:164:LYS:O	1:D:165:ALA:C	2.58	0.40
3:G:1257:NAP:H3D	4:G:1258:J47:N1	2.36	0.40
1:H:100:GLU:HG3	1:H:101:ASP:N	2.35	0.40
1:G:45:ARG:HD3	5:G:2035:HOH:O	2.21	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	256/282 (91%)	248 (97%)	8 (3%)	0	100	100
1	B	253/282 (90%)	239 (94%)	14 (6%)	0	100	100
1	C	255/282 (90%)	243 (95%)	12 (5%)	0	100	100
1	D	255/282 (90%)	244 (96%)	11 (4%)	0	100	100
1	E	253/282 (90%)	243 (96%)	10 (4%)	0	100	100
1	F	253/282 (90%)	239 (94%)	14 (6%)	0	100	100
1	G	256/282 (91%)	244 (95%)	12 (5%)	0	100	100
1	H	255/282 (90%)	241 (94%)	13 (5%)	1 (0%)	34	29
All	All	2036/2256 (90%)	1941 (95%)	94 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	47	GLU

### 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	211/234 (90%)	206 (98%)	5 (2%)	49	51
1	B	209/234 (89%)	205 (98%)	4 (2%)	57	61
1	C	211/234 (90%)	206 (98%)	5 (2%)	49	51
1	D	210/234 (90%)	204 (97%)	6 (3%)	42	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	209/234 (89%)	209 (100%)	0	100	100
1	F	209/234 (89%)	204 (98%)	5 (2%)	49	51
1	G	211/234 (90%)	204 (97%)	7 (3%)	38	37
1	H	211/234 (90%)	203 (96%)	8 (4%)	33	31
All	All	1681/1872 (90%)	1641 (98%)	40 (2%)	49	51

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	59	GLU
1	A	79	GLN
1	A	138	GLU
1	A	216	PRO
1	B	4	LEU
1	B	55	LEU
1	B	209	LYS
1	B	218	LYS
1	C	55	LEU
1	C	138	GLU
1	C	196	LEU
1	C	209	LYS
1	C	250	SER
1	D	4	LEU
1	D	40	ARG
1	D	50	LYS
1	D	59	GLU
1	D	64	GLN
1	D	145	THR
1	F	4	LEU
1	F	18	ARG
1	F	55	LEU
1	F	112	GLU
1	F	138	GLU
1	G	18	ARG
1	G	55	LEU
1	G	101	ASP
1	G	112	GLU
1	G	196	LEU
1	G	209	LYS
1	G	256	LYS

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Mol	Chain	Res	Type
1	H	4	LEU
1	H	30	GLN
1	H	41	LYS
1	H	42	GLU
1	H	44	SER
1	H	51	LEU
1	H	64	GLN
1	H	100	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	D	30	GLN
1	D	253	HIS
1	E	3	ASN
1	E	118	GLN
1	F	56	ASN
1	G	253	HIS
1	H	3	ASN
1	H	118	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 monosaccharides 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
2	GLU	F	1259	-	8,9,9	1.18	1 (12%)	10,11,11	1.38	1 (10%)
3	NAP	E	1257	-	45,52,52	1.63	3 (6%)	56,80,80	1.52	6 (10%)
3	NAP	H	1257	-	45,52,52	1.69	3 (6%)	56,80,80	1.38	4 (7%)
4	J47	A	1258	-	19,19,19	0.16	0	25,26,26	0.54	0
2	GLU	G	1259	-	8,9,9	1.25	1 (12%)	10,11,11	1.23	2 (20%)
2	GLU	E	1259	-	8,9,9	1.21	1 (12%)	10,11,11	1.09	0
2	GLU	B	1259	-	8,9,9	1.08	0	10,11,11	1.70	3 (30%)
2	GLU	A	1259	-	8,9,9	1.23	1 (12%)	10,11,11	1.18	1 (10%)
3	NAP	A	1257	-	45,52,52	1.67	4 (8%)	56,80,80	1.38	5 (8%)
3	NAP	B	1257	-	45,52,52	1.57	3 (6%)	56,80,80	1.57	9 (16%)
3	NAP	C	1257	-	45,52,52	1.54	3 (6%)	56,80,80	1.61	8 (14%)
3	NAP	F	1257	-	45,52,52	1.49	3 (6%)	56,80,80	1.65	6 (10%)
4	J47	E	1258	-	19,19,19	0.17	0	25,26,26	0.40	0
4	J47	B	1258	-	19,19,19	0.29	0	25,26,26	0.53	0
4	J47	F	1258	-	19,19,19	0.20	0	25,26,26	0.62	0
4	J47	C	1258	-	19,19,19	0.30	0	25,26,26	0.63	1 (4%)
3	NAP	D	1257	-	45,52,52	1.56	3 (6%)	56,80,80	1.37	6 (10%)
4	J47	H	1258	-	19,19,19	0.16	0	25,26,26	0.62	1 (4%)
2	GLU	C	1259	-	8,9,9	1.25	1 (12%)	10,11,11	1.24	1 (10%)
4	J47	D	1258	-	19,19,19	0.17	0	25,26,26	0.60	1 (4%)
3	NAP	G	1257	-	45,52,52	1.59	4 (8%)	56,80,80	1.69	7 (12%)
4	J47	G	1258	-	19,19,19	0.33	0	25,26,26	0.57	1 (4%)

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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	F	1259	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	E	1257	-	-	4/31/67/67	0/5/5/5
3	NAP	H	1257	-	-	7/31/67/67	0/5/5/5
4	J47	A	1258	-	-	0/6/6/6	0/2/2/2
2	GLU	G	1259	-	-	6/9/9/9	-
2	GLU	E	1259	-	-	5/9/9/9	-
2	GLU	B	1259	-	-	4/9/9/9	-
2	GLU	A	1259	-	-	4/9/9/9	-
3	NAP	A	1257	-	-	7/31/67/67	0/5/5/5
3	NAP	B	1257	-	-	7/31/67/67	0/5/5/5
3	NAP	C	1257	-	-	7/31/67/67	0/5/5/5
3	NAP	F	1257	-	-	6/31/67/67	0/5/5/5
4	J47	E	1258	-	-	0/6/6/6	0/2/2/2
4	J47	B	1258	-	-	0/6/6/6	0/2/2/2
4	J47	F	1258	-	-	1/6/6/6	0/2/2/2
4	J47	C	1258	-	-	0/6/6/6	0/2/2/2
3	NAP	D	1257	-	-	7/31/67/67	0/5/5/5
4	J47	H	1258	-	-	0/6/6/6	0/2/2/2
2	GLU	C	1259	-	-	5/9/9/9	-
4	J47	D	1258	-	-	0/6/6/6	0/2/2/2
3	NAP	G	1257	-	-	6/31/67/67	0/5/5/5
4	J47	G	1258	-	-	1/6/6/6	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1257	NAP	O7N-C7N	8.72	1.40	1.24
3	A	1257	NAP	O7N-C7N	8.32	1.40	1.24
3	D	1257	NAP	O7N-C7N	8.23	1.39	1.24
3	E	1257	NAP	O7N-C7N	8.01	1.39	1.24
3	B	1257	NAP	O7N-C7N	7.95	1.39	1.24
3	G	1257	NAP	O7N-C7N	7.78	1.39	1.24
3	C	1257	NAP	O7N-C7N	7.58	1.38	1.24
3	F	1257	NAP	O7N-C7N	7.19	1.37	1.24
3	A	1257	NAP	C2A-N3A	4.09	1.38	1.32
3	H	1257	NAP	C2A-N3A	4.09	1.38	1.32
3	E	1257	NAP	C2A-N3A	3.95	1.38	1.32
3	F	1257	NAP	C2A-N3A	3.88	1.38	1.32
3	B	1257	NAP	C2A-N3A	3.58	1.37	1.32
3	D	1257	NAP	C2A-N3A	3.58	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1257	NAP	C2A-N3A	3.41	1.37	1.32
3	G	1257	NAP	C2A-N3A	3.33	1.37	1.32
3	H	1257	NAP	C2A-N1A	2.71	1.38	1.33
3	D	1257	NAP	C2A-N1A	2.65	1.38	1.33
3	C	1257	NAP	C2A-N1A	2.61	1.38	1.33
3	G	1257	NAP	C2A-N1A	2.54	1.38	1.33
3	F	1257	NAP	C2A-N1A	2.46	1.38	1.33
2	G	1259	GLU	CG-CD	2.42	1.56	1.50
3	E	1257	NAP	C2A-N1A	2.40	1.38	1.33
3	A	1257	NAP	C2A-N1A	2.36	1.38	1.33
2	C	1259	GLU	CG-CD	2.35	1.56	1.50
3	B	1257	NAP	C2A-N1A	2.26	1.38	1.33
3	A	1257	NAP	C2N-N1N	2.16	1.37	1.35
2	F	1259	GLU	CG-CD	2.12	1.55	1.50
2	A	1259	GLU	CG-CD	2.10	1.55	1.50
3	G	1257	NAP	O4B-C4B	-2.06	1.40	1.45
2	E	1259	GLU	CG-CD	2.03	1.55	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1257	NAP	N3A-C2A-N1A	-6.34	118.77	128.68
3	G	1257	NAP	O7N-C7N-C3N	-6.34	112.05	119.63
3	A	1257	NAP	N3A-C2A-N1A	-6.26	118.90	128.68
3	F	1257	NAP	N3A-C2A-N1A	-6.02	119.27	128.68
3	C	1257	NAP	N3A-C2A-N1A	-5.91	119.43	128.68
3	F	1257	NAP	C3N-C7N-N7N	5.78	124.69	117.75
3	E	1257	NAP	N3A-C2A-N1A	-5.68	119.80	128.68
3	B	1257	NAP	N3A-C2A-N1A	-5.57	119.98	128.68
3	D	1257	NAP	N3A-C2A-N1A	-5.48	120.11	128.68
3	G	1257	NAP	N3A-C2A-N1A	-5.40	120.24	128.68
3	G	1257	NAP	C3N-C7N-N7N	4.93	123.67	117.75
3	C	1257	NAP	O7N-C7N-C3N	-4.88	113.79	119.63
3	E	1257	NAP	C3N-C7N-N7N	4.73	123.43	117.75
3	B	1257	NAP	C3N-C7N-N7N	4.51	123.16	117.75
3	F	1257	NAP	O7N-C7N-C3N	-4.30	114.48	119.63
3	B	1257	NAP	O7N-C7N-C3N	-4.18	114.64	119.63
3	E	1257	NAP	O4D-C1D-C2D	-4.07	100.98	106.93
3	D	1257	NAP	C3N-C7N-N7N	4.06	122.62	117.75
3	C	1257	NAP	C3N-C7N-N7N	3.87	122.39	117.75
3	A	1257	NAP	C3N-C7N-N7N	3.76	122.27	117.75
3	H	1257	NAP	C3N-C7N-N7N	3.76	122.26	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1257	NAP	C2N-C3N-C4N	3.37	122.08	118.26
3	C	1257	NAP	C3N-C2N-N1N	-3.28	117.22	120.43
3	G	1257	NAP	C2N-C3N-C4N	3.24	121.93	118.26
3	F	1257	NAP	O4B-C1B-C2B	-3.06	101.28	106.59
3	E	1257	NAP	C1B-N9A-C4A	-3.05	121.28	126.64
3	E	1257	NAP	O7N-C7N-C3N	-2.95	116.11	119.63
3	A	1257	NAP	O7N-C7N-C3N	-2.75	116.34	119.63
3	D	1257	NAP	O4B-C1B-C2B	-2.71	101.89	106.59
3	D	1257	NAP	C1B-N9A-C4A	-2.69	121.91	126.64
2	B	1259	GLU	O-C-CA	-2.66	112.77	122.14
3	E	1257	NAP	C4A-C5A-N7A	-2.52	106.78	109.40
3	G	1257	NAP	O4D-C1D-C2D	-2.50	103.28	106.93
3	B	1257	NAP	O2N-PN-O1N	2.49	124.53	112.24
3	G	1257	NAP	C3N-C2N-N1N	-2.48	118.00	120.43
3	B	1257	NAP	C2N-C3N-C4N	2.47	121.06	118.26
2	F	1259	GLU	O-C-CA	-2.43	113.55	122.14
3	F	1257	NAP	C2N-C3N-C4N	2.43	121.01	118.26
4	D	1258	J47	C7-C2-C1	2.40	121.91	119.57
3	H	1257	NAP	O2N-PN-O1N	2.40	124.11	112.24
3	H	1257	NAP	O4B-C1B-C2B	-2.40	102.43	106.59
3	F	1257	NAP	O2N-PN-O1N	2.34	123.80	112.24
3	A	1257	NAP	C3D-C2D-C1D	-2.30	97.52	100.98
3	B	1257	NAP	C3N-C2N-N1N	-2.28	118.20	120.43
2	B	1259	GLU	CB-CA-C	-2.28	104.87	110.30
4	C	1258	J47	C7-C2-C1	2.26	121.77	119.57
2	B	1259	GLU	OE1-CD-CG	-2.26	115.84	123.08
3	B	1257	NAP	O4B-C1B-C2B	-2.24	102.69	106.59
3	C	1257	NAP	C2A-N1A-C6A	2.21	122.54	118.75
3	A	1257	NAP	C1B-N9A-C4A	-2.21	122.76	126.64
3	D	1257	NAP	O7N-C7N-C3N	-2.19	117.01	119.63
2	C	1259	GLU	O-C-CA	-2.19	114.42	122.14
3	D	1257	NAP	O2N-PN-O1N	2.17	122.97	112.24
3	C	1257	NAP	C4A-C5A-N7A	-2.16	107.14	109.40
3	G	1257	NAP	O5B-C5B-C4B	-2.15	101.58	108.99
3	B	1257	NAP	C3B-C2B-C1B	-2.12	98.91	102.89
2	A	1259	GLU	OE1-CD-CG	-2.08	116.40	123.08
3	C	1257	NAP	O2N-PN-O1N	2.06	122.43	112.24
3	B	1257	NAP	O5B-C5B-C4B	-2.06	101.91	108.99
4	H	1258	J47	C7-C2-C1	2.05	121.57	119.57
2	G	1259	GLU	OE1-CD-CG	-2.04	116.54	123.08
2	G	1259	GLU	O-C-CA	-2.03	114.96	122.14
4	G	1258	J47	C7-C2-C1	2.03	121.55	119.57

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1259	GLU	C-CA-CB-CG
2	B	1259	GLU	C-CA-CB-CG
2	G	1259	GLU	C-CA-CB-CG
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	A	1257	NAP	O4D-C1D-N1N-C6N
3	B	1257	NAP	C5D-O5D-PN-O1N
3	B	1257	NAP	C5D-O5D-PN-O2N
3	B	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
3	D	1257	NAP	C5D-O5D-PN-O1N
3	D	1257	NAP	C5D-O5D-PN-O2N
3	D	1257	NAP	O4D-C1D-N1N-C2N
3	E	1257	NAP	C5D-O5D-PN-O1N
3	E	1257	NAP	C5D-O5D-PN-O2N
3	F	1257	NAP	C5D-O5D-PN-O1N
3	F	1257	NAP	C5D-O5D-PN-O2N
3	F	1257	NAP	O4D-C1D-N1N-C2N
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	H	1257	NAP	C5D-O5D-PN-O1N
3	H	1257	NAP	C5D-O5D-PN-O2N
3	H	1257	NAP	O4D-C1D-N1N-C2N
2	B	1259	GLU	CA-CB-CG-CD
2	C	1259	GLU	CA-CB-CG-CD
2	E	1259	GLU	O-C-CA-N
2	G	1259	GLU	OXT-C-CA-CB
3	D	1257	NAP	PN-O3-PA-O5B
3	F	1257	NAP	PN-O3-PA-O5B
2	A	1259	GLU	OXT-C-CA-CB
2	B	1259	GLU	OXT-C-CA-CB
2	C	1259	GLU	OXT-C-CA-CB
2	F	1259	GLU	OXT-C-CA-CB
3	D	1257	NAP	C5D-O5D-PN-O3
2	F	1259	GLU	O-C-CA-CB
2	C	1259	GLU	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	A	1259	GLU	CA-CB-CG-CD
2	E	1259	GLU	CA-CB-CG-CD
2	A	1259	GLU	O-C-CA-CB
2	B	1259	GLU	O-C-CA-CB
2	G	1259	GLU	O-C-CA-CB
2	F	1259	GLU	CA-CB-CG-CD
2	G	1259	GLU	CA-CB-CG-CD
3	B	1257	NAP	O4B-C4B-C5B-O5B
2	E	1259	GLU	O-C-CA-CB
2	E	1259	GLU	OXT-C-CA-N
3	B	1257	NAP	PA-O3-PN-O1N
3	B	1257	NAP	PA-O3-PN-O2N
3	C	1257	NAP	PA-O3-PN-O1N
3	H	1257	NAP	PA-O3-PN-O1N
3	H	1257	NAP	PA-O3-PN-O2N
3	F	1257	NAP	O4B-C4B-C5B-O5B
3	G	1257	NAP	PN-O3-PA-O5B
3	G	1257	NAP	O4B-C4B-C5B-O5B
4	G	1258	J47	N1-C1-C2-C3
2	E	1259	GLU	OXT-C-CA-CB
3	A	1257	NAP	C5D-O5D-PN-O3
3	A	1257	NAP	C2D-C1D-N1N-C6N
3	B	1257	NAP	C5D-O5D-PN-O3
3	C	1257	NAP	C5D-O5D-PN-O3
3	E	1257	NAP	C5D-O5D-PN-O3
3	F	1257	NAP	C5D-O5D-PN-O3
3	G	1257	NAP	C5D-O5D-PN-O3
3	H	1257	NAP	C5D-O5D-PN-O3
4	F	1258	J47	N1-C1-C2-C7
2	C	1259	GLU	OE2-CD-CG-CB
3	C	1257	NAP	PA-O3-PN-O2N
3	D	1257	NAP	PA-O3-PN-O2N
3	A	1257	NAP	O4B-C4B-C5B-O5B
3	C	1257	NAP	O4B-C4B-C5B-O5B
3	D	1257	NAP	O4B-C4B-C5B-O5B
3	E	1257	NAP	O4B-C4B-C5B-O5B
3	H	1257	NAP	O4B-C4B-C5B-O5B
2	F	1259	GLU	OXT-C-CA-N
2	C	1259	GLU	OE1-CD-CG-CB
2	G	1259	GLU	N-CA-CB-CG
2	G	1259	GLU	OXT-C-CA-N

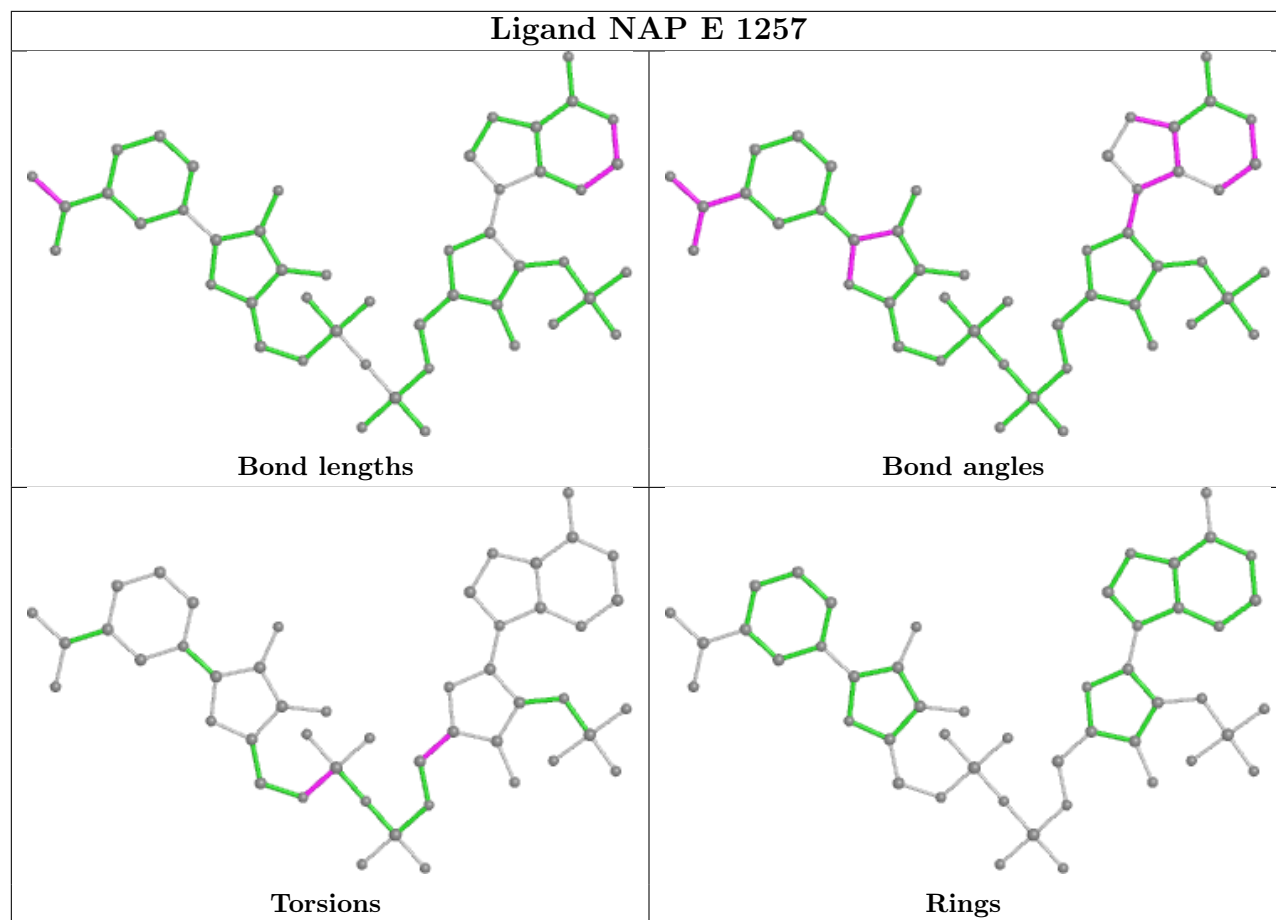
There are no ring outliers.

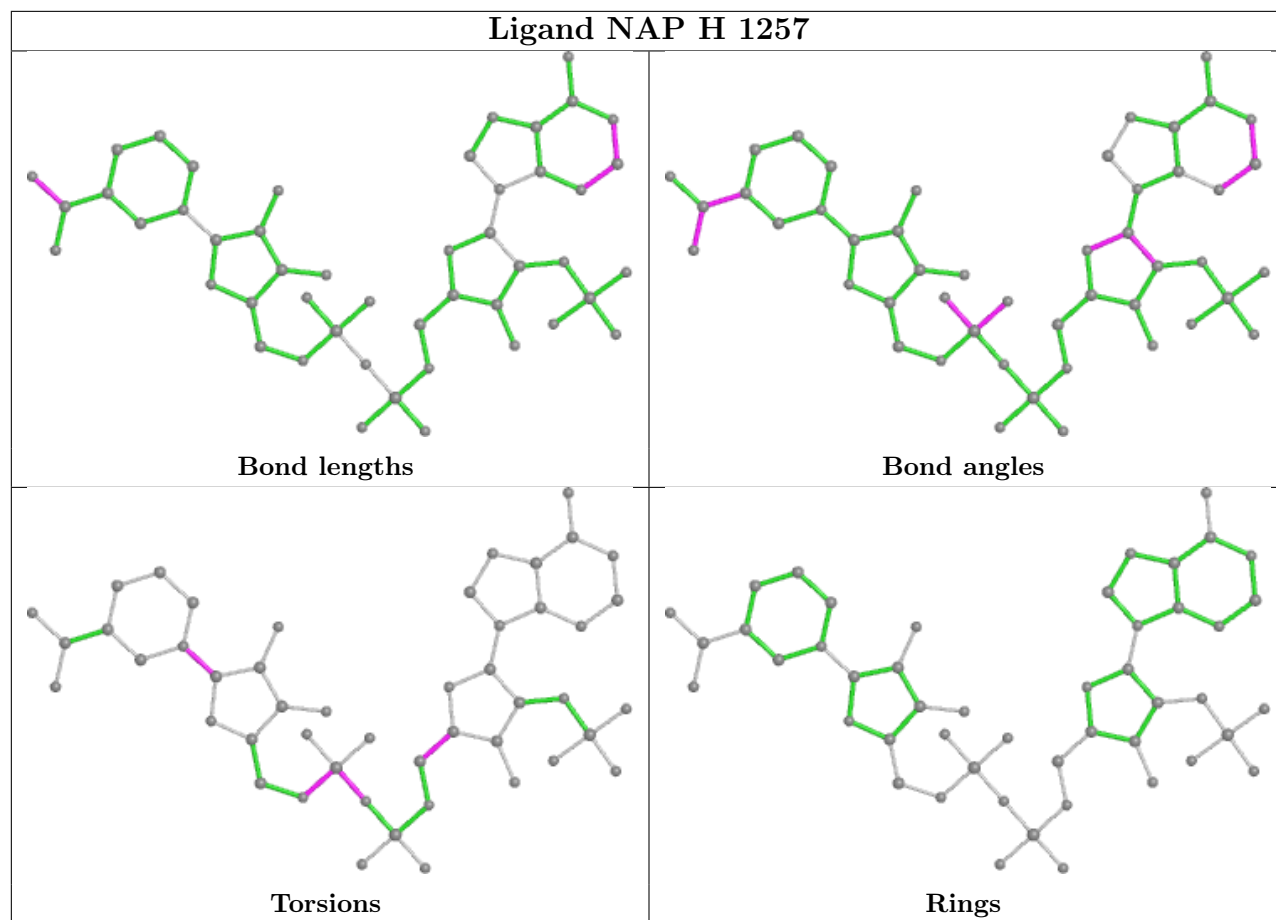


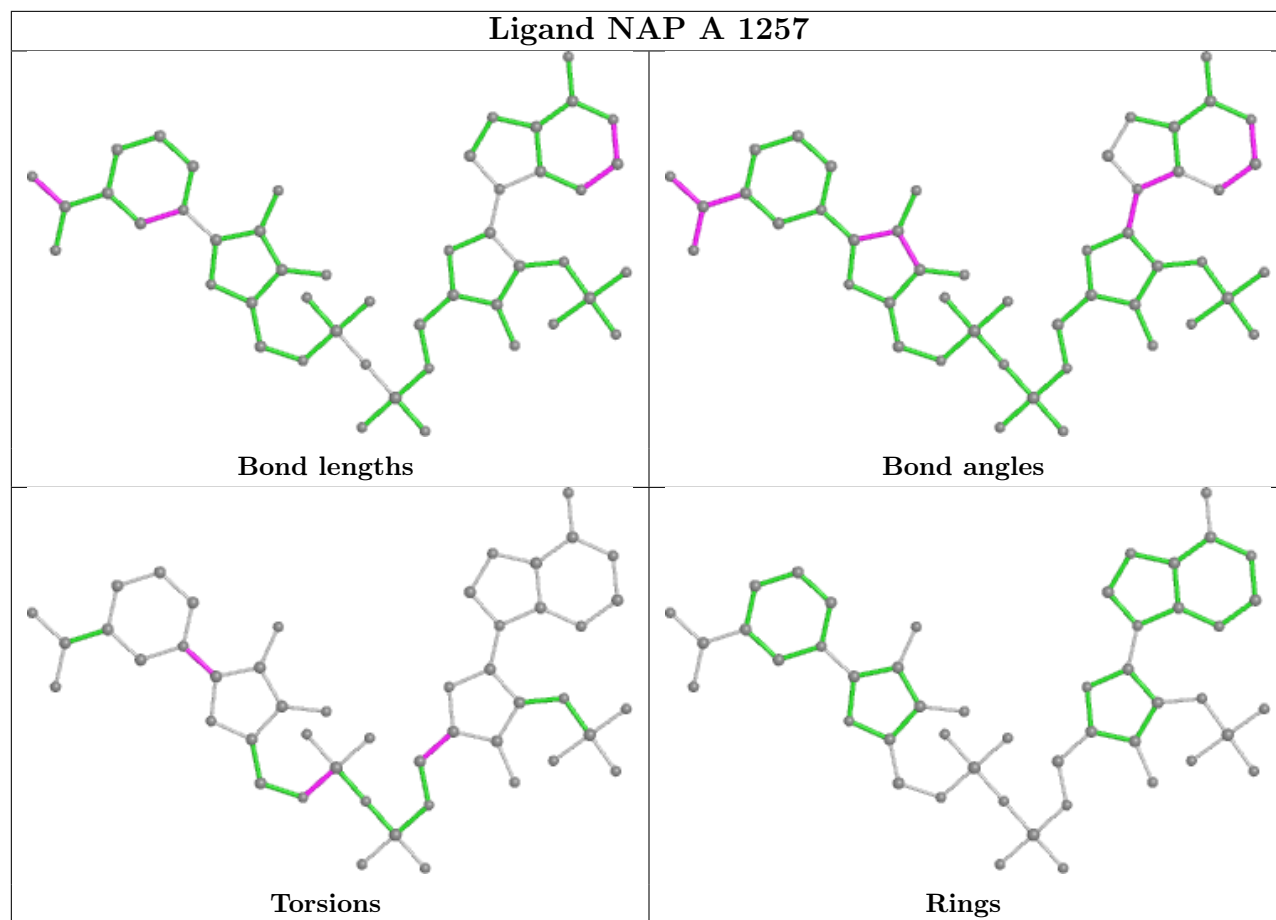
16 monomers are involved in 27 short contacts:

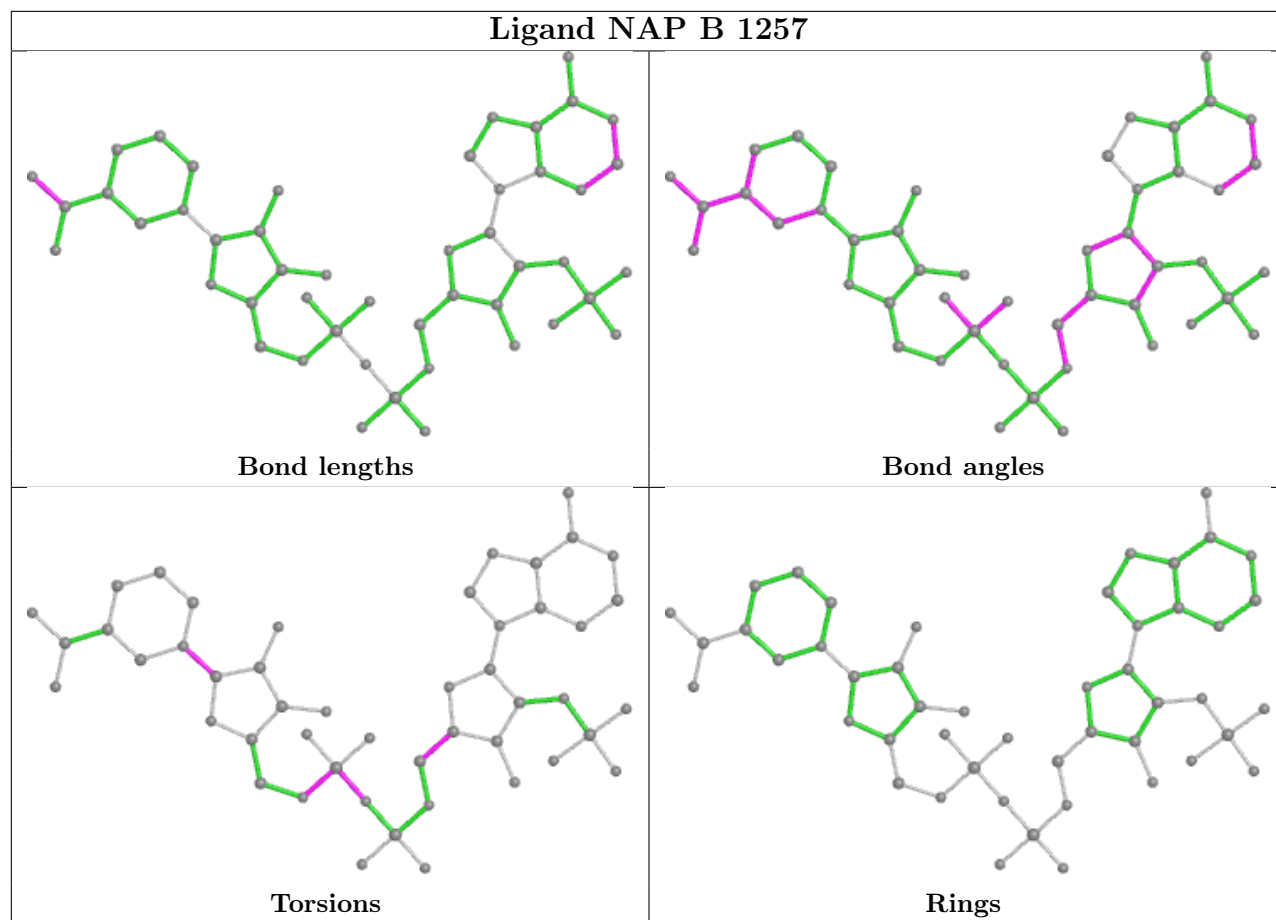
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1259	GLU	1	0
3	H	1257	NAP	2	0
4	A	1258	J47	1	0
2	G	1259	GLU	2	0
2	B	1259	GLU	5	0
2	A	1259	GLU	2	0
3	B	1257	NAP	3	0
3	F	1257	NAP	1	0
4	E	1258	J47	1	0
4	B	1258	J47	2	0
4	F	1258	J47	3	0
4	C	1258	J47	1	0
3	D	1257	NAP	1	0
4	D	1258	J47	1	0
3	G	1257	NAP	2	0
4	G	1258	J47	2	0

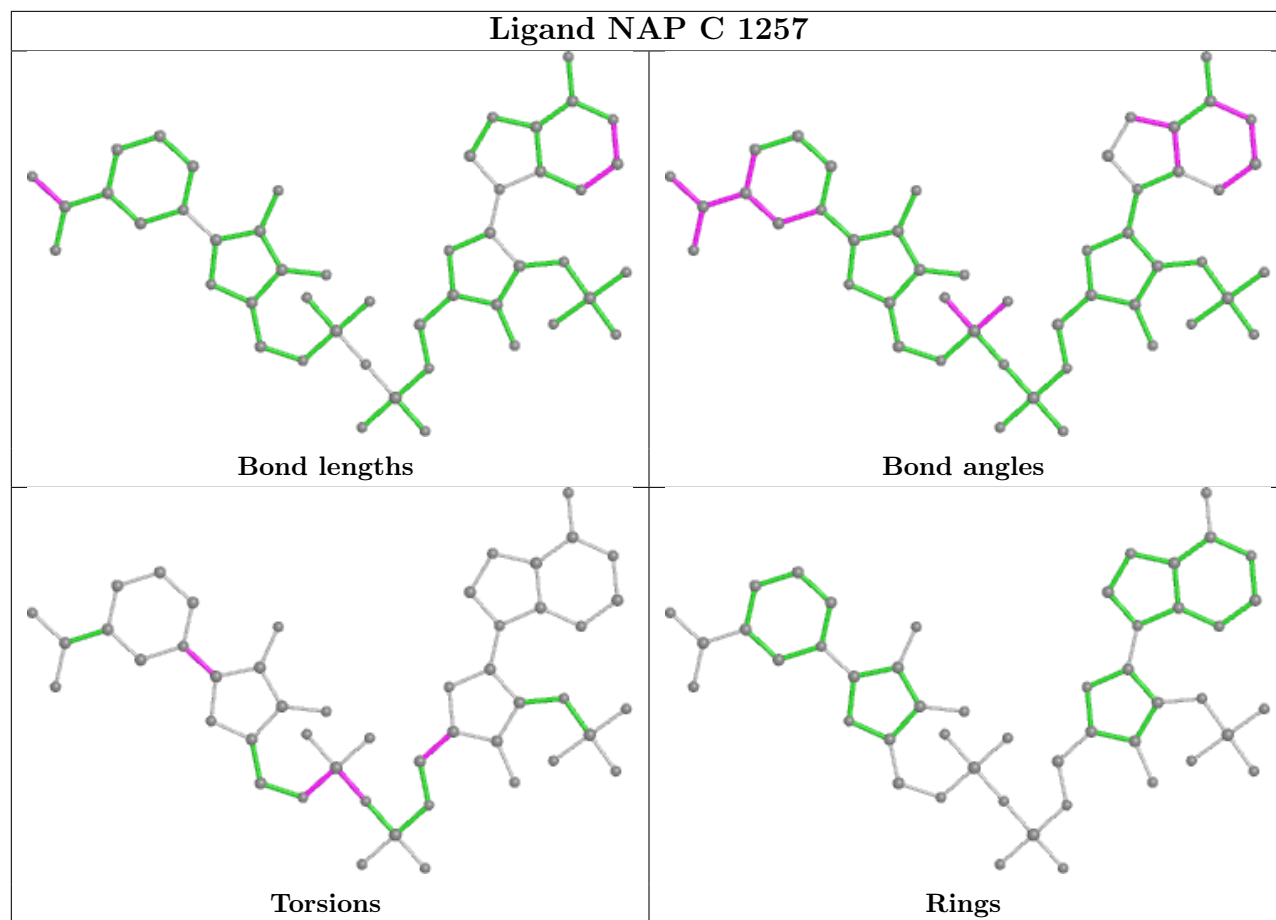
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

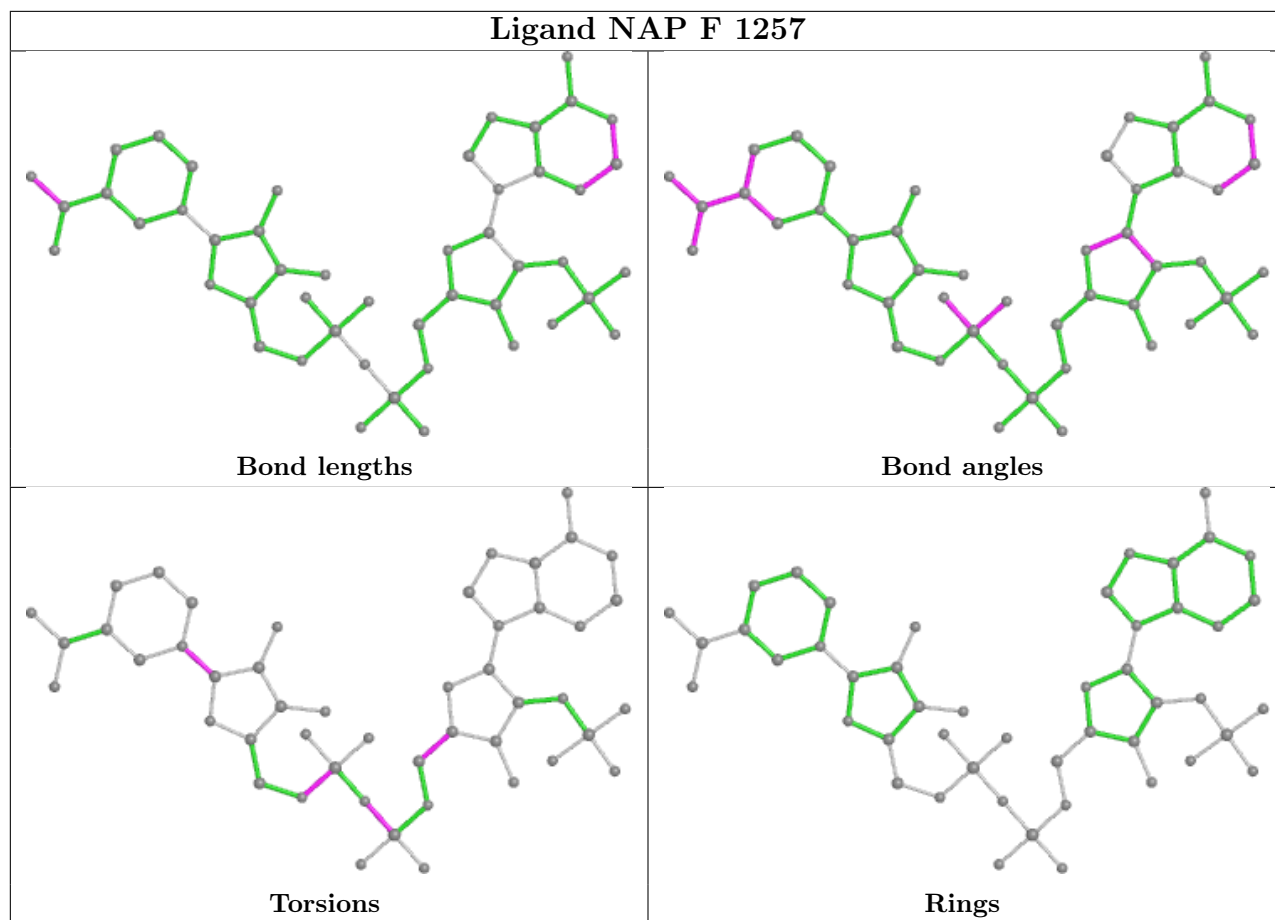


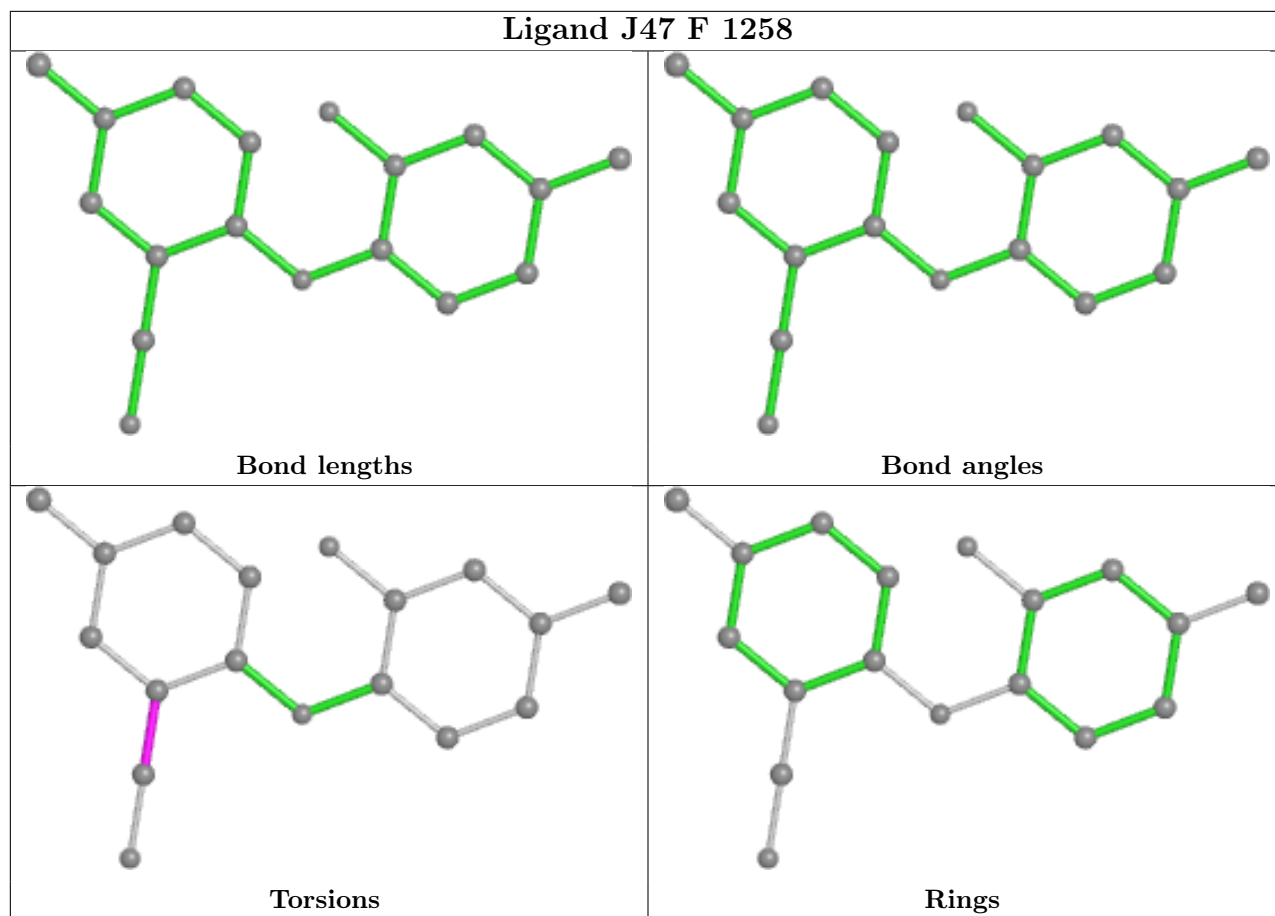




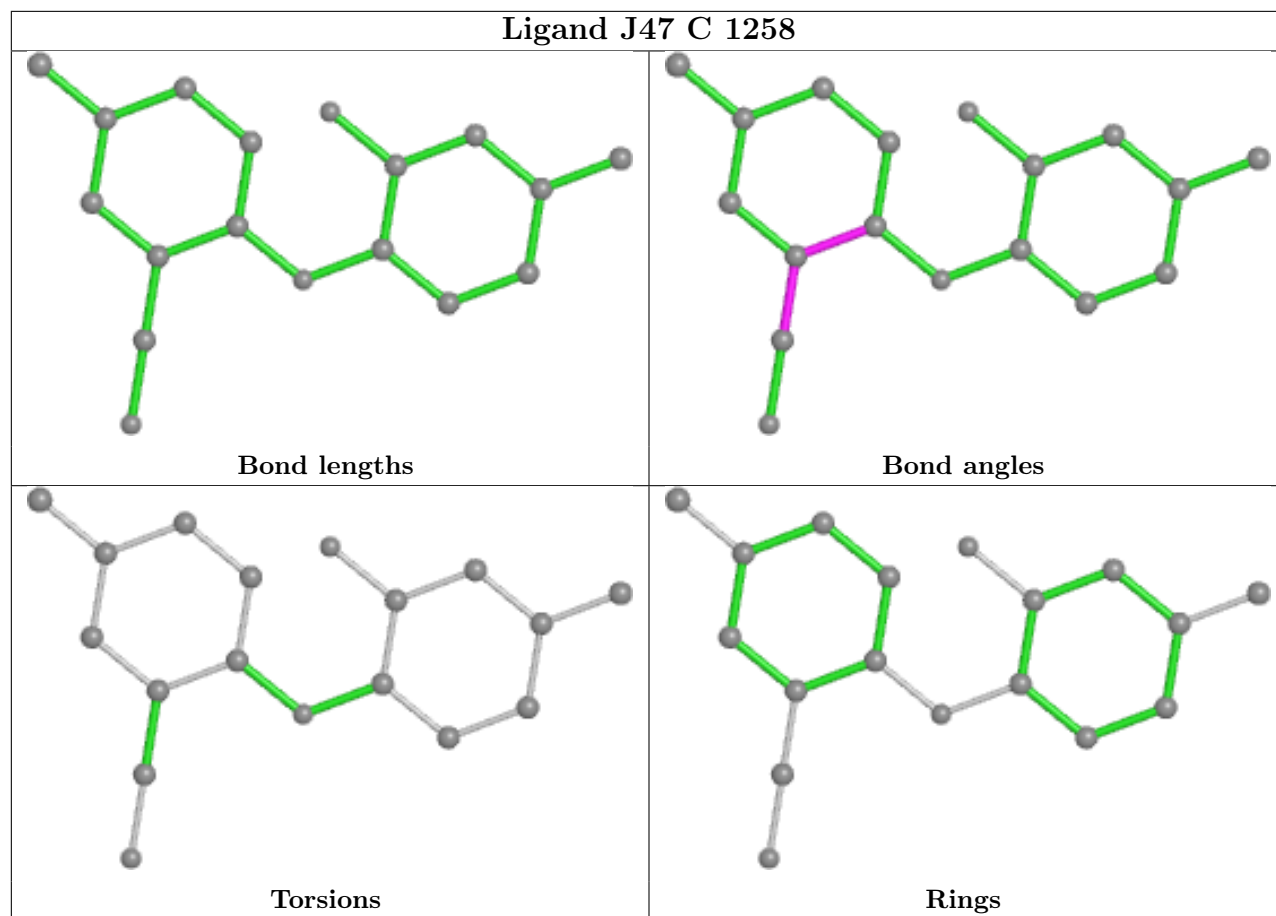


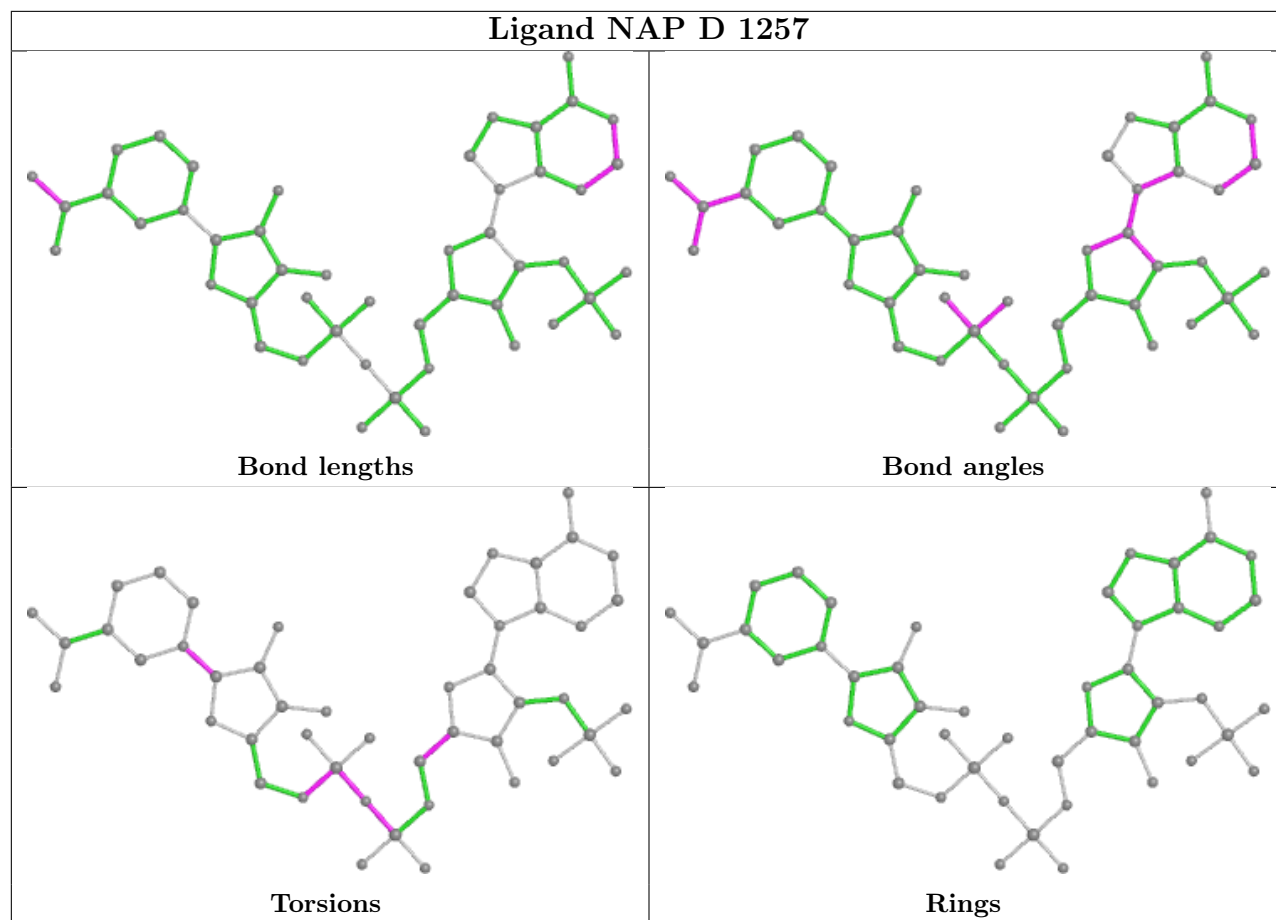


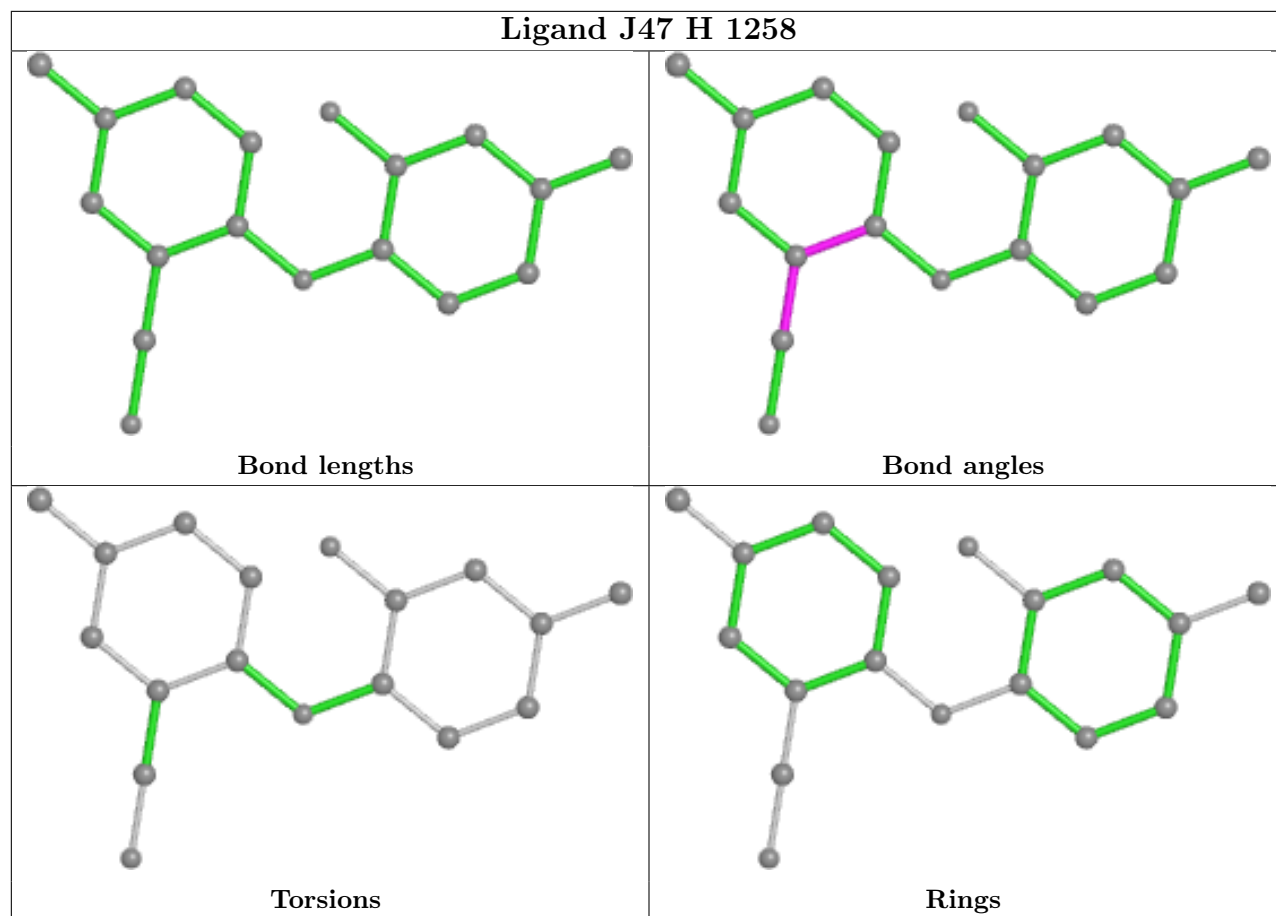


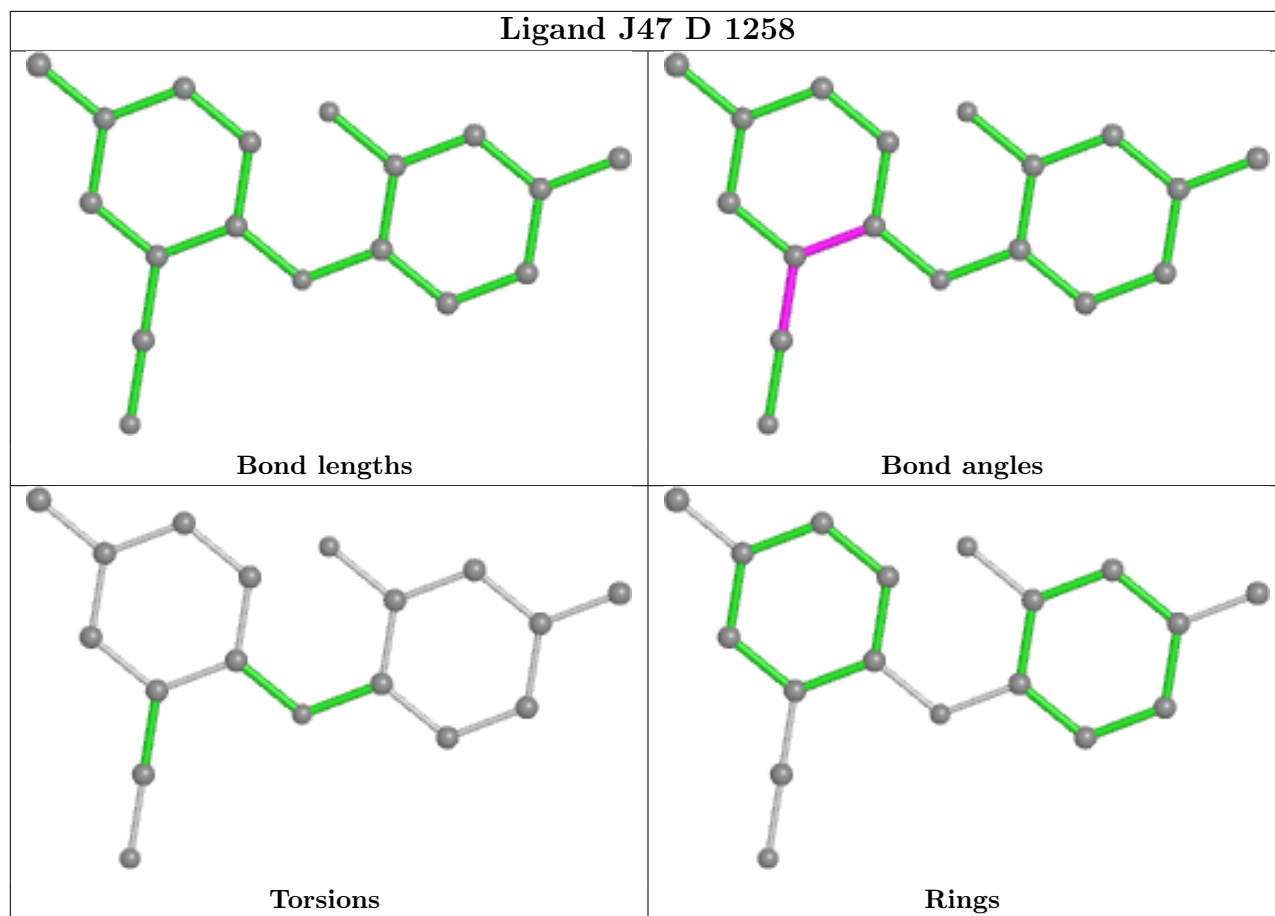


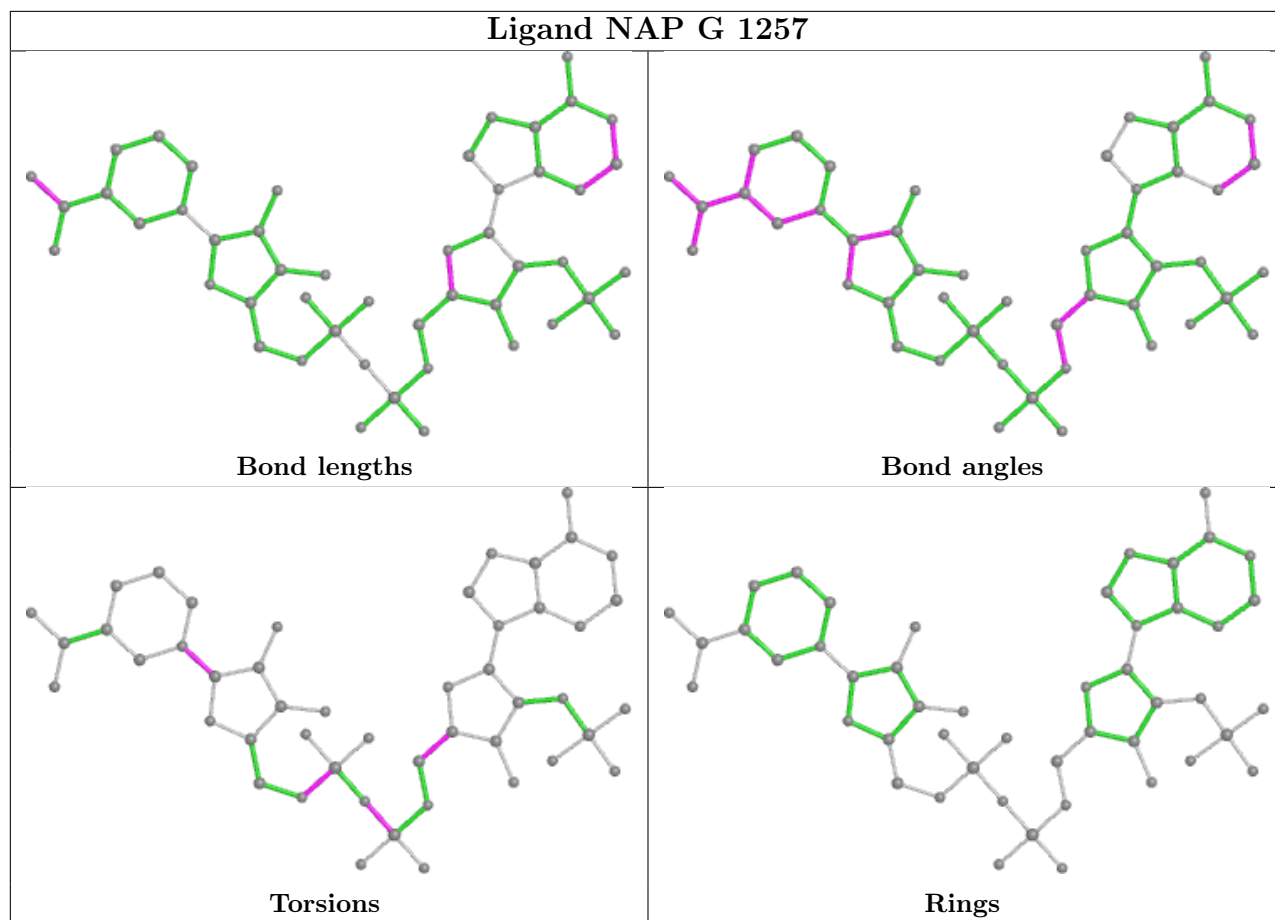


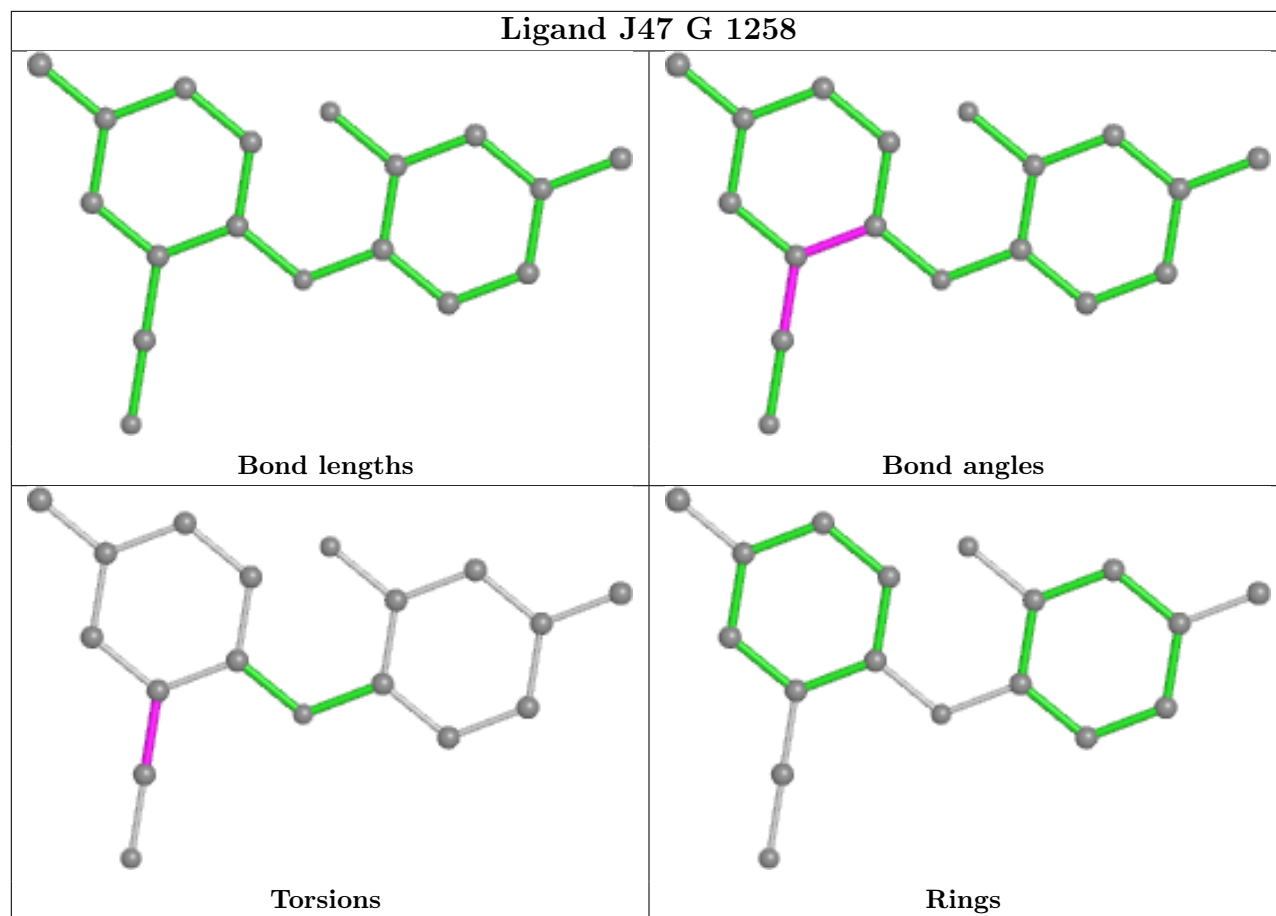












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	254/282 (90%)	-0.06	2 (0%) 86 89	22, 31, 49, 62	0
1	B	254/282 (90%)	0.06	5 (1%) 65 72	21, 33, 52, 65	0
1	C	254/282 (90%)	-0.02	2 (0%) 86 89	20, 34, 55, 69	0
1	D	254/282 (90%)	0.10	11 (4%) 35 45	23, 38, 66, 89	0
1	E	254/282 (90%)	-0.09	3 (1%) 79 83	21, 31, 50, 66	0
1	F	254/282 (90%)	-0.05	2 (0%) 86 89	21, 33, 52, 63	0
1	G	254/282 (90%)	0.02	3 (1%) 79 83	19, 35, 55, 68	0
1	H	254/282 (90%)	0.02	10 (3%) 39 48	21, 38, 71, 98	0
All	All	2032/2256 (90%)	-0.00	38 (1%) 66 74	19, 34, 57, 98	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	58	PRO	3.7
1	C	58	PRO	3.4
1	D	43	ARG	3.2
1	H	6	ASN	3.2
1	D	104	GLY	3.1
1	G	58	PRO	3.1
1	H	103	ARG	3.1
1	H	99	MET	3.1
1	D	103	ARG	3.1
1	H	52	LEU	3.1
1	D	52	LEU	3.0
1	E	6	ASN	3.0
1	D	99	MET	2.8
1	G	6	ASN	2.7
1	H	58	PRO	2.7
1	C	6	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	59	GLU	2.7
1	H	44	SER	2.6
1	E	58	PRO	2.6
1	B	148	LEU	2.5
1	D	200	GLY	2.5
1	H	43	ARG	2.4
1	F	148	LEU	2.4
1	B	85	GLY	2.3
1	A	6	ASN	2.3
1	H	56	ASN	2.3
1	D	54	GLN	2.3
1	H	200	GLY	2.2
1	D	47[A]	GLU	2.2
1	F	6	ASN	2.2
1	E	254	ALA	2.2
1	G	60	ALA	2.2
1	A	254	ALA	2.1
1	D	46	LYS	2.1
1	B	58	PRO	2.1
1	B	60	ALA	2.0
1	B	59	GLU	2.0
1	H	209[A]	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	GLU	F	1259	10/10	0.64	0.24	67,76,78,78	0

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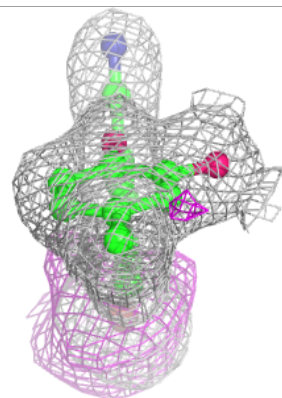
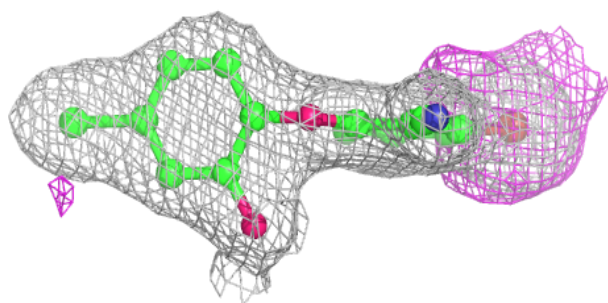
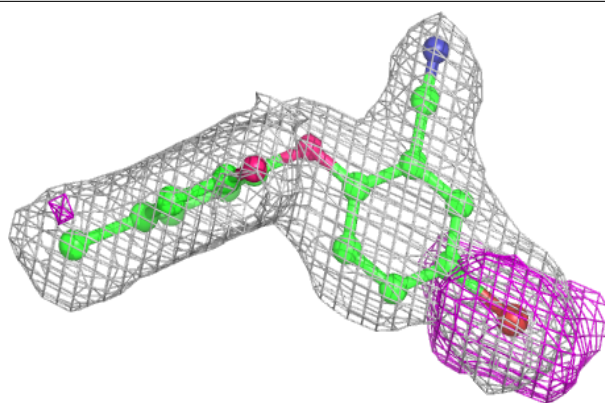
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLU	G	1259	10/10	0.65	0.27	57,75,76,76	0
2	GLU	B	1259	10/10	0.68	0.20	64,70,71,71	0
2	GLU	C	1259	10/10	0.69	0.26	68,73,75,75	0
2	GLU	A	1259	10/10	0.73	0.21	70,76,77,80	0
2	GLU	E	1259	10/10	0.74	0.27	62,74,75,75	0
4	J47	D	1258	18/18	0.89	0.14	37,40,50,60	0
4	J47	H	1258	18/18	0.92	0.11	38,40,52,63	0
4	J47	G	1258	18/18	0.93	0.12	25,30,41,50	0
4	J47	A	1258	18/18	0.93	0.13	28,30,34,44	0
4	J47	E	1258	18/18	0.94	0.11	24,29,35,45	0
4	J47	F	1258	18/18	0.94	0.10	27,31,40,49	0
4	J47	C	1258	18/18	0.94	0.11	24,32,40,47	0
4	J47	B	1258	18/18	0.94	0.12	26,31,38,48	0
3	NAP	D	1257	48/48	0.96	0.09	33,39,57,64	0
3	NAP	C	1257	48/48	0.97	0.10	26,34,39,42	0
3	NAP	F	1257	48/48	0.97	0.11	28,33,38,40	0
3	NAP	G	1257	48/48	0.97	0.11	24,31,37,38	0
3	NAP	H	1257	48/48	0.97	0.09	29,38,61,64	0
3	NAP	E	1257	48/48	0.98	0.11	22,30,35,36	0
3	NAP	A	1257	48/48	0.98	0.11	23,30,35,40	0
3	NAP	B	1257	48/48	0.98	0.12	27,32,37,40	0

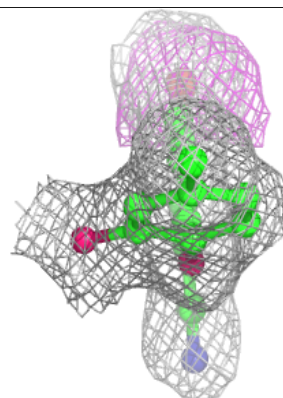
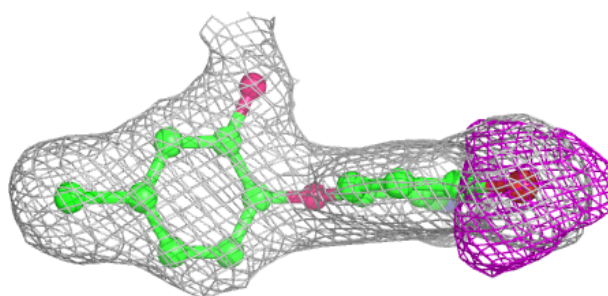
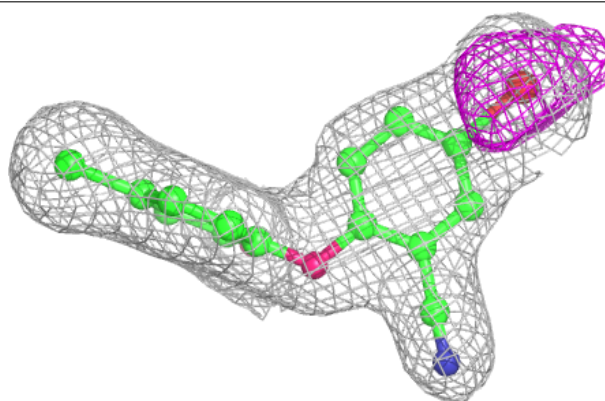
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around J47 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)

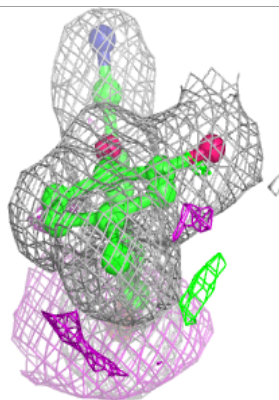
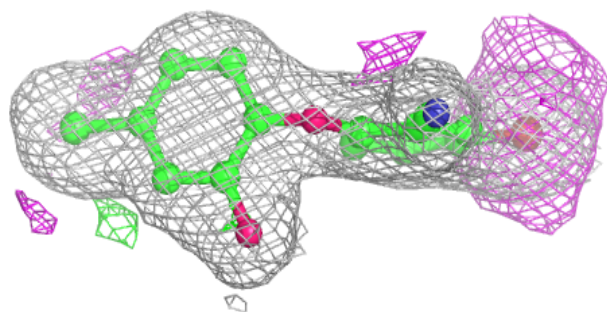
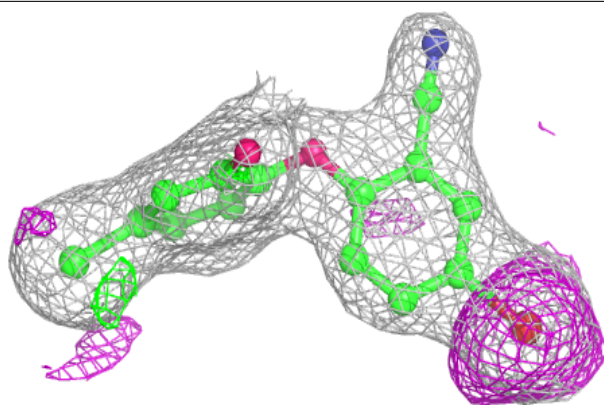
**Electron density around J47 H 1258:**

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

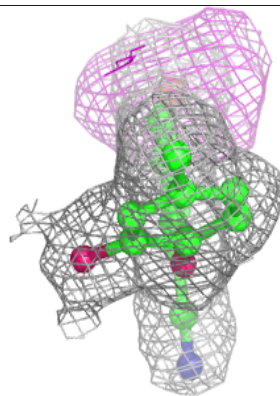
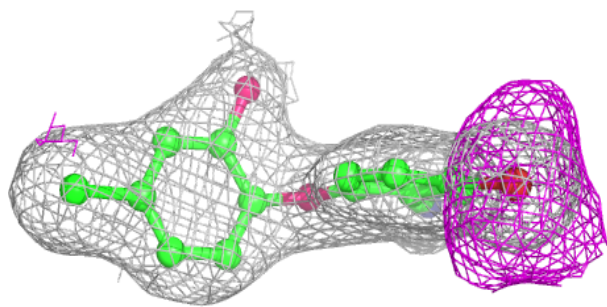
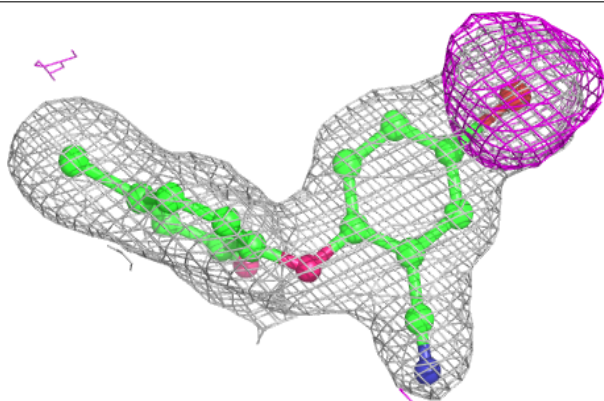


**Electron density around J47 G 1258:**

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

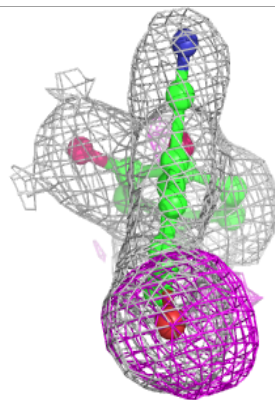
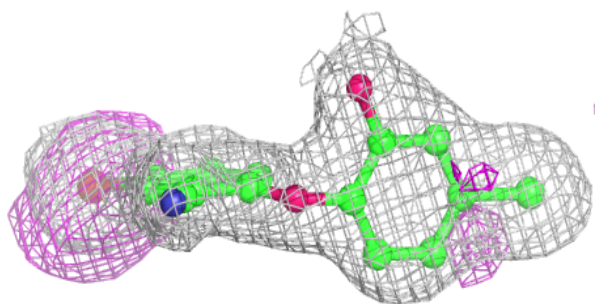
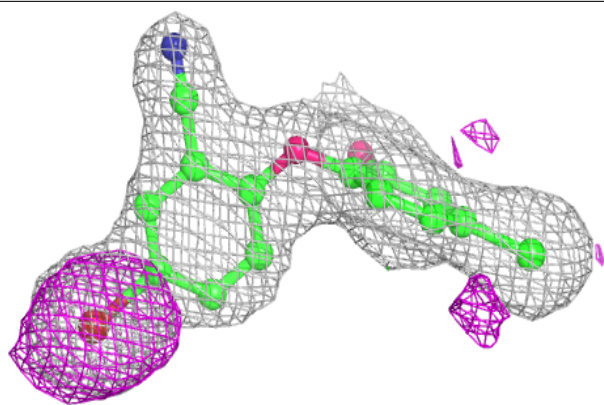
**Electron density around J47 F 1258:**

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

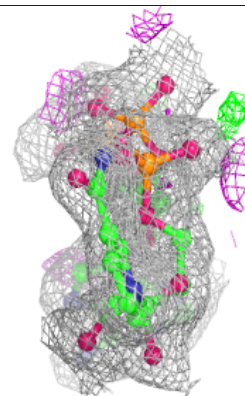
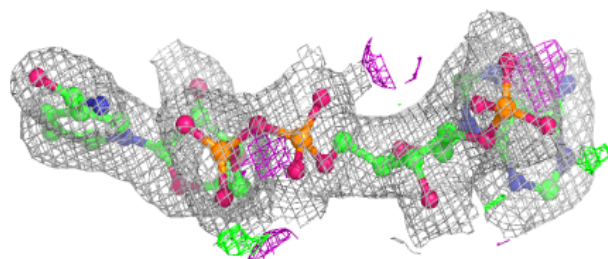
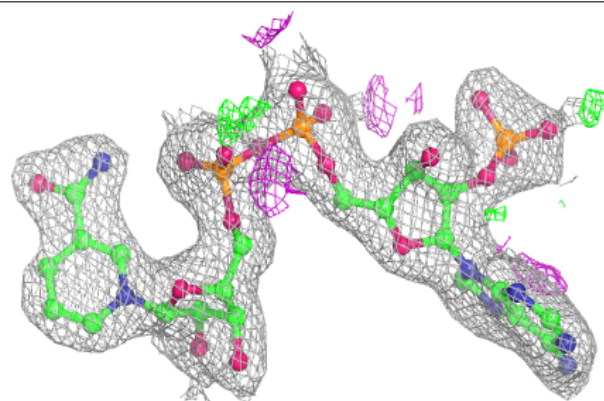


**Electron density around J47 C 1258:**

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

**Electron density around NAP D 1257:**

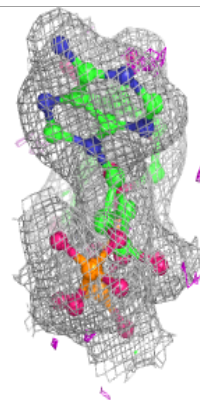
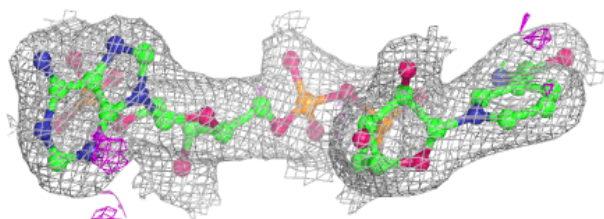
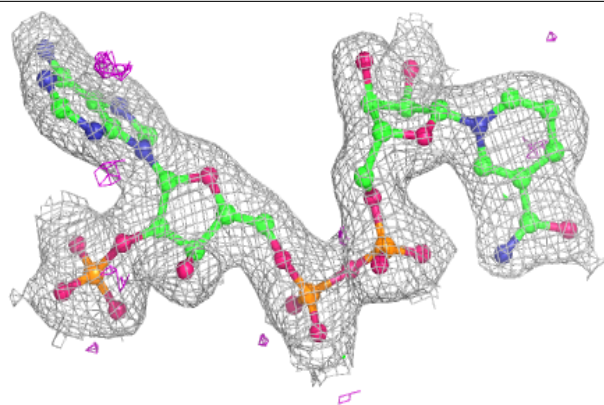
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



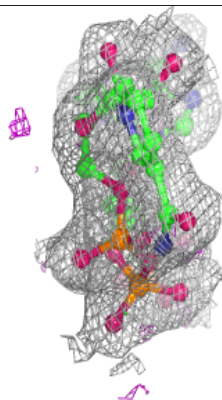
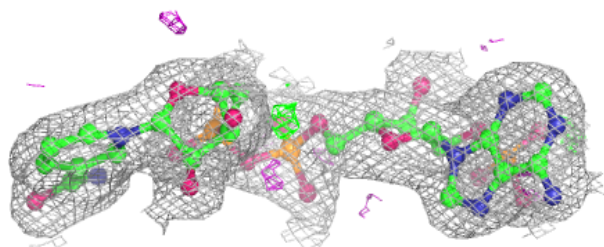
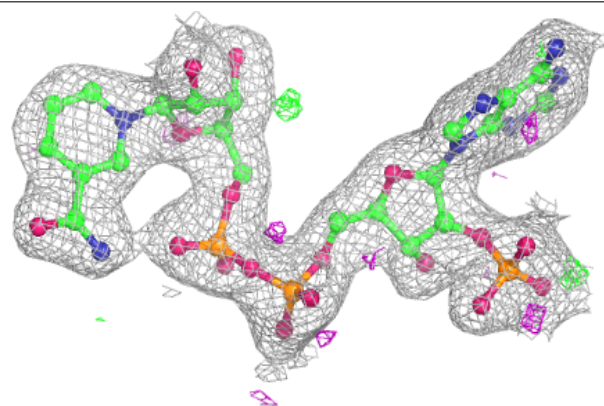


**Electron density around NAP C 1257:**

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

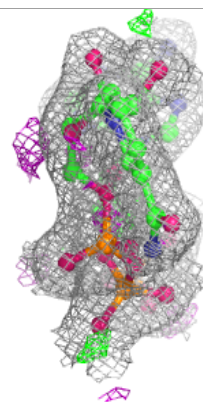
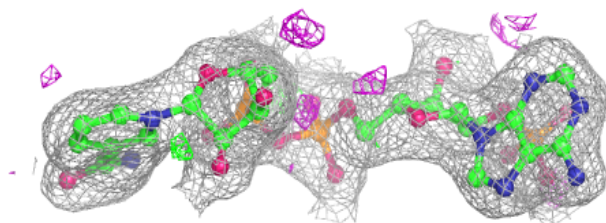
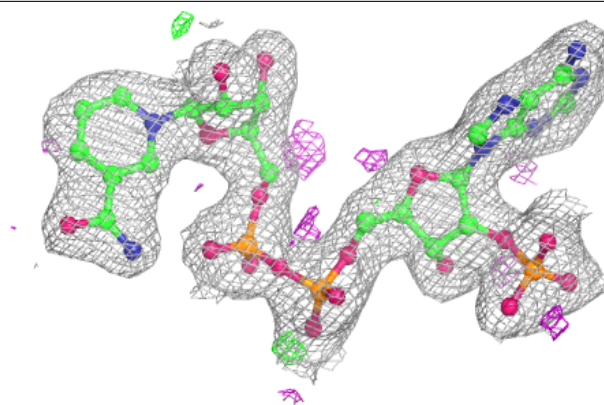
**Electron density around NAP F 1257:**

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

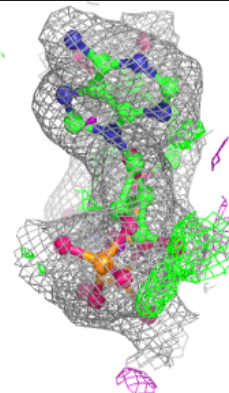
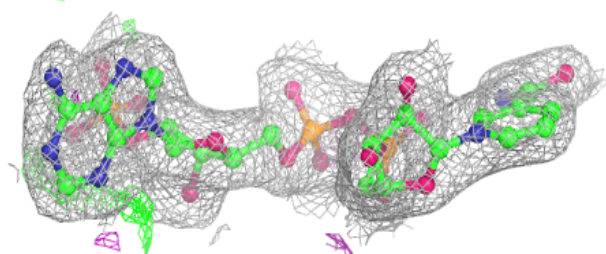
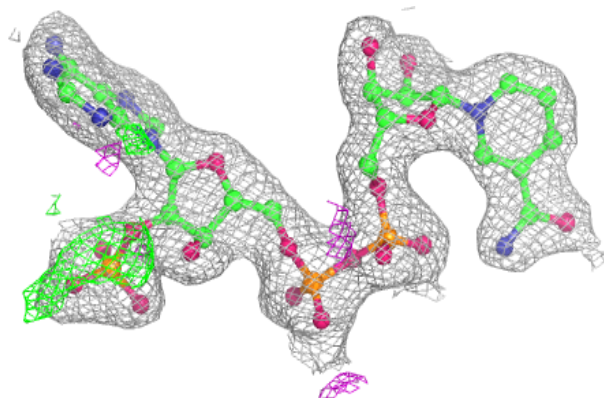


**Electron density around NAP G 1257:**

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

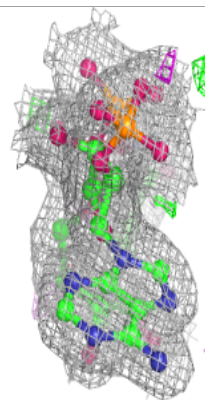
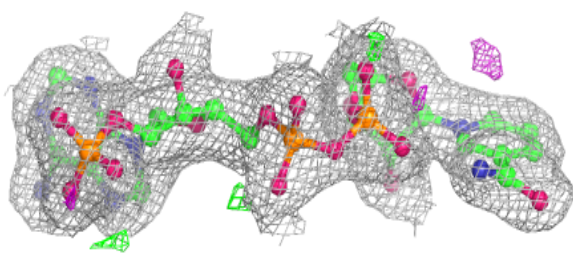
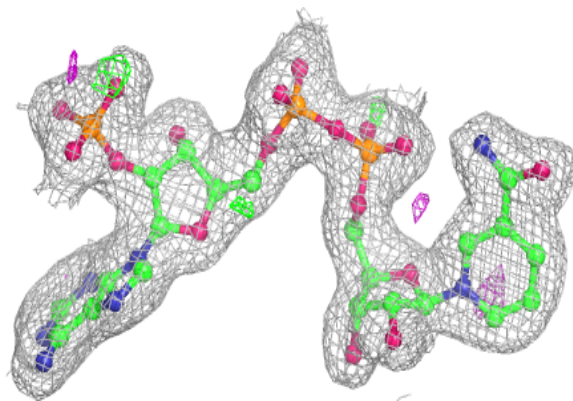
**Electron density around NAP H 1257:**

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

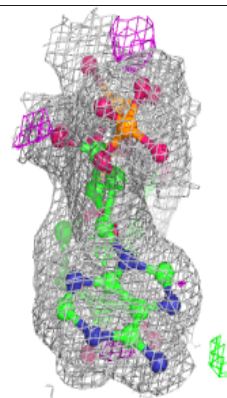
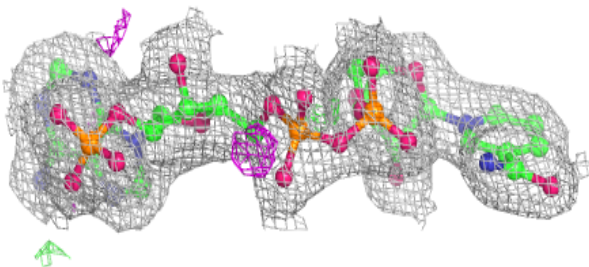
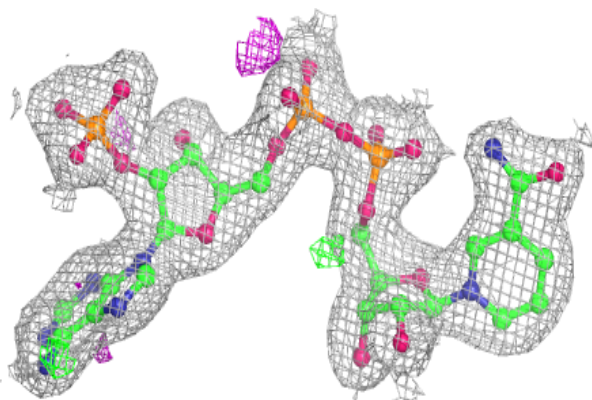


**Electron density around NAP E 1257:**

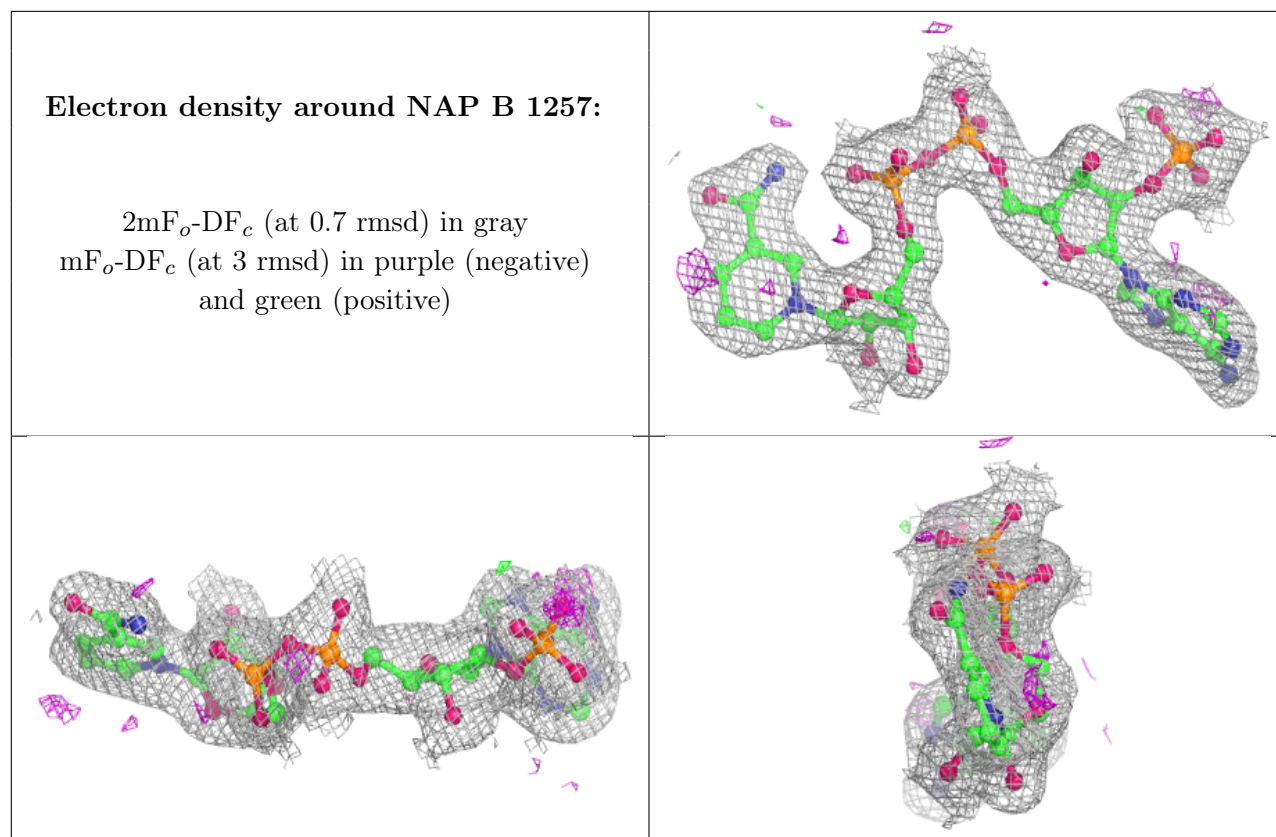
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP 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)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.