



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 03:09 AM BST

PDB ID : 4D44  
Title : Crystal structure of S. aureus FabI in complex with NADP and 5-ethyl- 4-fluoro-2-((2-fluoropyridin-3-yl)oxy)phenol  
Authors : Schiebel, J.; Chang, A.; Tonge, P.J.; Sotriffer, C.A.; Kisker, C.  
Deposited on : 2014-10-26  
Resolution : 1.80 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.

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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 : 1.8.5 (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

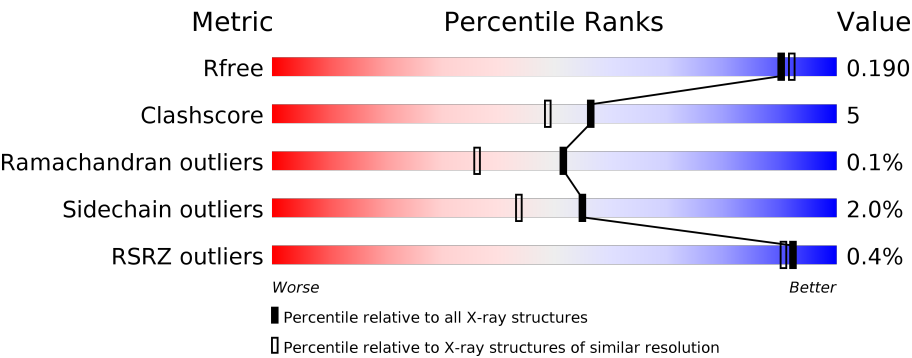
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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><div></div><div>79%9%10%</div></div>
1	B	282	<div><div></div><div>82%8%10%</div></div>
1	C	282	<div><div></div><div>81%9%10%</div></div>
1	D	282	<div><div>%</div><div>79%11%10%</div></div>
1	E	282	<div><div></div><div>81%8%10%</div></div>
1	F	282	<div><div></div><div>82%8%10%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	282	<div><div>%</div><div><div></div><div>78%</div><div>12%</div><div>10%</div></div></div>
1	H	282	<div><div>%</div><div><div></div><div>80%</div><div>9%</div><div>10%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18237 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	12	0
			2044	1284	357	398	5			
1	B	254	Total	C	N	O	S	0	12	0
			2044	1284	356	399	5			
1	C	254	Total	C	N	O	S	0	12	0
			2046	1285	359	397	5			
1	D	254	Total	C	N	O	S	0	6	0
			1995	1256	349	386	4			
1	E	254	Total	C	N	O	S	0	13	0
			2052	1289	359	399	5			
1	F	254	Total	C	N	O	S	0	11	0
			2038	1280	356	397	5			
1	G	254	Total	C	N	O	S	0	13	0
			2052	1289	360	398	5			
1	H	254	Total	C	N	O	S	0	3	0
			1971	1241	340	386	4			

There are 216 discrepancies between the modelled and reference sequences:

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

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

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

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

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

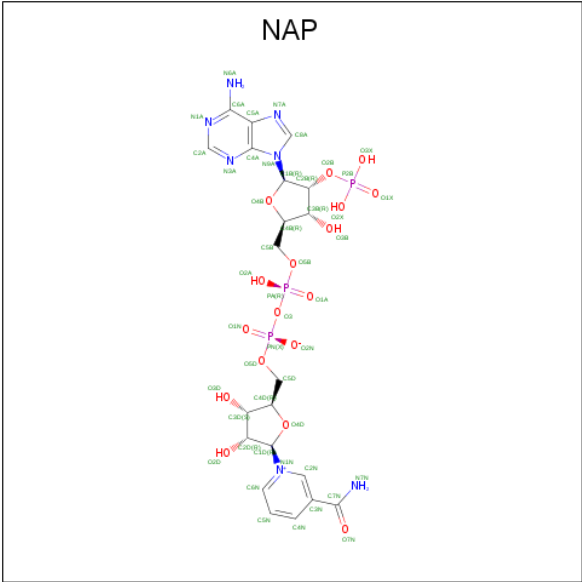
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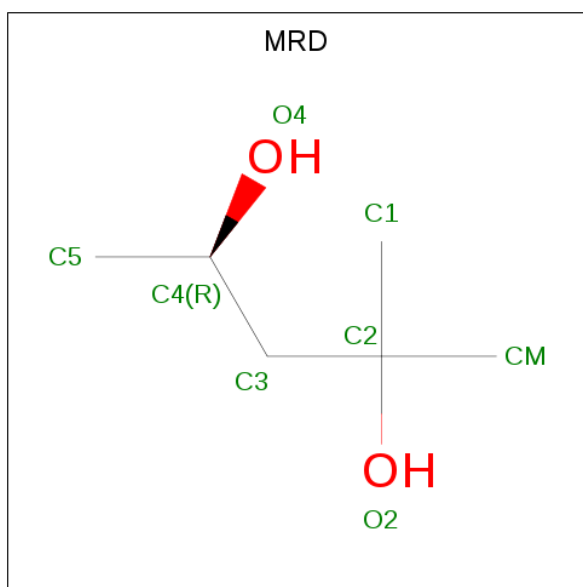
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8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

- Molecule 2 is 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>).



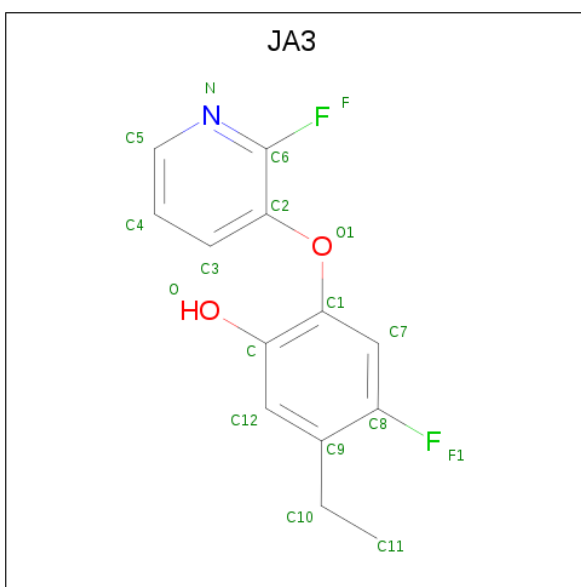
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G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

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is 5-ethyl-4-fluoro-2-[(2-fluoropyridin-3-yl)oxy]phenol (three-letter code: JA3) (formula: C<sub>13</sub>H<sub>11</sub>F<sub>2</sub>NO<sub>2</sub>).



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

- Molecule 5 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
5	B	1	Total	C	N	O	0	0
			10	5	1	4		
5	C	1	Total	C	N	O	0	0
			10	5	1	4		
5	E	1	Total	C	N	O	0	0
			10	5	1	4		
5	F	1	Total	C	N	O	0	0
			10	5	1	4		
5	G	1	Total	C	N	O	0	0
			10	5	1	4		
5	H	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	218	Total	O	0	0
			218	218		
6	B	190	Total	O	0	0
			190	190		
6	C	168	Total	O	0	0
			168	168		
6	D	122	Total	O	0	0
			122	122		
6	E	195	Total	O	0	0
			195	195		
6	F	168	Total	O	0	0
			168	168		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	154	Total 154	O 154	0	0
6	H	128	Total 128	O 128	0	0

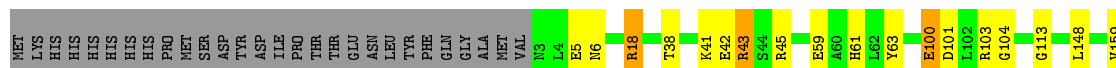
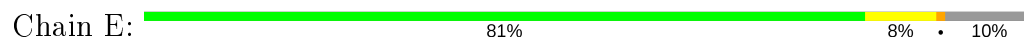


- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

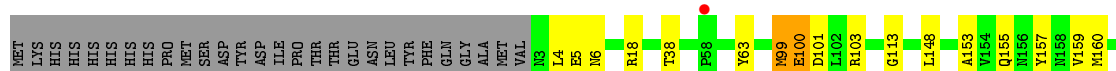
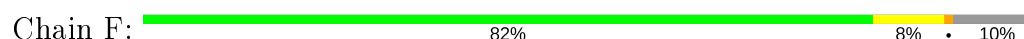




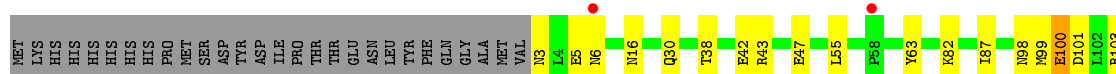
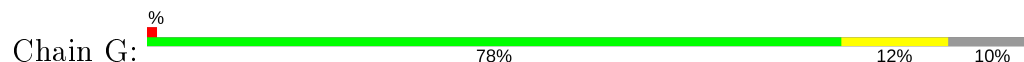
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



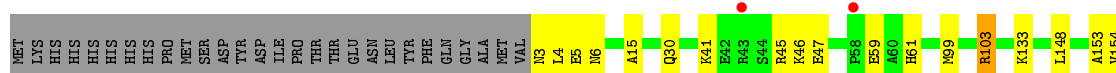
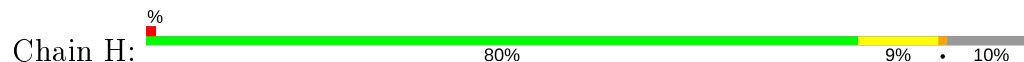
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



- 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, $\alpha$ , $\beta$ , $\gamma$	89.97Å 94.74Å 94.80Å 98.06° 97.38° 112.18°	Depositor
Resolution (Å)	33.64 – 1.80 32.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (33.64-1.80) 97.5 (32.93-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.140 , 0.170 0.165 , 0.190	Depositor DCC
$R_{free}$ test set	12770 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	18237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, NAP, JA3

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	0.74	0/2080	0.92	3/2799 (0.1%)
1	B	0.71	1/2080 (0.0%)	0.86	0/2799
1	C	0.67	0/2082	0.87	2/2801 (0.1%)
1	D	0.65	1/2034 (0.0%)	0.82	2/2738 (0.1%)
1	E	0.75	0/2091	0.94	5/2813 (0.2%)
1	F	0.69	1/2071 (0.0%)	0.83	0/2787
1	G	0.67	0/2091	0.85	1/2813 (0.0%)
1	H	0.66	0/2001	0.87	5/2696 (0.2%)
All	All	0.69	3/16530 (0.0%)	0.87	18/22246 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	GLU	CB-CG	5.96	1.63	1.52
1	D	168	GLU	CB-CG	5.39	1.62	1.52
1	F	168	GLU	CB-CG	5.00	1.61	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	ARG	NE-CZ-NH1	-11.04	114.78	120.30
1	E	43	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	G	43	ARG	NE-CZ-NH1	-8.50	116.05	120.30
1	C	43	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	H	228	LYS	CD-CE-NZ	-6.76	96.15	111.70
1	D	228	LYS	CD-CE-NZ	-6.54	96.65	111.70
1	E	18[A]	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	E	18[B]	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	18[A]	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	18[B]	ARG	NE-CZ-NH2	-5.81	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	208	LEU	CA-CB-CG	5.66	128.31	115.30
1	H	103	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	H	184	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	H	177	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	103	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	43	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	E	18[A]	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	18[B]	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2044	0	2060	37	0
1	B	2044	0	2058	19	0
1	C	2046	0	2065	18	0
1	D	1995	0	2020	21	0
1	E	2052	0	2071	26	0
1	F	2038	0	2052	22	0
1	G	2052	0	2073	25	1
1	H	1971	0	1981	18	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
2	E	48	0	25	0	0
2	F	48	0	25	0	0
2	G	48	0	25	0	0
2	H	48	0	25	1	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
3	C	8	0	14	1	0
3	E	8	0	14	0	0
3	F	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	16	0	28	2	0
3	H	8	0	14	1	0
4	A	18	0	10	0	0
4	B	18	0	10	0	0
4	C	36	0	21	0	0
4	E	36	0	21	0	0
4	G	36	0	21	0	0
5	B	10	0	5	0	0
5	C	10	0	5	1	0
5	E	10	0	5	0	0
5	F	10	0	5	3	0
5	G	10	0	5	2	0
5	H	10	0	5	0	0
6	A	218	0	0	10	1
6	B	190	0	0	7	0
6	C	168	0	0	5	0
6	D	122	0	0	5	0
6	E	195	0	0	5	0
6	F	168	0	0	4	0
6	G	154	0	0	5	0
6	H	128	0	0	5	0
All	All	18237	0	16805	168	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (168) 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:G:98:ASN:HB3	1:G:100[B]:GLU:HG2	1.25	1.11
3:G:1261:MRD:H1C3	6:G:2065:HOH:O	1.48	1.11
1:A:18[B]:ARG:HG3	1:A:18[B]:ARG:HH11	1.22	1.05
3:F:1258:MRD:H1C3	6:F:2076:HOH:O	1.55	1.04
1:G:100[B]:GLU:OE1	1:G:100[B]:GLU:N	1.94	1.01
3:H:1257:MRD:H1C3	6:H:2052:HOH:O	1.61	0.98
3:B:1259:MRD:H1C3	6:B:2091:HOH:O	1.67	0.93
1:A:42[B]:GLU:OE1	1:A:45:ARG:NH2	2.02	0.91
1:G:101[B]:ASP:OD2	6:G:2073:HOH:O	1.86	0.91
1:H:3:ASN:HD21	1:H:5:GLU:HG3	1.34	0.91
6:D:2048:HOH:O	3:G:1259:MRD:H1C3	1.71	0.89
1:H:154:VAL:HG11	6:H:2082:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:ASN:CB	1:G:100[B]:GLU:HG2	2.08	0.84
1:E:42[B]:GLU:OE1	1:E:45:ARG:NH2	2.09	0.84
1:F:203:GLY:H	5:F:1257:GLU:HB2	1.41	0.84
1:D:100:GLU:OE1	6:D:2054:HOH:O	1.96	0.83
1:H:154:VAL:CG1	6:H:2082:HOH:O	2.26	0.82
1:B:101[B]:ASP:OD2	6:B:2100:HOH:O	1.97	0.82
6:A:2111:HOH:O	1:E:42[A]:GLU:OE2	1.97	0.81
3:C:1260:MRD:H1C3	6:C:2081:HOH:O	1.82	0.80
1:C:101[B]:ASP:OD2	6:C:2091:HOH:O	1.99	0.79
1:G:103[B]:ARG:NH1	5:G:1260:GLU:O	2.16	0.78
6:E:2165:HOH:O	1:G:155[A]:GLN:NE2	2.17	0.78
1:A:154:VAL:HG11	6:A:2132:HOH:O	1.83	0.78
1:A:101[B]:ASP:OD2	6:A:2092:HOH:O	2.02	0.76
1:B:42[B]:GLU:OE2	6:B:2046:HOH:O	2.05	0.74
1:F:253:HIS:HD2	6:F:2163:HOH:O	1.69	0.74
1:E:101[B]:ASP:OD2	6:E:2090:HOH:O	2.04	0.73
1:A:154:VAL:CG1	6:A:2132:HOH:O	2.38	0.69
1:F:99[A]:MET:CE	1:F:200:GLY:HA2	2.22	0.69
1:A:101[B]:ASP:OD2	1:A:113:GLY:HA3	1.92	0.68
1:D:64:GLN:CD	6:D:2037:HOH:O	2.32	0.67
1:A:18[B]:ARG:NH1	1:A:18[B]:ARG:HG3	2.00	0.66
1:G:101[B]:ASP:OD2	1:G:113:GLY:HA3	1.96	0.66
1:F:155:GLN:NE2	6:F:2119:HOH:O	2.28	0.65
1:A:3:ASN:ND2	1:A:5:GLU:H	1.95	0.65
1:B:101[B]:ASP:OD2	1:B:113:GLY:HA3	1.96	0.65
1:B:101[A]:ASP:HB3	1:B:159:VAL:CG1	2.27	0.65
1:F:99[A]:MET:HE2	1:F:200:GLY:HA2	1.79	0.64
1:A:155[A]:GLN:NE2	6:A:2101:HOH:O	2.30	0.63
1:A:43:ARG:HG2	1:E:100[A]:GLU:HG3	1.81	0.63
1:C:101[B]:ASP:OD2	1:C:113:GLY:HA3	1.99	0.63
1:G:203:GLY:H	5:G:1260:GLU:HB3	1.63	0.63
1:C:99[B]:MET:O	1:C:103[B]:ARG:HG2	1.99	0.62
1:A:104[B]:GLY:HA3	1:E:43:ARG:HH22	1.64	0.62
1:F:148:LEU:HD21	1:H:256:LYS:HG2	1.80	0.62
1:B:253:HIS:HD2	6:B:2089:HOH:O	1.82	0.62
1:D:40:ARG:HD3	2:D:400:NAP:C6A	2.29	0.62
1:D:210:GLU:HG3	1:D:214[B]:ARG:HD2	1.81	0.61
1:F:101[B]:ASP:OD2	1:F:113:GLY:HA3	1.99	0.61
1:C:203:GLY:H	5:C:1259:GLU:N	1.98	0.61
1:E:101[B]:ASP:OD2	1:E:113:GLY:HA3	2.00	0.61
1:G:98:ASN:HB3	1:G:100[B]:GLU:CG	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101[A]:ASP:HB3	1:B:159:VAL:HG11	1.83	0.60
1:H:15:ALA:O	1:H:47:GLU:HG2	2.01	0.59
1:D:60:ALA:HB1	1:D:62:LEU:HD11	1.83	0.59
1:A:103[A]:ARG:CZ	1:E:199:LYS:HE3	2.32	0.58
1:A:48:LEU:O	1:A:52:LEU:HD23	2.03	0.58
1:A:18[B]:ARG:CG	1:A:18[B]:ARG:HH11	2.08	0.58
1:D:42[B]:GLU:OE1	1:D:43:ARG:N	2.37	0.57
1:G:103[B]:ARG:NE	1:G:200:GLY:O	2.35	0.57
1:H:3:ASN:ND2	1:H:5:GLU:HG3	2.13	0.57
1:D:5:GLU:O	1:D:6:ASN:HB2	2.02	0.57
1:F:100[A]:GLU:HB2	6:F:2084:HOH:O	2.04	0.57
1:F:203:GLY:N	5:F:1257:GLU:HB2	2.15	0.57
1:E:18[A]:ARG:CD	6:E:2012:HOH:O	2.53	0.56
1:G:214:ARG:NH2	6:G:2139:HOH:O	2.35	0.56
1:E:101[A]:ASP:HB3	1:E:159:VAL:CG1	2.36	0.56
1:H:41:LYS:HG2	2:H:400:NAP:O2X	2.07	0.55
1:E:59:GLU:HG3	1:E:61:HIS:CE1	2.42	0.55
1:D:84:VAL:HG12	1:D:84:VAL:O	2.07	0.54
1:B:42[B]:GLU:OE1	6:B:2045:HOH:O	2.18	0.54
1:C:46:LYS:HE3	6:C:2034:HOH:O	2.07	0.54
1:C:101[A]:ASP:HB3	1:C:159:VAL:CG1	2.36	0.54
1:D:15:ALA:O	1:D:47:GLU:HG2	2.08	0.54
1:E:18[A]:ARG:HD3	6:E:2012:HOH:O	2.08	0.53
1:F:101[A]:ASP:HB3	1:F:159:VAL:CG1	2.39	0.53
1:D:194[A]:ARG:NH2	6:D:2096:HOH:O	2.13	0.53
1:F:99[A]:MET:HE3	1:F:200:GLY:HA2	1.89	0.53
1:E:148:LEU:HD21	1:G:256:LYS:HE3	1.91	0.53
1:G:99[B]:MET:HB2	1:G:100[B]:GLU:OE1	2.09	0.53
1:H:154:VAL:CG1	6:H:2089:HOH:O	2.56	0.53
1:A:64:GLN:HG2	6:A:2065:HOH:O	2.09	0.52
1:B:210:GLU:HG3	1:B:214:ARG:HD3	1.92	0.52
1:H:133:LYS:HE2	1:H:181:ASP:OD2	2.08	0.52
1:A:194:ARG:NH2	1:A:205:ASN:OD1	2.41	0.52
1:A:253:HIS:HD2	6:A:2052:HOH:O	1.92	0.52
1:B:256:LYS:HE3	1:D:148:LEU:HD21	1.91	0.52
1:F:203:GLY:H	5:F:1257:GLU:CB	2.16	0.52
1:G:3:ASN:OD1	1:G:5:GLU:HG3	2.10	0.51
1:B:196:LEU:O	1:B:199:LYS:HG2	2.11	0.51
1:D:103:ARG:NH2	1:D:200:GLY:O	2.44	0.50
1:G:16:ASN:HA	1:G:47:GLU:HG2	1.92	0.50
1:H:3:ASN:HD21	1:H:5:GLU:CG	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HD21	1:D:256:LYS:HG2	1.93	0.50
1:G:215:ALA:O	1:G:218:LYS:HD3	2.11	0.50
1:C:253:HIS:HD2	6:C:2048:HOH:O	1.94	0.49
1:D:41:LYS:HD3	1:D:43:ARG:HE	1.77	0.49
1:H:5:GLU:O	1:H:6:ASN:HB2	2.13	0.49
1:A:101[A]:ASP:HB3	1:A:159:VAL:CG1	2.42	0.49
1:A:103[A]:ARG:NH1	1:E:199:LYS:HE3	2.27	0.49
1:G:101[B]:ASP:CG	6:G:2073:HOH:O	2.40	0.49
1:A:100[A]:GLU:HB3	1:E:196:LEU:HD21	1.95	0.48
1:A:154:VAL:CG1	6:A:2146:HOH:O	2.61	0.48
1:E:18[A]:ARG:HD2	6:E:2012:HOH:O	2.14	0.48
1:H:103:ARG:NH2	1:H:200:GLY:O	2.47	0.48
1:F:101[A]:ASP:HB3	1:F:159:VAL:HG11	1.96	0.47
1:E:256:LYS:HE3	1:G:148:LEU:HD21	1.96	0.47
1:A:101[B]:ASP:CG	6:A:2092:HOH:O	2.49	0.47
1:F:196:LEU:O	1:F:199:LYS:HG2	2.14	0.47
1:H:154:VAL:HG13	6:H:2082:HOH:O	2.05	0.47
1:F:5:GLU:O	1:F:6:ASN:HB2	2.15	0.47
1:C:5:GLU:O	1:C:6:ASN:HB2	2.15	0.46
1:D:60:ALA:HB1	1:D:62:LEU:CD1	2.45	0.46
1:C:101[A]:ASP:HB3	1:C:159:VAL:HG11	1.97	0.46
1:A:133:LYS:HE2	1:A:181:ASP:OD2	2.16	0.45
1:A:3:ASN:HD21	1:A:5:GLU:H	1.64	0.45
1:B:101[A]:ASP:HB3	1:B:159:VAL:HG12	1.99	0.45
1:E:38:THR:HA	1:E:63:TYR:O	2.17	0.45
1:G:207:ILE:HD11	6:G:2111:HOH:O	2.16	0.45
1:E:5:GLU:O	1:E:6:ASN:HB2	2.17	0.44
1:A:148:LEU:HD21	1:C:256:LYS:HE3	1.98	0.44
1:D:39:TYR:HB2	1:D:44:SER:HB2	2.00	0.44
1:G:210:GLU:HG3	1:G:214:ARG:HD3	1.99	0.44
1:A:100[A]:GLU:HG3	1:E:43:ARG:HG2	1.98	0.44
1:A:18[B]:ARG:HD3	6:A:2017:HOH:O	2.18	0.44
1:A:157:TYR:CZ	1:A:160:MET:HG3	2.53	0.44
1:B:101[A]:ASP:O	1:B:159:VAL:HG12	2.18	0.43
1:G:87:ILE:O	1:G:136:MET:HG2	2.18	0.43
1:C:194[B]:ARG:CZ	6:C:2145:HOH:O	2.65	0.43
1:H:59:GLU:HG3	1:H:61:HIS:NE2	2.34	0.43
1:A:100[B]:GLU:HG2	1:A:100[B]:GLU:H	1.04	0.43
1:B:192:PRO:HG3	1:B:207:ILE:HG22	2.01	0.43
1:E:101[A]:ASP:HB3	1:E:159:VAL:HG11	1.99	0.43
1:C:59:GLU:HG3	1:C:61:HIS:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:TYR:CZ	1:B:153:ALA:HA	2.54	0.43
1:B:256:LYS:HD3	1:D:256:LYS:HD2	2.01	0.43
1:E:210:GLU:OE2	1:E:214[A]:ARG:HD3	2.19	0.43
1:E:256:LYS:HG2	1:G:148:LEU:HD21	2.00	0.43
1:F:256:LYS:HE3	1:H:148:LEU:HD21	2.00	0.43
1:A:100[B]:GLU:OE2	1:E:41:LYS:NZ	2.41	0.42
1:B:54:GLN:HG3	6:B:2052:HOH:O	2.18	0.42
1:F:196:LEU:HD12	1:F:196:LEU:HA	1.95	0.42
1:H:157:TYR:CZ	1:H:160:MET:HG3	2.54	0.42
1:E:236:ASP:OD2	1:H:228:LYS:HE2	2.20	0.42
1:G:173:TYR:CZ	1:H:153:ALA:HA	2.54	0.42
1:A:43:ARG:HH22	1:E:104[B]:GLY:HA3	1.83	0.42
1:A:3:ASN:ND2	1:A:3:ASN:C	2.73	0.42
1:C:192:PRO:HG3	1:C:207:ILE:HG22	2.01	0.42
1:B:207:ILE:HD11	6:B:2134:HOH:O	2.18	0.42
1:E:173:TYR:CZ	1:F:153:ALA:HA	2.54	0.42
1:C:173:TYR:CZ	1:D:153:ALA:HA	2.55	0.41
1:C:71[A]:GLU:HG2	1:C:75:ASN:ND2	2.35	0.41
1:G:38:THR:HA	1:G:63:TYR:O	2.20	0.41
1:G:5:GLU:O	1:G:6:ASN:HB2	2.21	0.41
1:A:256:LYS:HE3	1:C:148:LEU:HD21	2.02	0.41
1:F:38:THR:HA	1:F:63:TYR:O	2.21	0.41
1:D:194[A]:ARG:NE	6:D:2096:HOH:O	2.50	0.41
1:A:256:LYS:HG2	1:C:148:LEU:HD21	2.02	0.41
1:D:210:GLU:CG	1:D:214[B]:ARG:HD2	2.51	0.41
1:A:192:PRO:HG3	1:A:207:ILE:HG22	2.03	0.40
1:B:39:TYR:CE2	1:B:45[A]:ARG:HB2	2.55	0.40
1:C:157:TYR:CZ	1:C:160:MET:HG3	2.56	0.40
1:F:18:ARG:HH12	1:F:199:LYS:NZ	2.19	0.40
1:D:57:GLN:HA	1:D:58:PRO:HD3	1.99	0.40
1:F:157:TYR:CZ	1:F:160:MET:HG3	2.57	0.40
1:A:5:GLU:O	1:A:6:ASN:HB2	2.22	0.40
1:F:99[B]:MET:HE3	1:F:103[B]:ARG:CG	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:GLU:OE2	6:A:2072:HOH:O[1_565]	2.04	0.16



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	264/282 (94%)	255 (97%)	9 (3%)	0	100	100
1	B	264/282 (94%)	253 (96%)	11 (4%)	0	100	100
1	C	264/282 (94%)	257 (97%)	7 (3%)	0	100	100
1	D	258/282 (92%)	247 (96%)	11 (4%)	0	100	100
1	E	265/282 (94%)	255 (96%)	10 (4%)	0	100	100
1	F	263/282 (93%)	253 (96%)	10 (4%)	0	100	100
1	G	265/282 (94%)	257 (97%)	8 (3%)	0	100	100
1	H	255/282 (90%)	242 (95%)	11 (4%)	2 (1%)	19	7
All	All	2098/2256 (93%)	2019 (96%)	77 (4%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	45	ARG
1	H	46	LYS

### 5.3.2 Protein sidechains

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	218/234 (93%)	213 (98%)	5 (2%)	50	37
1	B	218/234 (93%)	213 (98%)	5 (2%)	50	37
1	C	218/234 (93%)	214 (98%)	4 (2%)	59	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	213/234 (91%)	206 (97%)	7 (3%)	38	23
1	E	219/234 (94%)	214 (98%)	5 (2%)	50	37
1	F	217/234 (93%)	212 (98%)	5 (2%)	50	37
1	G	219/234 (94%)	211 (96%)	8 (4%)	34	19
1	H	210/234 (90%)	207 (99%)	3 (1%)	67	59
All	All	1732/1872 (92%)	1690 (98%)	42 (2%)	55	36

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	100[A]	GLU
1	A	100[B]	GLU
1	A	155[A]	GLN
1	A	155[B]	GLN
1	B	4	LEU
1	B	55	LEU
1	B	112	GLU
1	B	138	GLU
1	B	255	ILE
1	C	55	LEU
1	C	100[A]	GLU
1	C	100[B]	GLU
1	C	216	PRO
1	D	4	LEU
1	D	30	GLN
1	D	46	LYS
1	D	50	LYS
1	D	121	SER
1	D	194[A]	ARG
1	D	194[B]	ARG
1	E	100[A]	GLU
1	E	100[B]	GLU
1	E	103[A]	ARG
1	E	103[B]	ARG
1	E	216	PRO
1	F	4	LEU
1	F	99[A]	MET
1	F	99[B]	MET
1	F	100[A]	GLU

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Mol	Chain	Res	Type
1	F	100[B]	GLU
1	G	30	GLN
1	G	55	LEU
1	G	82	LYS
1	G	100[A]	GLU
1	G	100[B]	GLU
1	G	112	GLU
1	G	216	PRO
1	G	255	ILE
1	H	4	LEU
1	H	30	GLN
1	H	99	MET

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
1	A	253	HIS
1	B	54	GLN
1	B	253	HIS
1	C	253	HIS
1	F	253	HIS
1	H	3	ASN
1	H	68	GLN
1	H	155	GLN
1	H	253	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GLU	B	1258	-	2,9,9	0.34	0	2,11,11	1.61	1 (50%)
5	GLU	G	1260	-	2,9,9	0.32	0	2,11,11	1.48	1 (50%)
4	JA3	E	1258	-	19,19,19	0.68	1 (5%)	23,26,26	0.93	2 (8%)
2	NAP	H	400	-	45,52,52	1.56	5 (11%)	56,80,80	2.08	13 (23%)
4	JA3	C	1257	-	19,19,19	0.44	0	23,26,26	1.09	1 (4%)
4	JA3	G	1258	-	19,19,19	0.65	1 (5%)	23,26,26	1.06	3 (13%)
5	GLU	C	1259	-	2,9,9	0.33	0	2,11,11	1.59	1 (50%)
5	GLU	H	1259	-	2,9,9	0.36	0	2,11,11	2.79	1 (50%)
4	JA3	A	1259	-	19,19,19	0.45	0	23,26,26	1.00	2 (8%)
2	NAP	B	400	-	45,52,52	1.63	6 (13%)	56,80,80	1.90	12 (21%)
2	NAP	C	400	-	45,52,52	1.56	7 (15%)	56,80,80	1.70	8 (14%)
4	JA3	E	1257	-	19,19,19	0.41	0	23,26,26	1.49	2 (8%)
2	NAP	E	400	-	45,52,52	1.57	5 (11%)	56,80,80	1.74	7 (12%)
3	MRD	B	1259	-	7,7,7	0.63	0	9,10,10	1.17	1 (11%)
3	MRD	A	1257	-	7,7,7	0.78	0	9,10,10	1.25	1 (11%)
3	MRD	F	1258	-	7,7,7	0.65	0	9,10,10	0.92	1 (11%)
2	NAP	A	400	-	45,52,52	1.53	5 (11%)	56,80,80	2.14	9 (16%)
5	GLU	E	1259	-	2,9,9	0.40	0	2,11,11	1.23	0
3	MRD	E	1260	-	7,7,7	0.69	0	9,10,10	0.85	1 (11%)
3	MRD	C	1260	-	7,7,7	0.58	0	9,10,10	0.81	0
4	JA3	C	1258	-	19,19,19	0.37	0	23,26,26	1.18	3 (13%)
2	NAP	D	400	-	45,52,52	1.60	3 (6%)	56,80,80	1.50	9 (16%)
5	GLU	F	1257	-	2,9,9	0.35	0	2,11,11	1.48	1 (50%)
3	MRD	G	1259	-	7,7,7	0.62	0	9,10,10	0.81	1 (11%)
3	MRD	H	1257	-	7,7,7	0.72	0	9,10,10	1.30	1 (11%)
3	MRD	G	1261	-	7,7,7	0.51	0	9,10,10	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	JA3	B	1257	-	19,19,19	0.51	0	23,26,26	1.19	2 (8%)
2	NAP	F	400	-	45,52,52	1.48	6 (13%)	56,80,80	1.86	12 (21%)
4	JA3	G	1257	-	19,19,19	0.49	0	23,26,26	1.47	2 (8%)
2	NAP	G	400	-	45,52,52	1.50	5 (11%)	56,80,80	1.85	9 (16%)

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
5	GLU	B	1258	-	-	1/3/9/9	-
5	GLU	G	1260	-	-	2/3/9/9	-
4	JA3	E	1258	-	-	0/6/6/6	0/2/2/2
2	NAP	H	400	-	-	6/31/67/67	0/5/5/5
4	JA3	C	1257	-	-	0/6/6/6	0/2/2/2
4	JA3	G	1258	-	-	0/6/6/6	0/2/2/2
5	GLU	C	1259	-	-	1/3/9/9	-
5	GLU	H	1259	-	-	2/3/9/9	-
4	JA3	A	1259	-	-	0/6/6/6	0/2/2/2
2	NAP	B	400	-	-	6/31/67/67	0/5/5/5
2	NAP	C	400	-	-	5/31/67/67	0/5/5/5
4	JA3	E	1257	-	-	0/6/6/6	0/2/2/2
2	NAP	E	400	-	-	7/31/67/67	0/5/5/5
3	MRD	B	1259	-	-	0/5/5/5	-
3	MRD	A	1257	-	-	0/5/5/5	-
3	MRD	F	1258	-	-	0/5/5/5	-
2	NAP	A	400	-	-	6/31/67/67	0/5/5/5
5	GLU	E	1259	-	-	3/3/9/9	-
3	MRD	E	1260	-	-	0/5/5/5	-
3	MRD	C	1260	-	-	0/5/5/5	-
4	JA3	C	1258	-	-	0/6/6/6	0/2/2/2
2	NAP	D	400	-	-	7/31/67/67	0/5/5/5
5	GLU	F	1257	-	-	2/3/9/9	-
3	MRD	G	1259	-	-	0/5/5/5	-
3	MRD	H	1257	-	-	0/5/5/5	-
3	MRD	G	1261	-	-	0/5/5/5	-
4	JA3	B	1257	-	-	0/6/6/6	0/2/2/2
2	NAP	F	400	-	-	5/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	JA3	G	1257	-	-	0/6/6/6	0/2/2/2
2	NAP	G	400	-	-	8/31/67/67	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	NAP	O7N-C7N	7.82	1.39	1.24
2	C	400	NAP	O7N-C7N	6.95	1.37	1.24
2	H	400	NAP	O7N-C7N	6.76	1.37	1.24
2	B	400	NAP	O7N-C7N	6.53	1.36	1.24
2	G	400	NAP	O7N-C7N	6.43	1.36	1.24
2	E	400	NAP	O7N-C7N	6.39	1.36	1.24
2	A	400	NAP	O7N-C7N	6.36	1.36	1.24
2	F	400	NAP	O7N-C7N	5.02	1.33	1.24
2	E	400	NAP	C2A-N3A	4.33	1.39	1.32
2	B	400	NAP	C2A-N3A	4.15	1.38	1.32
2	D	400	NAP	C2A-N3A	4.13	1.38	1.32
2	F	400	NAP	C2N-N1N	3.80	1.39	1.35
2	H	400	NAP	C2A-N3A	3.75	1.38	1.32
2	A	400	NAP	C2A-N3A	3.63	1.38	1.32
2	H	400	NAP	P2B-O2B	3.52	1.66	1.59
2	G	400	NAP	P2B-O2B	3.38	1.65	1.59
2	E	400	NAP	C2N-N1N	3.35	1.39	1.35
2	G	400	NAP	C2A-N3A	3.31	1.37	1.32
2	C	400	NAP	C2A-N3A	3.28	1.37	1.32
2	B	400	NAP	P2B-O2B	3.26	1.65	1.59
2	F	400	NAP	C2A-N3A	3.24	1.37	1.32
2	F	400	NAP	P2B-O2B	3.12	1.65	1.59
2	B	400	NAP	C2N-N1N	3.06	1.38	1.35
2	E	400	NAP	P2B-O2B	2.97	1.64	1.59
2	C	400	NAP	P2B-O2B	2.80	1.64	1.59
2	B	400	NAP	C2A-N1A	2.48	1.38	1.33
2	F	400	NAP	C2A-N1A	2.43	1.38	1.33
2	G	400	NAP	C2A-N1A	2.42	1.38	1.33
2	H	400	NAP	C2A-N1A	2.36	1.38	1.33
2	D	400	NAP	C2A-N1A	2.33	1.38	1.33
2	A	400	NAP	P2B-O2B	2.32	1.63	1.59
2	G	400	NAP	C2N-N1N	2.30	1.37	1.35
4	G	1258	JA3	C2-C6	-2.29	1.36	1.40
2	C	400	NAP	C2N-N1N	2.26	1.37	1.35
2	C	400	NAP	O4B-C4B	-2.26	1.39	1.45
2	A	400	NAP	C2A-N1A	2.24	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	NAP	C2A-N1A	2.20	1.38	1.33
2	H	400	NAP	C2N-N1N	2.17	1.37	1.35
2	B	400	NAP	PN-O2N	-2.16	1.45	1.55
2	A	400	NAP	C2N-N1N	-2.09	1.32	1.35
4	E	1258	JA3	C2-C6	-2.08	1.37	1.40
2	C	400	NAP	PN-O2N	-2.06	1.45	1.55
2	F	400	NAP	PN-O2N	-2.06	1.45	1.55
2	C	400	NAP	C2A-N1A	2.00	1.37	1.33

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NAP	C3N-C7N-N7N	8.58	128.04	117.75
2	A	400	NAP	O7N-C7N-C3N	-7.54	110.61	119.63
2	G	400	NAP	C3N-C7N-N7N	7.03	126.18	117.75
2	G	400	NAP	N3A-C2A-N1A	-6.89	117.91	128.68
2	H	400	NAP	N3A-C2A-N1A	-6.87	117.95	128.68
2	H	400	NAP	C3N-C7N-N7N	6.71	125.80	117.75
2	B	400	NAP	C3N-C7N-N7N	6.63	125.70	117.75
2	F	400	NAP	C3N-C7N-N7N	6.27	125.27	117.75
2	C	400	NAP	N3A-C2A-N1A	-6.08	119.17	128.68
4	G	1257	JA3	O1-C2-C6	-5.78	114.81	119.89
2	E	400	NAP	C3N-C7N-N7N	5.74	124.64	117.75
2	C	400	NAP	C3N-C7N-N7N	5.46	124.30	117.75
2	H	400	NAP	O7N-C7N-C3N	-5.45	113.11	119.63
2	E	400	NAP	N3A-C2A-N1A	-5.43	120.19	128.68
2	A	400	NAP	N3A-C2A-N1A	-5.42	120.20	128.68
2	B	400	NAP	O7N-C7N-C3N	-5.11	113.52	119.63
2	F	400	NAP	N3A-C2A-N1A	-4.94	120.95	128.68
4	E	1257	JA3	O1-C2-C6	-4.67	115.78	119.89
2	D	400	NAP	C3N-C7N-N7N	4.60	123.27	117.75
2	B	400	NAP	C6N-N1N-C2N	-4.40	117.96	121.97
2	E	400	NAP	O7N-C7N-C3N	-4.37	114.41	119.63
2	F	400	NAP	C2N-C3N-C4N	4.24	123.07	118.26
2	E	400	NAP	C2N-C3N-C4N	4.13	122.94	118.26
4	E	1257	JA3	C3-C2-C6	4.08	121.52	118.11
2	F	400	NAP	O2N-PN-O1N	4.06	132.30	112.24
2	B	400	NAP	C2N-C3N-C4N	4.03	122.83	118.26
2	H	400	NAP	C2N-C3N-C4N	3.91	122.69	118.26
2	D	400	NAP	N3A-C2A-N1A	-3.82	122.71	128.68
5	H	1259	GLU	CB-CG-CD	-3.81	105.41	113.59
4	C	1257	JA3	O1-C2-C6	-3.72	116.62	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NAP	N3A-C2A-N1A	-3.72	122.87	128.68
2	A	400	NAP	C5N-C6N-N1N	3.50	125.42	120.40
2	C	400	NAP	O7N-C7N-N7N	-3.49	117.63	122.58
4	B	1257	JA3	C3-C2-C6	3.45	120.99	118.11
2	G	400	NAP	O7N-C7N-C3N	-3.44	115.52	119.63
2	A	400	NAP	C6N-C5N-C4N	-3.41	114.49	119.44
2	F	400	NAP	C6N-N1N-C2N	-3.39	118.89	121.97
2	F	400	NAP	O7N-C7N-N7N	-3.36	117.81	122.58
2	H	400	NAP	O2N-PN-O1N	3.35	128.82	112.24
2	D	400	NAP	O4B-C1B-C2B	-3.32	100.82	106.59
3	B	1259	MRD	CM-C2-C1	-3.28	103.74	110.57
2	G	400	NAP	C2A-N1A-C6A	3.27	124.35	118.75
2	H	400	NAP	O3X-P2B-O2X	3.25	120.06	107.64
2	A	400	NAP	O4D-C1D-C2D	-3.25	102.18	106.93
4	C	1258	JA3	C3-C2-C6	3.24	120.82	118.11
2	E	400	NAP	C3N-C2N-N1N	-3.16	117.34	120.43
2	H	400	NAP	C1B-N9A-C4A	-3.07	121.25	126.64
4	B	1257	JA3	O1-C2-C6	-3.06	117.20	119.89
2	A	400	NAP	O4B-C1B-C2B	-3.05	101.29	106.59
3	H	1257	MRD	CM-C2-C1	-3.04	104.23	110.57
2	G	400	NAP	O7N-C7N-N7N	-3.02	118.28	122.58
2	C	400	NAP	O4B-C1B-C2B	-3.02	101.34	106.59
2	H	400	NAP	O3X-P2B-O1X	-2.97	99.06	110.68
2	B	400	NAP	C4A-C5A-N7A	-2.95	106.32	109.40
2	B	400	NAP	O2N-PN-O1N	2.94	126.79	112.24
2	D	400	NAP	O7N-C7N-C3N	-2.94	116.12	119.63
2	G	400	NAP	O4B-C1B-C2B	-2.91	101.53	106.59
2	F	400	NAP	C4A-C5A-N7A	-2.87	106.41	109.40
4	C	1258	JA3	O1-C2-C6	-2.82	117.41	119.89
3	A	1257	MRD	CM-C2-C1	-2.79	104.75	110.57
2	F	400	NAP	O7N-C7N-C3N	-2.79	116.30	119.63
2	G	400	NAP	O3X-P2B-O2X	2.66	117.82	107.64
2	A	400	NAP	C2A-N1A-C6A	2.66	123.31	118.75
2	D	400	NAP	O2N-PN-O1N	2.65	125.33	112.24
4	E	1258	JA3	O1-C2-C6	-2.61	117.59	119.89
2	H	400	NAP	O4B-C1B-C2B	-2.59	102.10	106.59
4	G	1258	JA3	C3-C2-C6	2.58	120.27	118.11
2	F	400	NAP	C3N-C2N-N1N	-2.50	117.98	120.43
2	C	400	NAP	C2A-N1A-C6A	2.50	123.03	118.75
2	H	400	NAP	C2A-N1A-C6A	2.48	122.99	118.75
4	G	1257	JA3	C3-C2-C6	2.47	120.17	118.11
2	B	400	NAP	C5N-C6N-N1N	2.45	123.92	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	NAP	C5N-C6N-N1N	2.45	123.92	120.40
2	B	400	NAP	C1B-N9A-C4A	-2.45	122.34	126.64
4	A	1259	JA3	C3-C2-C6	2.41	120.12	118.11
3	F	1258	MRD	CM-C2-C1	-2.40	105.56	110.57
2	G	400	NAP	C1B-N9A-C4A	-2.36	122.50	126.64
2	H	400	NAP	C3N-C2N-N1N	-2.35	118.13	120.43
4	C	1258	JA3	F-C6-N	2.34	121.00	115.21
2	C	400	NAP	O2A-PA-O1A	2.27	123.44	112.24
5	C	1259	GLU	CB-CG-CD	-2.25	108.75	113.59
3	E	1260	MRD	CM-C2-C1	-2.20	105.98	110.57
2	H	400	NAP	C5N-C4N-C3N	-2.20	117.74	120.34
2	F	400	NAP	O4D-C1D-C2D	-2.19	103.73	106.93
2	C	400	NAP	C2N-C3N-C4N	2.18	120.72	118.26
2	D	400	NAP	C1B-N9A-C4A	-2.17	122.83	126.64
2	G	400	NAP	C2N-C3N-C4N	2.17	120.71	118.26
2	B	400	NAP	C5N-C4N-C3N	-2.16	117.79	120.34
2	B	400	NAP	O2A-PA-O1A	2.14	122.82	112.24
2	C	400	NAP	C3D-C2D-C1D	-2.13	97.77	100.98
2	D	400	NAP	O2X-P2B-O1X	2.13	119.00	110.68
2	E	400	NAP	O4B-C1B-C2B	-2.10	102.95	106.59
2	B	400	NAP	O3X-P2B-O2X	2.09	115.64	107.64
5	G	1260	GLU	CB-CG-CD	-2.08	109.12	113.59
4	G	1258	JA3	F-C6-N	2.08	120.36	115.21
2	E	400	NAP	O2N-PN-O1N	2.07	122.47	112.24
2	F	400	NAP	C1B-N9A-C4A	-2.05	123.03	126.64
4	E	1258	JA3	C3-C2-C6	2.04	119.82	118.11
3	G	1259	MRD	CM-C2-C1	-2.04	106.31	110.57
5	F	1257	GLU	CB-CG-CD	-2.04	109.21	113.59
2	A	400	NAP	O2N-PN-O1N	2.04	122.30	112.24
4	G	1258	JA3	O1-C2-C6	-2.03	118.10	119.89
5	B	1258	GLU	CB-CG-CD	-2.03	109.22	113.59
2	H	400	NAP	O2A-PA-O1A	2.03	122.28	112.24
2	D	400	NAP	C5N-C4N-C3N	-2.03	117.95	120.34
4	A	1259	JA3	O1-C2-C6	-2.00	118.13	119.89
2	D	400	NAP	N6A-C6A-N1A	2.00	122.73	118.57

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1258	GLU	CA-CB-CG-CD
5	G	1260	GLU	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
5	G	1260	GLU	C-CA-CB-CG
2	H	400	NAP	PN-O3-PA-O5B
2	H	400	NAP	C5D-O5D-PN-O1N
2	H	400	NAP	O4D-C1D-N1N-C2N
5	C	1259	GLU	CA-CB-CG-CD
5	H	1259	GLU	C-CA-CB-CG
2	B	400	NAP	PN-O3-PA-O5B
2	B	400	NAP	C5D-O5D-PN-O1N
2	B	400	NAP	C5D-O5D-PN-O2N
2	B	400	NAP	O4D-C1D-N1N-C2N
2	C	400	NAP	C5D-O5D-PN-O1N
2	C	400	NAP	C5D-O5D-PN-O2N
2	C	400	NAP	O4D-C1D-N1N-C2N
2	E	400	NAP	PN-O3-PA-O5B
2	E	400	NAP	C5D-O5D-PN-O1N
2	E	400	NAP	C5D-O5D-PN-O2N
2	E	400	NAP	O4D-C1D-N1N-C2N
2	A	400	NAP	C5D-O5D-PN-O1N
2	A	400	NAP	C5D-O5D-PN-O2N
2	A	400	NAP	O4D-C1D-N1N-C2N
5	E	1259	GLU	N-CA-CB-CG
5	E	1259	GLU	C-CA-CB-CG
2	D	400	NAP	PN-O3-PA-O5B
2	D	400	NAP	C5D-O5D-PN-O1N
2	D	400	NAP	C5D-O5D-PN-O2N
2	D	400	NAP	O4D-C1D-N1N-C2N
5	F	1257	GLU	N-CA-CB-CG
5	F	1257	GLU	C-CA-CB-CG
2	F	400	NAP	C5D-O5D-PN-O1N
2	F	400	NAP	O4D-C1D-N1N-C2N
2	G	400	NAP	C5D-O5D-PN-O1N
2	G	400	NAP	C5D-O5D-PN-O2N
2	G	400	NAP	O4D-C1D-N1N-C2N
2	G	400	NAP	O4D-C1D-N1N-C6N
5	E	1259	GLU	CA-CB-CG-CD
2	A	400	NAP	PN-O3-PA-O5B
2	G	400	NAP	PN-O3-PA-O5B
2	D	400	NAP	C2B-O2B-P2B-O3X
2	D	400	NAP	C5D-O5D-PN-O3
2	H	400	NAP	C5D-O5D-PN-O2N
2	F	400	NAP	C5D-O5D-PN-O2N
5	H	1259	GLU	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	H	400	NAP	O4B-C4B-C5B-O5B
2	H	400	NAP	C5D-O5D-PN-O3
2	B	400	NAP	C5D-O5D-PN-O3
2	C	400	NAP	C5D-O5D-PN-O3
2	E	400	NAP	C2B-O2B-P2B-O3X
2	E	400	NAP	C5D-O5D-PN-O3
2	A	400	NAP	C5D-O5D-PN-O3
2	F	400	NAP	C5D-O5D-PN-O3
2	G	400	NAP	C5D-O5D-PN-O3
2	B	400	NAP	O4B-C4B-C5B-O5B
2	C	400	NAP	O4B-C4B-C5B-O5B
2	G	400	NAP	C5B-O5B-PA-O2A
2	E	400	NAP	O4B-C4B-C5B-O5B
2	A	400	NAP	O4B-C4B-C5B-O5B
2	D	400	NAP	O4B-C4B-C5B-O5B
2	F	400	NAP	O4B-C4B-C5B-O5B
2	G	400	NAP	O4B-C4B-C5B-O5B

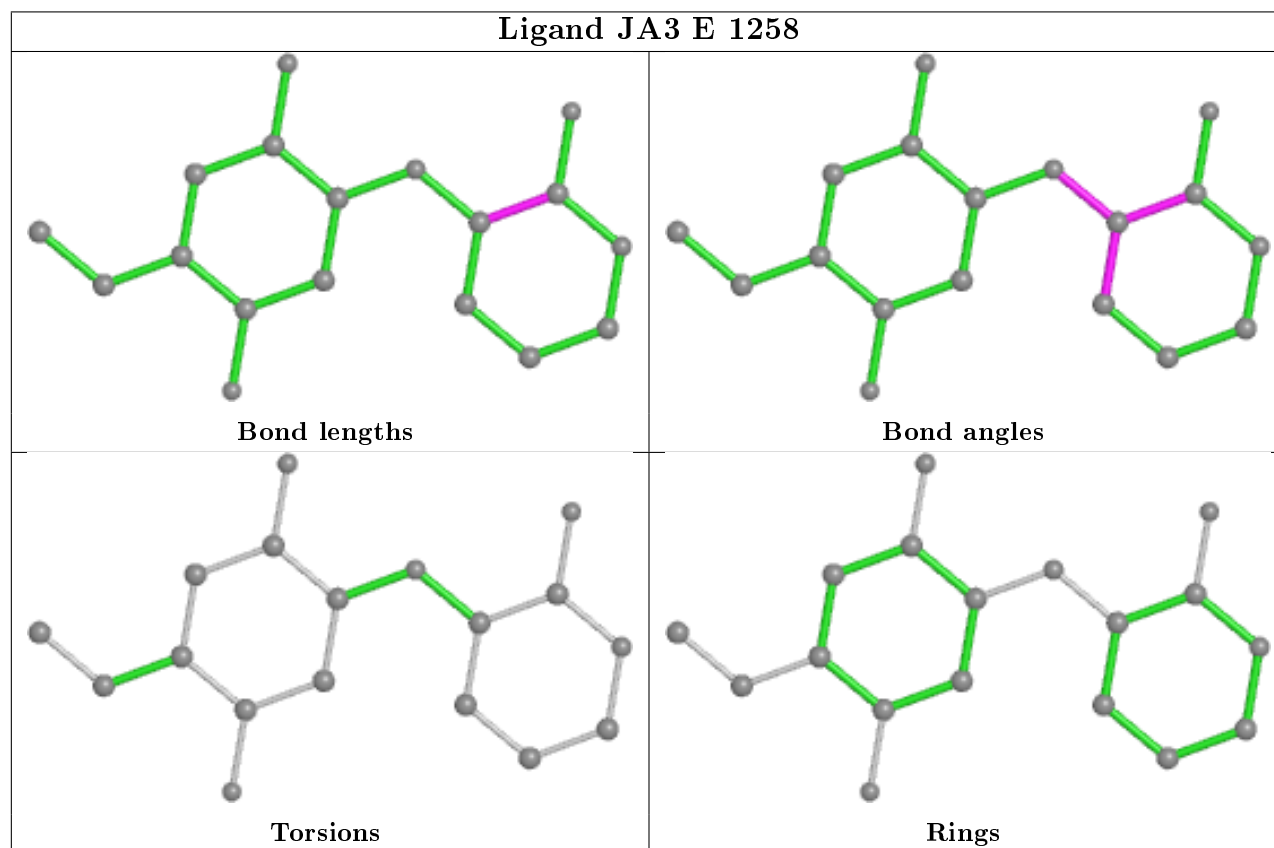
There are no ring outliers.

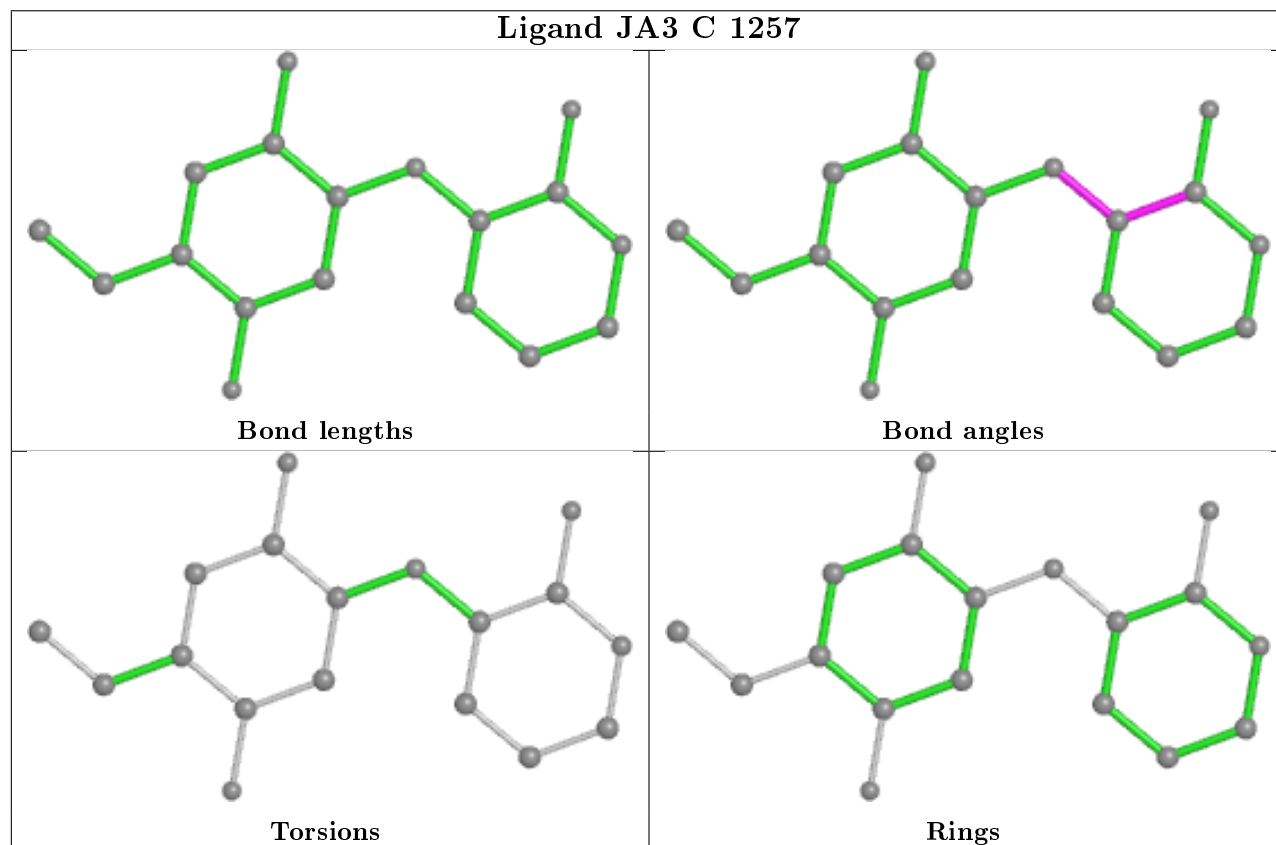
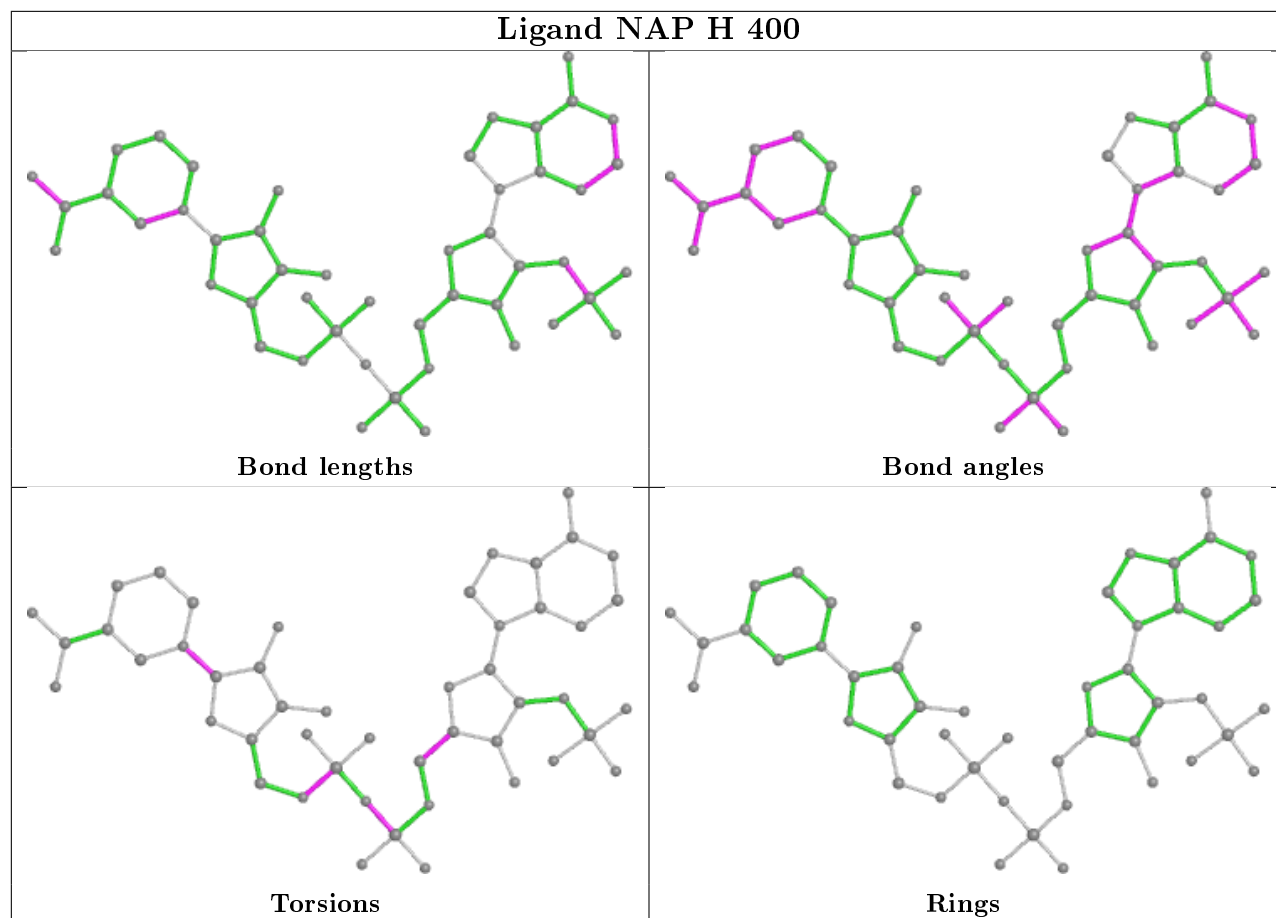
11 monomers are involved in 14 short contacts:

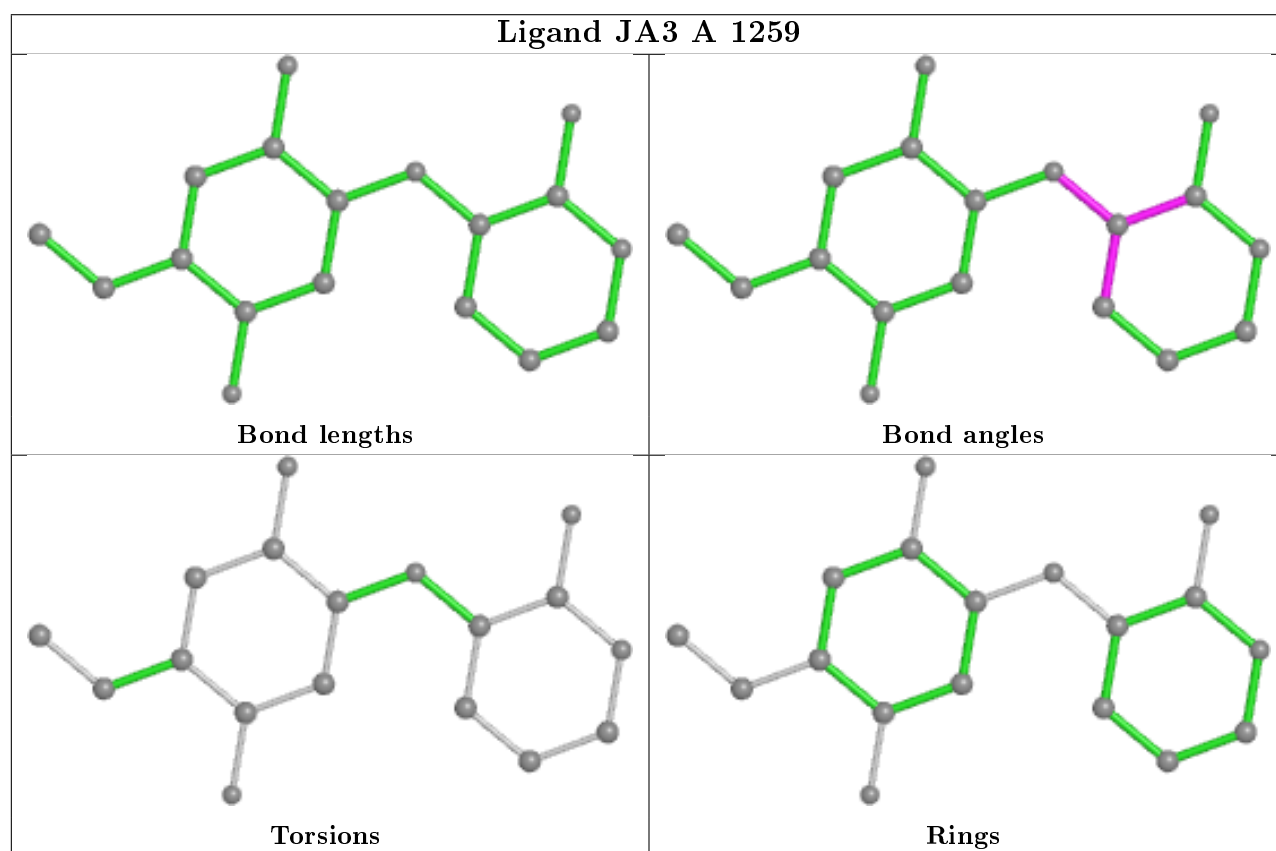
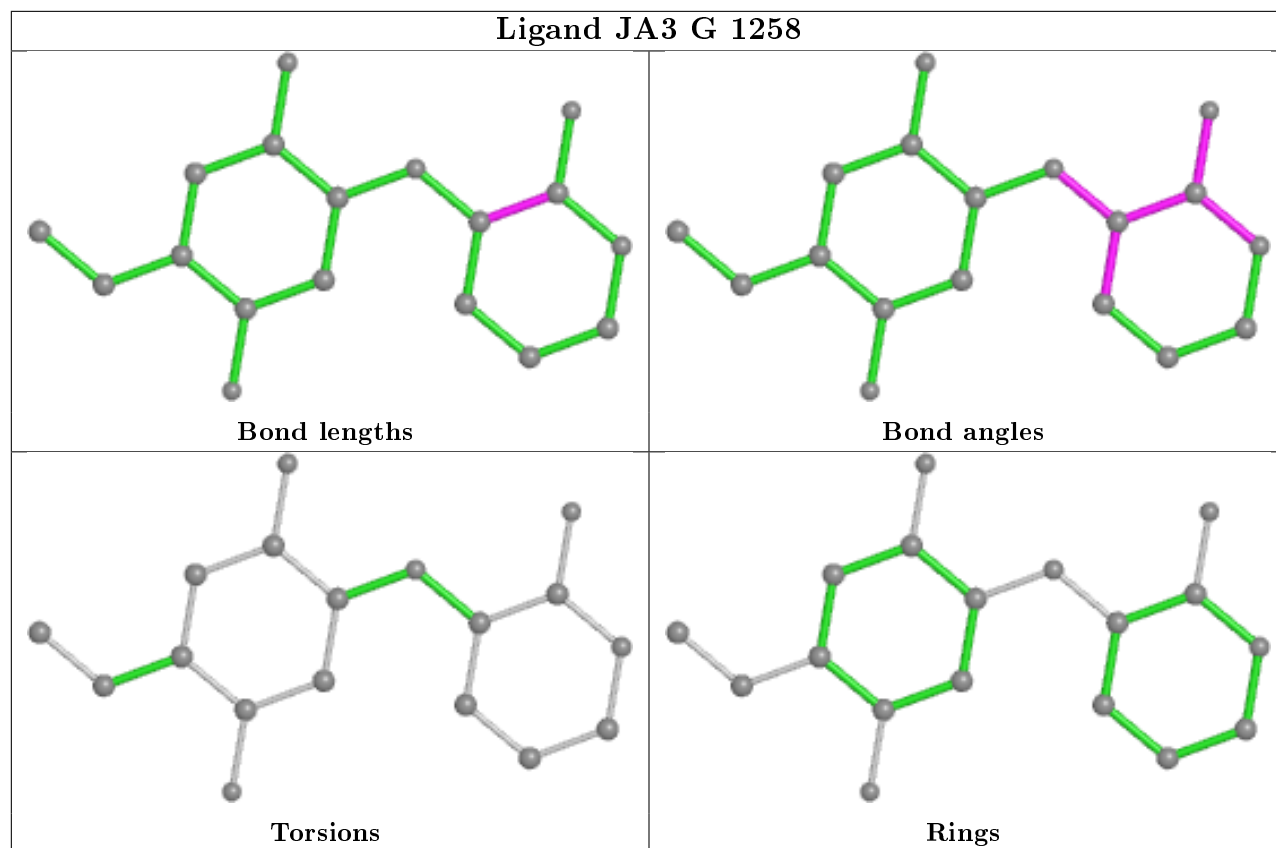
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1260	GLU	2	0
2	H	400	NAP	1	0
5	C	1259	GLU	1	0
3	B	1259	MRD	1	0
3	F	1258	MRD	1	0
3	C	1260	MRD	1	0
2	D	400	NAP	1	0
5	F	1257	GLU	3	0
3	G	1259	MRD	1	0
3	H	1257	MRD	1	0
3	G	1261	MRD	1	0

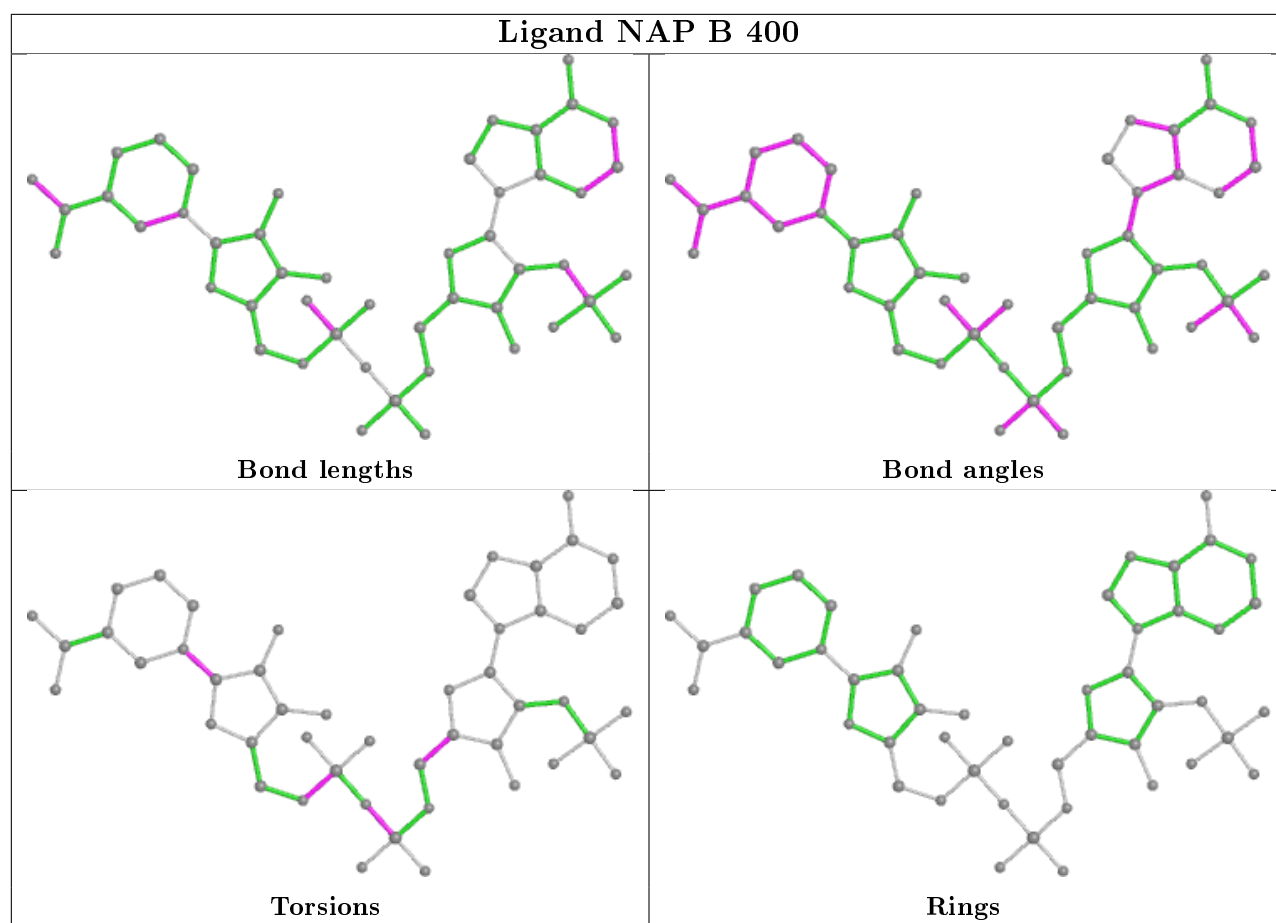
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

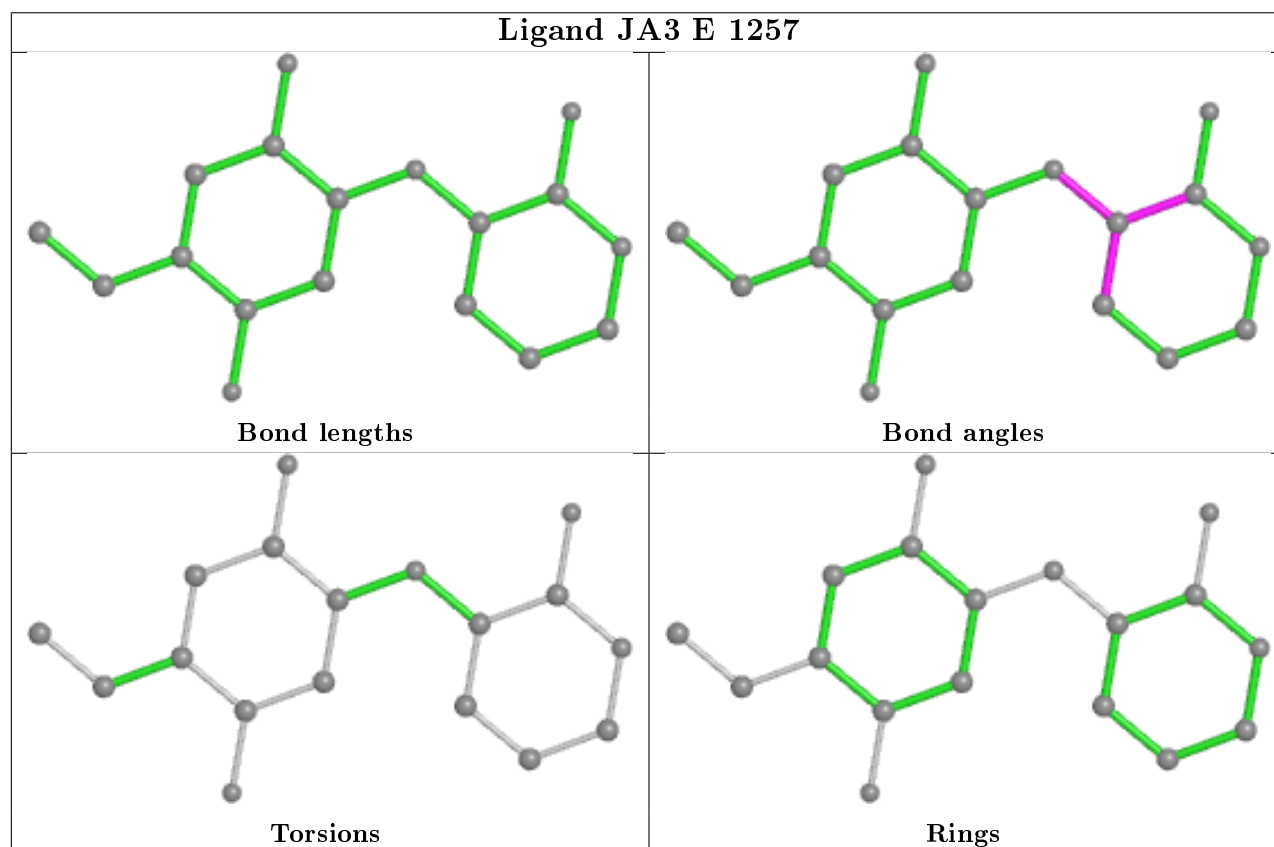
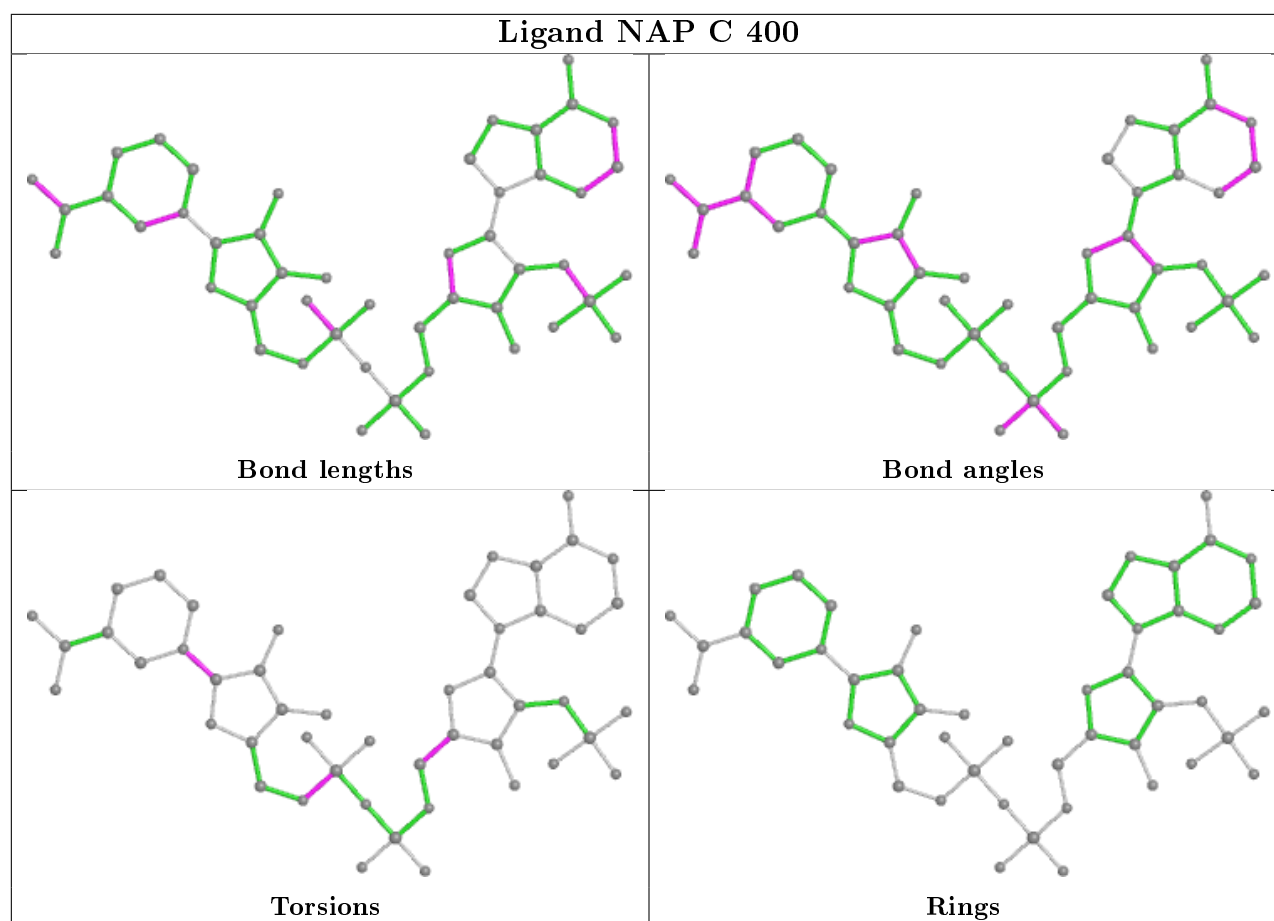
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



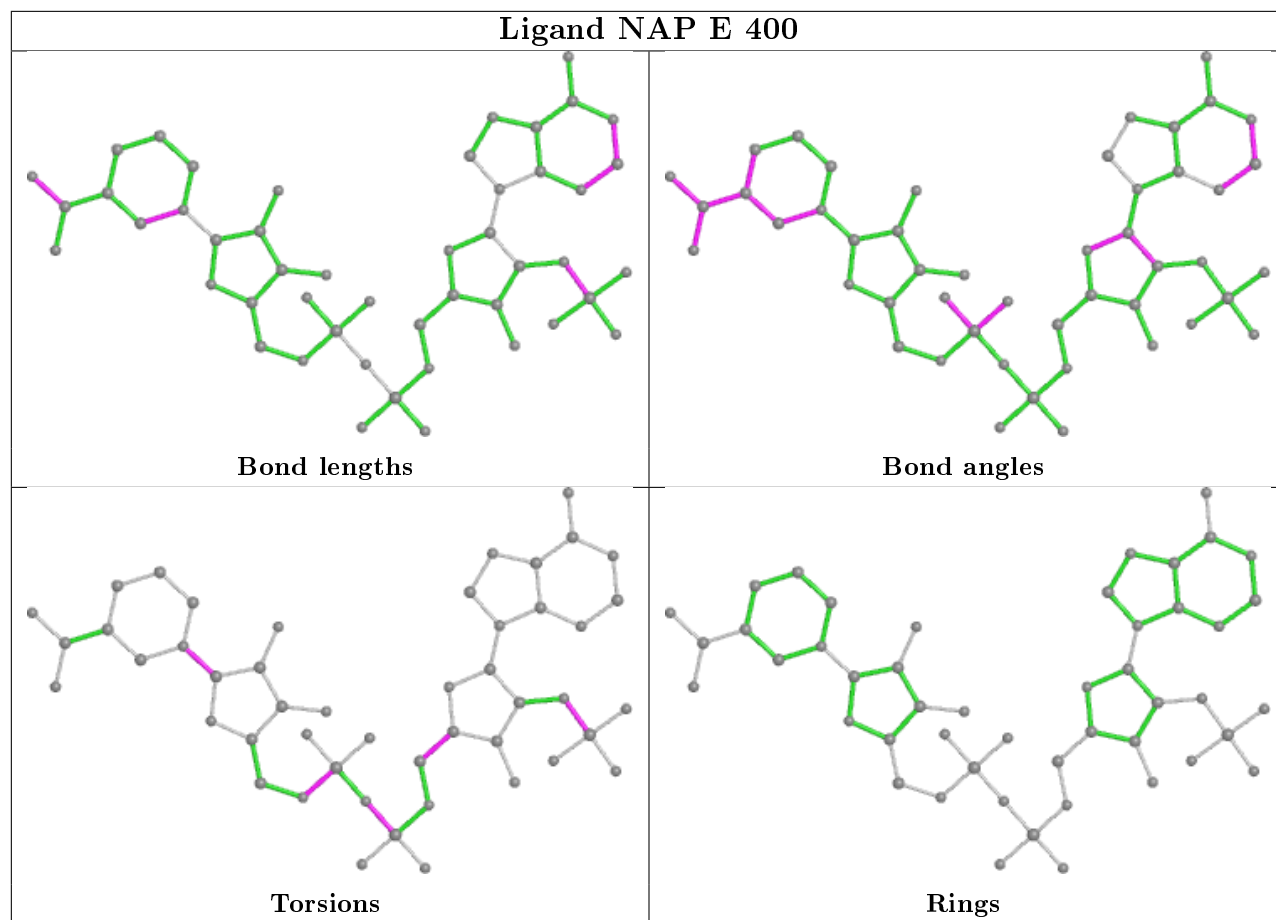


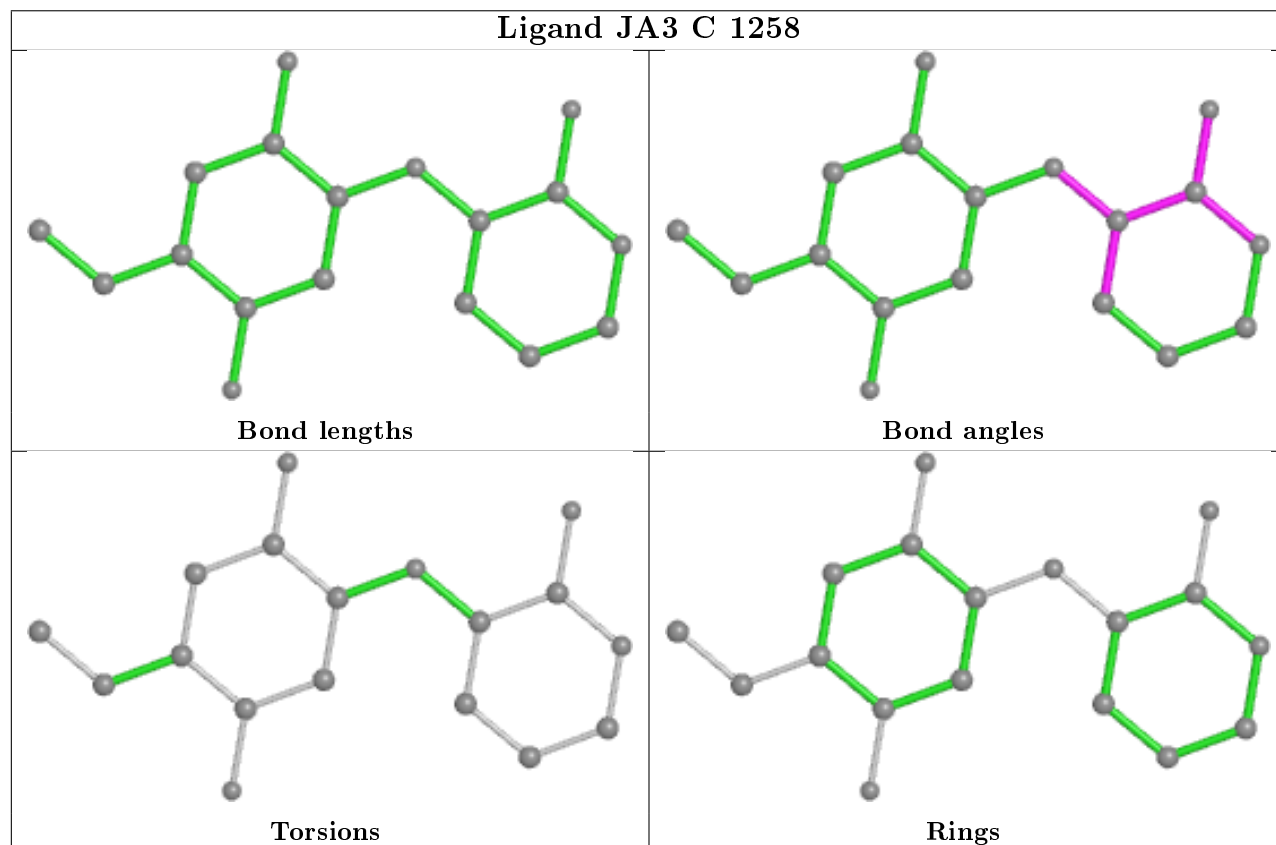
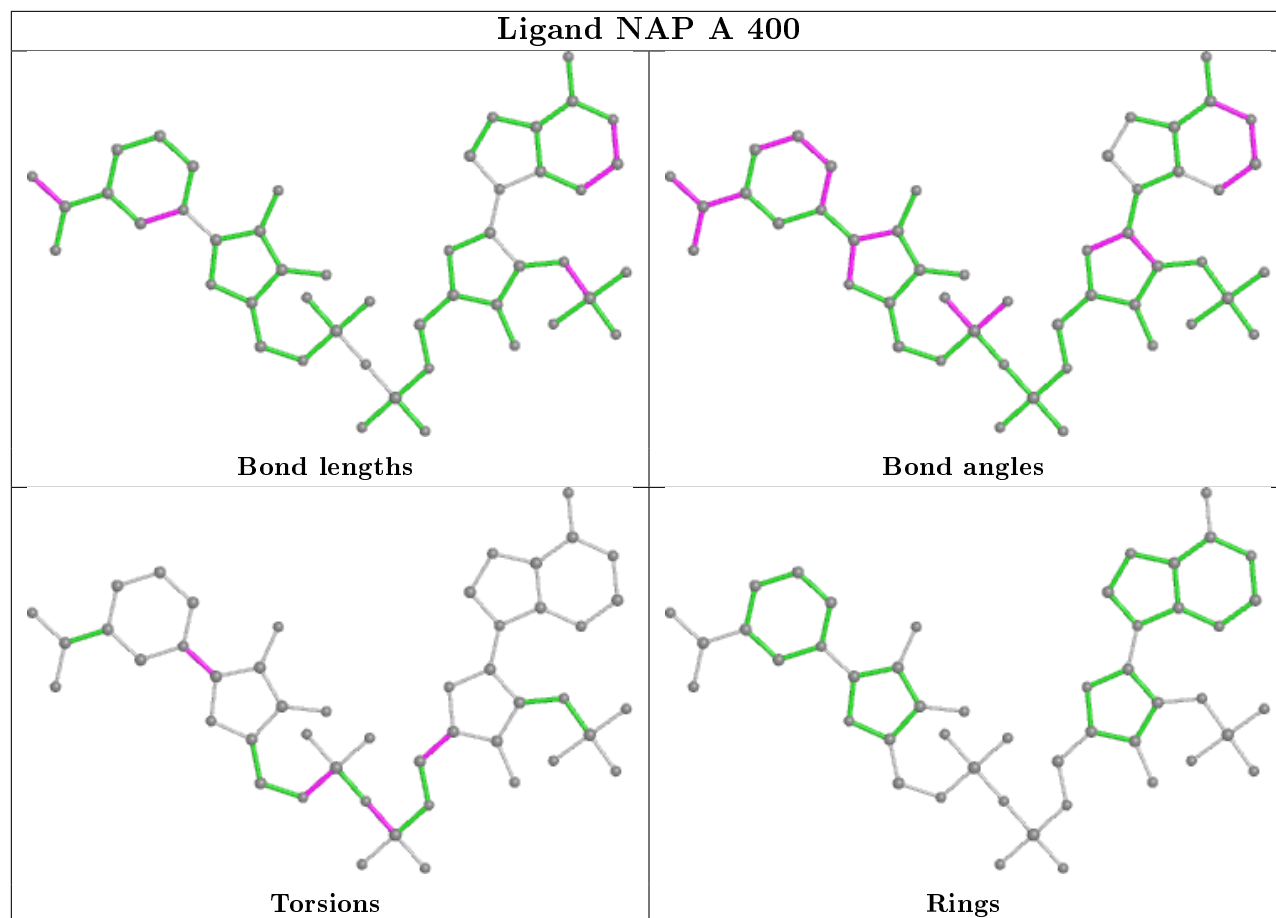


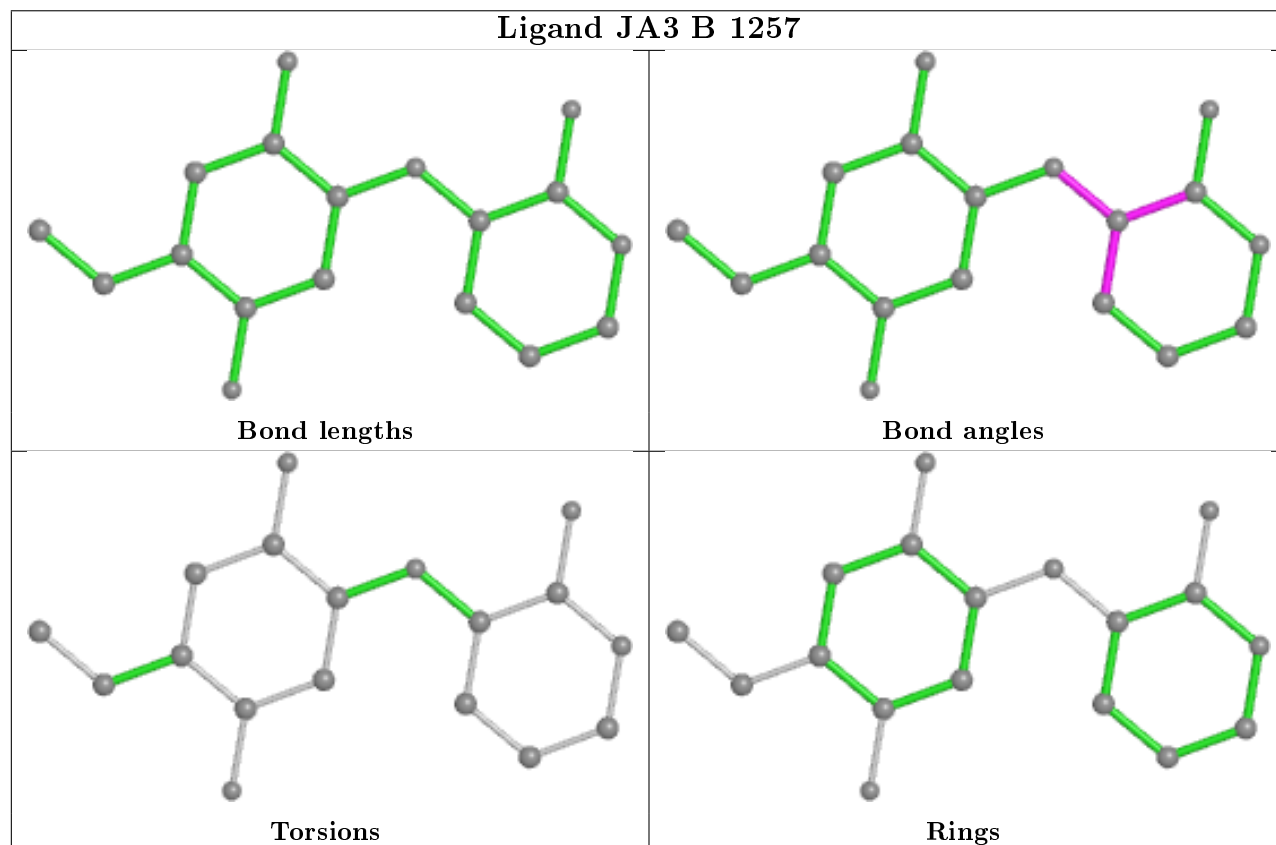
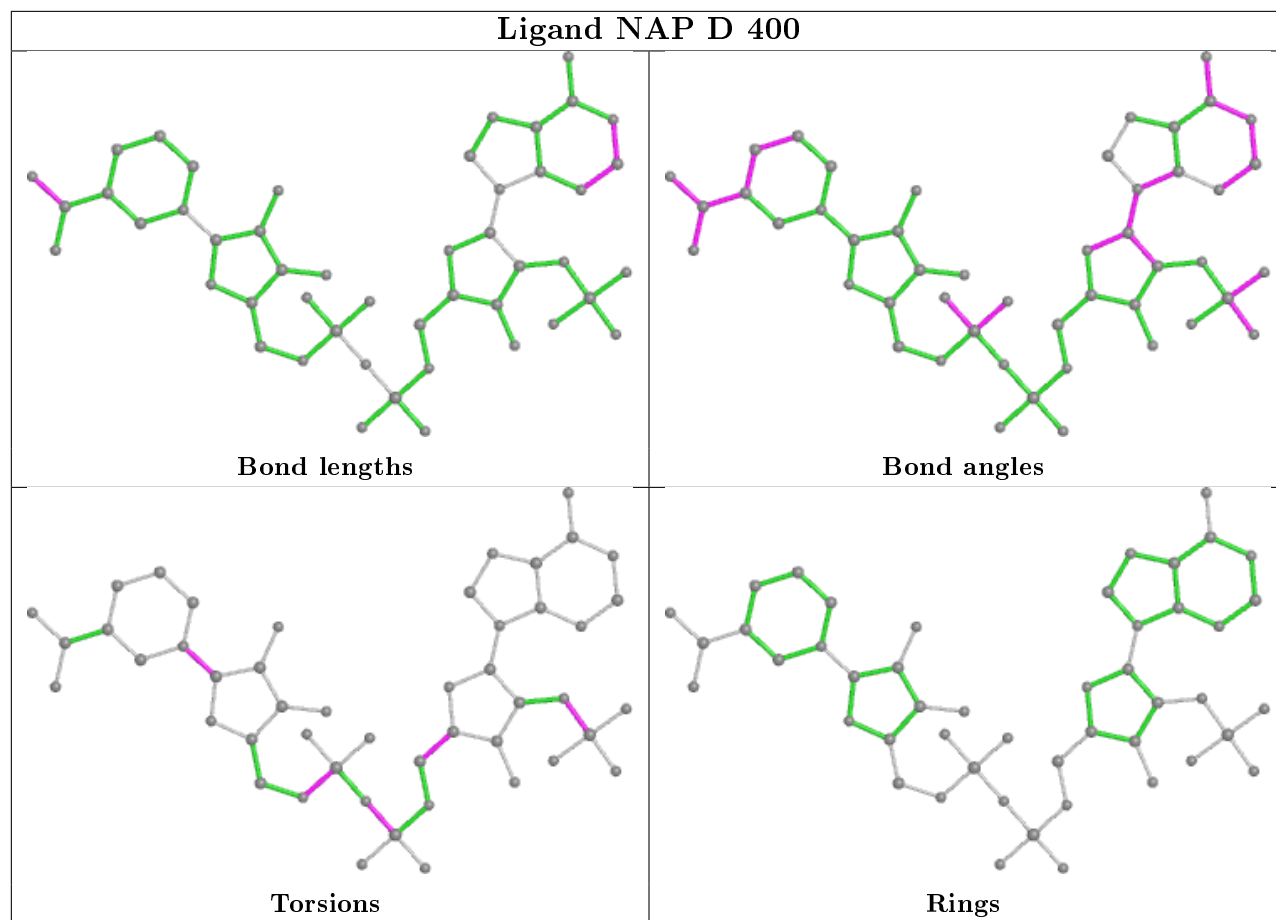


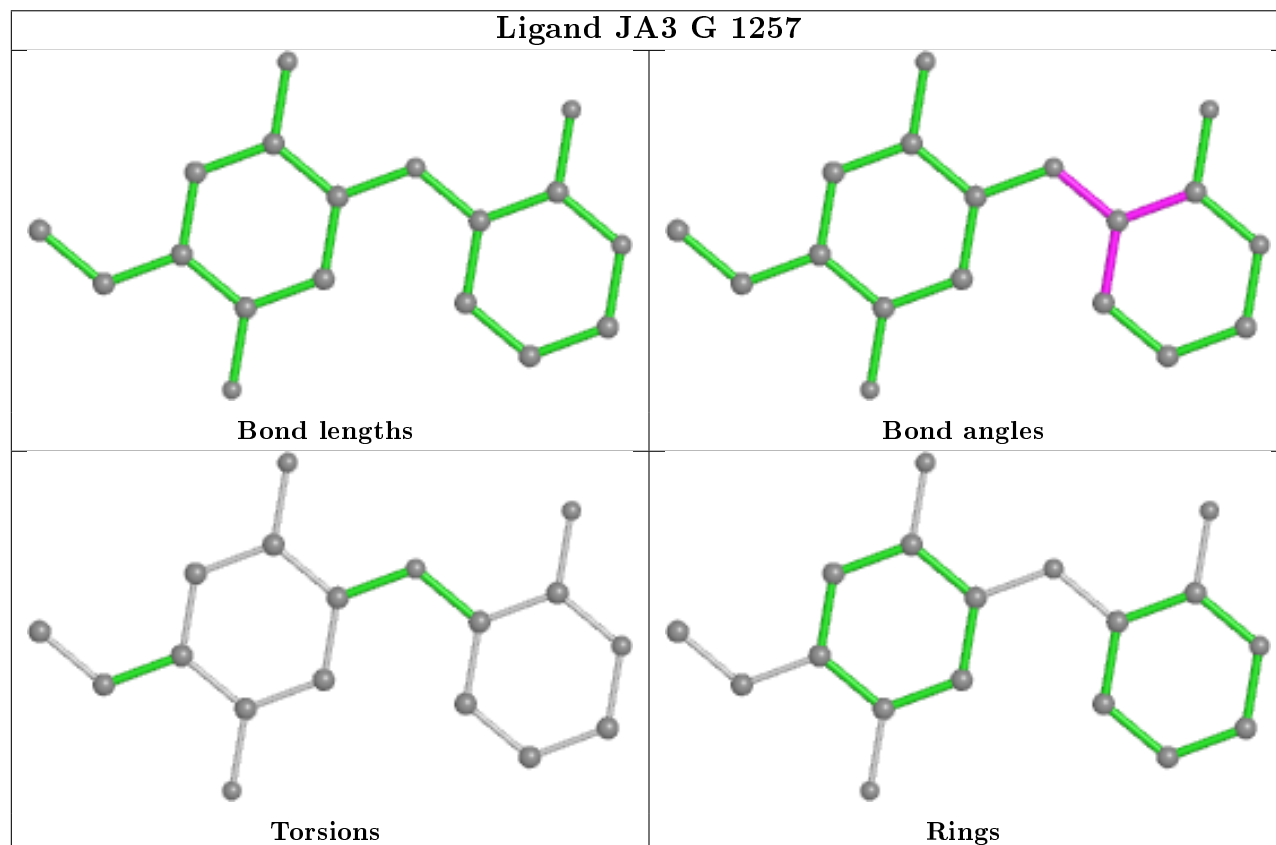
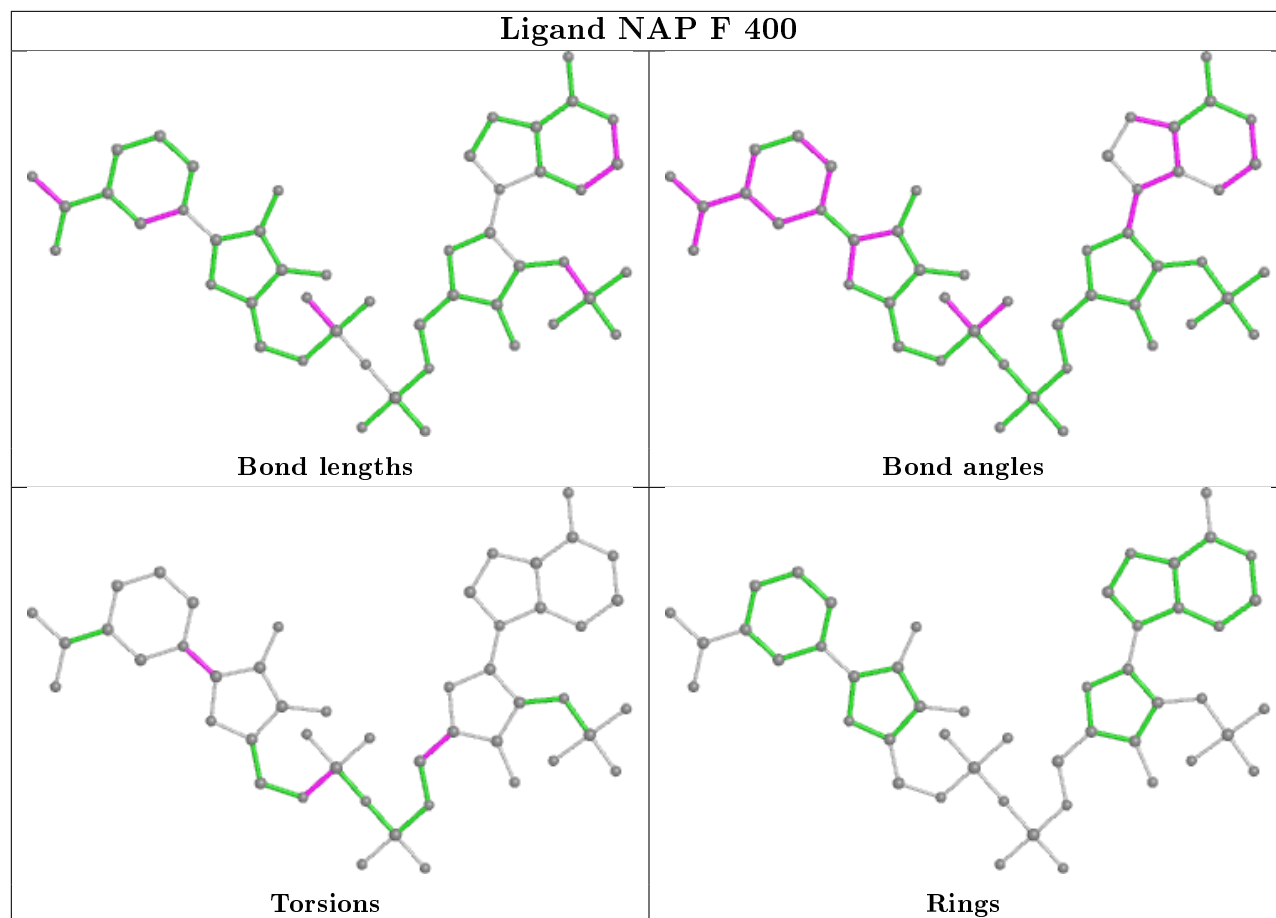


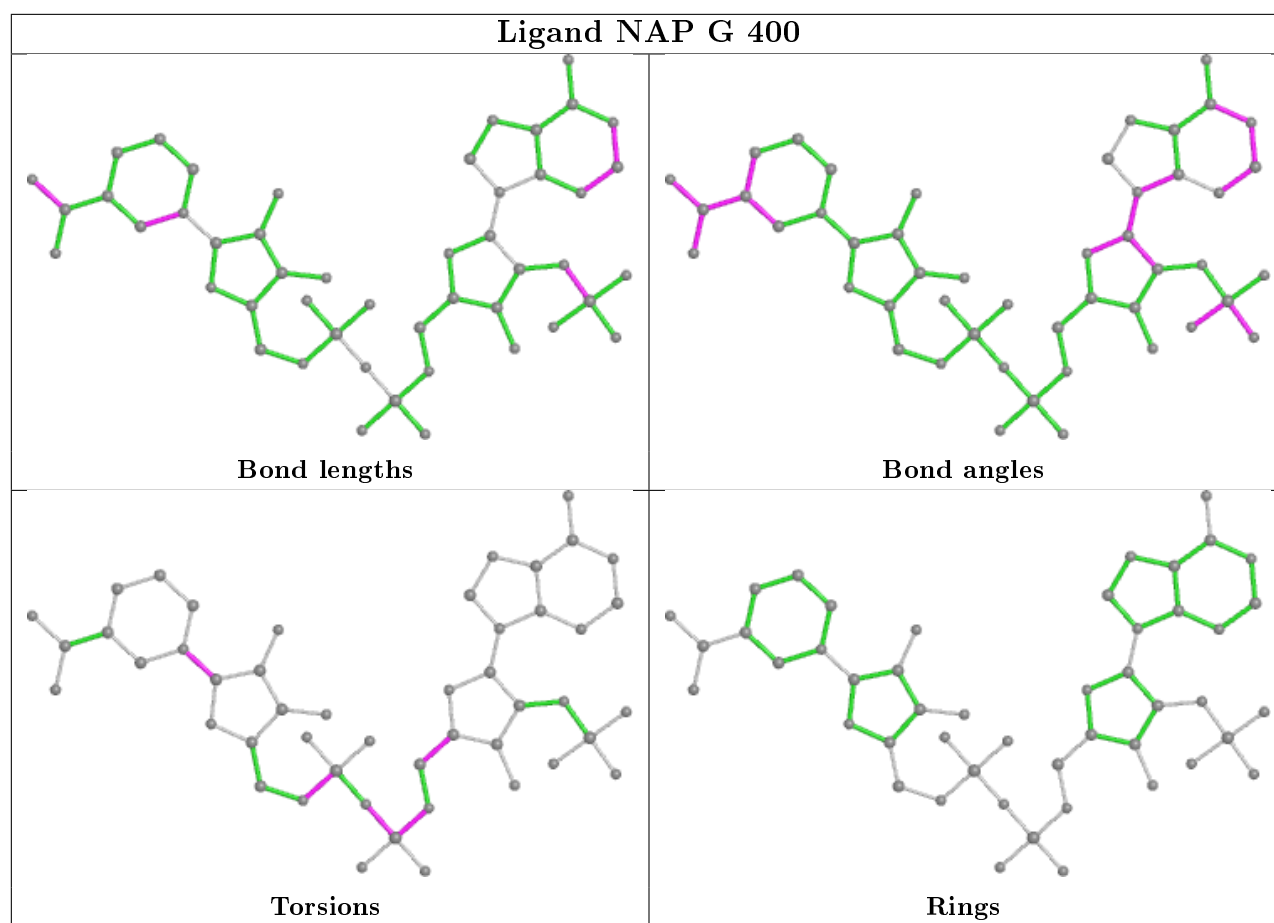












## 5.7 Other polymers [i](#)

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%)	-0.57	0	100 100	13, 23, 43, 59	0
1	B	254/282 (90%)	-0.63	0	100 100	15, 24, 47, 61	0
1	C	254/282 (90%)	-0.53	1 (0%)	92 90	17, 26, 46, 61	0
1	D	254/282 (90%)	-0.49	2 (0%)	86 84	18, 30, 55, 70	0
1	E	254/282 (90%)	-0.58	0	100 100	15, 23, 42, 56	0
1	F	254/282 (90%)	-0.56	1 (0%)	92 90	16, 26, 48, 63	0
1	G	254/282 (90%)	-0.56	2 (0%)	86 84	16, 26, 46, 65	0
1	H	254/282 (90%)	-0.47	2 (0%)	86 84	17, 29, 55, 79	0
All	All	2032/2256 (90%)	-0.55	8 (0%)	92 90	13, 26, 49, 79	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	43	ARG	3.5
1	H	58	PRO	3.5
1	D	58	PRO	3.1
1	D	43	ARG	2.5
1	G	58	PRO	2.5
1	F	58	PRO	2.4
1	C	6	ASN	2.3
1	G	6	ASN	2.3

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

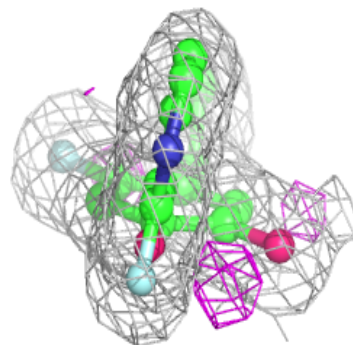
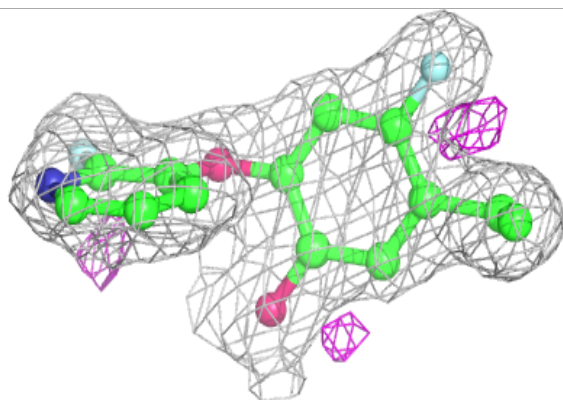
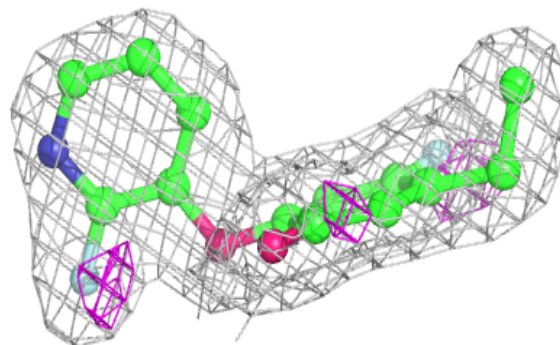
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GLU	E	1259	10/10	0.45	0.27	63,73,74,75	0
5	GLU	C	1259	10/10	0.57	0.21	63,76,77,77	0
5	GLU	B	1258	10/10	0.59	0.21	70,78,79,80	0
3	MRD	E	1260	8/8	0.59	0.26	49,59,62,64	0
5	GLU	G	1260	10/10	0.60	0.26	69,81,83,84	0
5	GLU	H	1259	10/10	0.60	0.23	64,68,71,72	0
5	GLU	F	1257	10/10	0.60	0.20	70,77,78,78	0
3	MRD	B	1259	8/8	0.68	0.21	39,57,63,63	0
3	MRD	C	1260	8/8	0.71	0.21	50,57,60,60	0
3	MRD	F	1258	8/8	0.74	0.18	39,53,57,59	0
3	MRD	A	1257	8/8	0.75	0.17	39,46,51,54	0
3	MRD	H	1257	8/8	0.79	0.24	40,51,54,55	0
3	MRD	G	1261	8/8	0.79	0.20	43,57,62,62	0
3	MRD	G	1259	8/8	0.82	0.20	39,52,54,54	0
4	JA3	C	1258	18/18	0.95	0.07	24,27,32,33	0
4	JA3	G	1258	18/18	0.96	0.07	22,26,29,29	0
2	NAP	D	400	48/48	0.96	0.09	22,28,48,55	0
4	JA3	C	1257	18/18	0.97	0.09	19,22,26,29	0
2	NAP	H	400	48/48	0.97	0.08	21,26,38,42	0
4	JA3	B	1257	18/18	0.97	0.07	19,23,27,27	0
4	JA3	G	1257	18/18	0.97	0.07	18,21,24,27	0
2	NAP	B	400	48/48	0.98	0.08	19,21,27,29	0
2	NAP	C	400	48/48	0.98	0.09	19,23,30,32	0
4	JA3	E	1257	18/18	0.98	0.09	16,19,24,27	0
2	NAP	E	400	48/48	0.98	0.09	15,20,25,26	0
4	JA3	E	1258	18/18	0.98	0.06	19,23,29,29	0
2	NAP	F	400	48/48	0.98	0.07	19,23,29,32	0
4	JA3	A	1259	18/18	0.98	0.08	16,20,24,26	0
2	NAP	G	400	48/48	0.98	0.08	18,22,28,31	0
2	NAP	A	400	48/48	0.99	0.09	13,20,24,27	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 JA3 C 1258:**

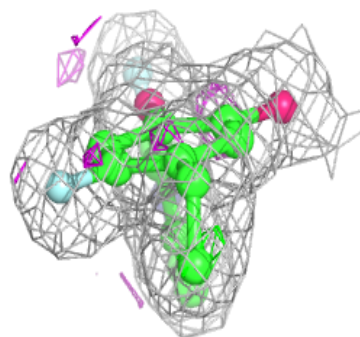
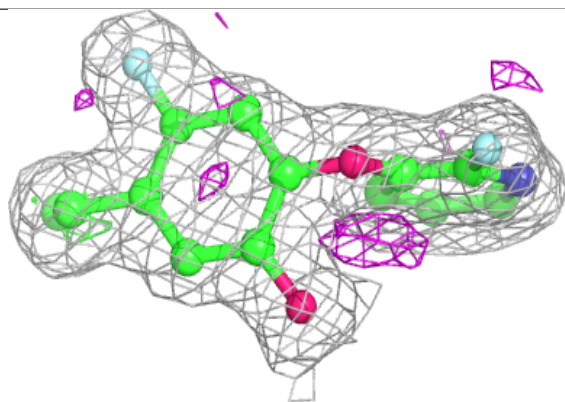
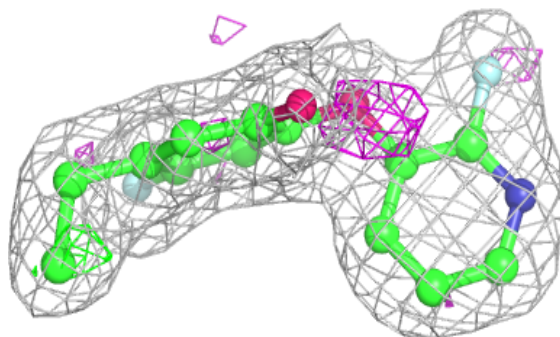
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



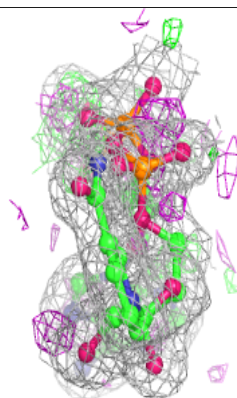
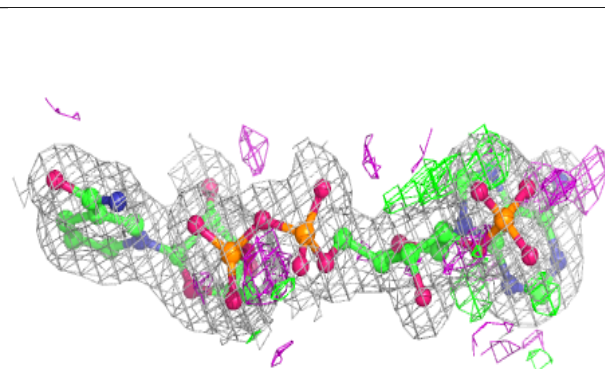
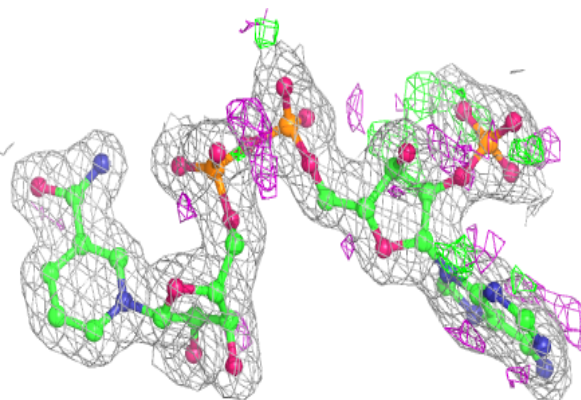


**Electron density around JA3 G 1258:**

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

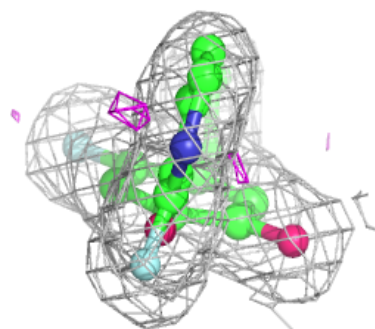
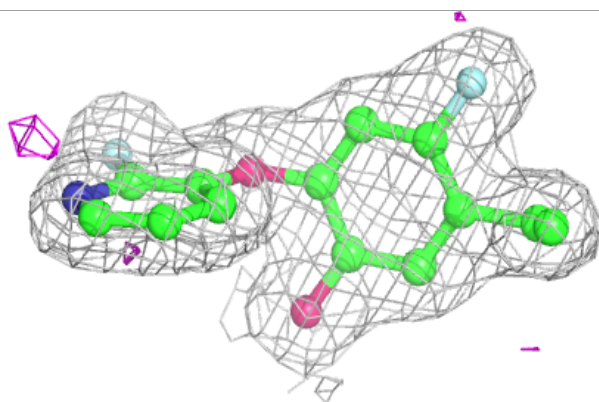
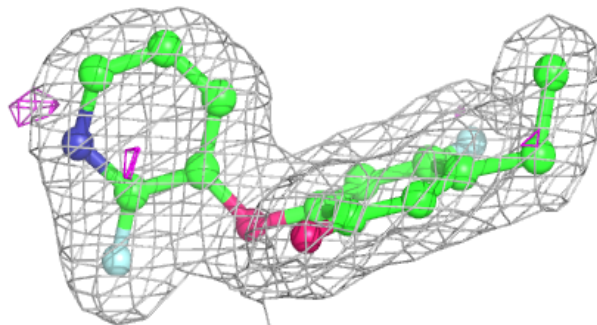
**Electron density around NAP D 400:**

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

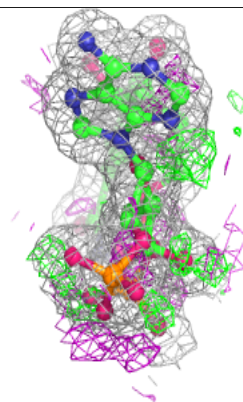
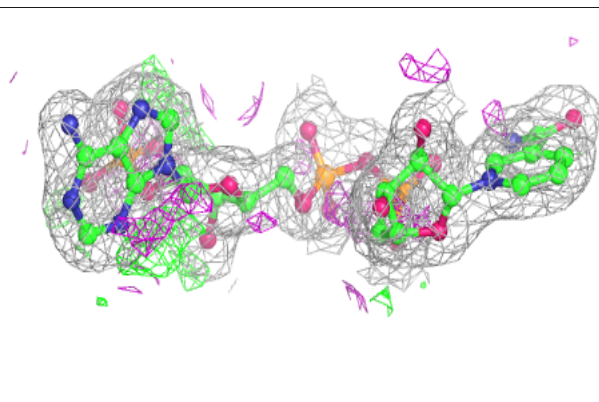
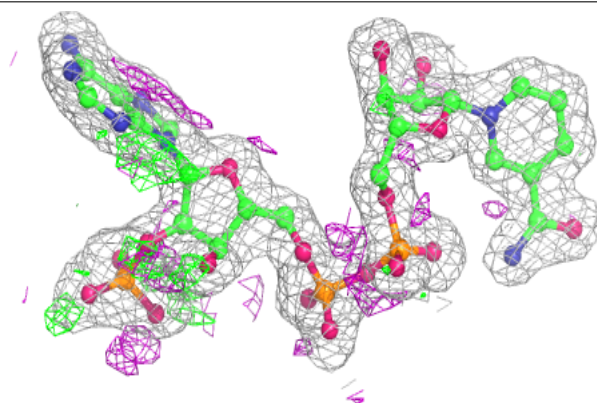


**Electron density around JA3 C 1257:**

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

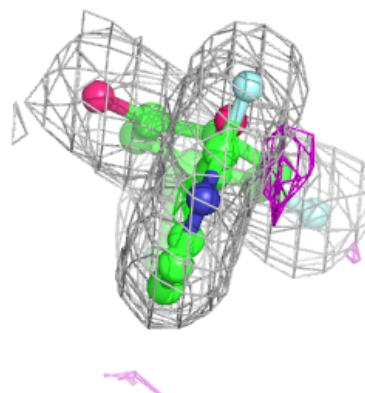
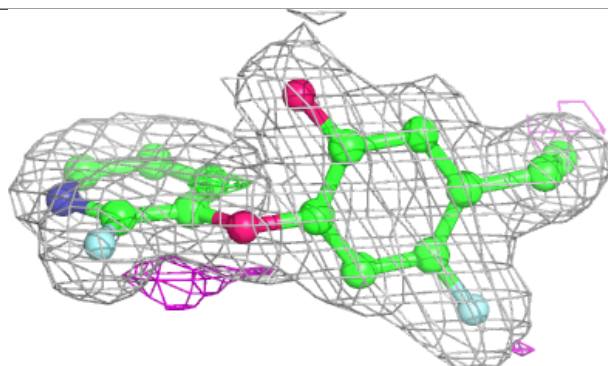
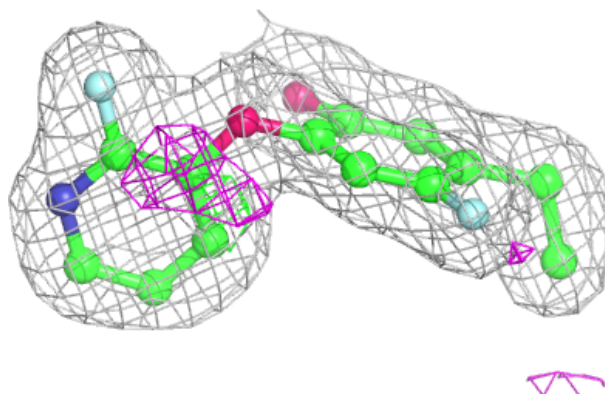
**Electron density around NAP H 400:**

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

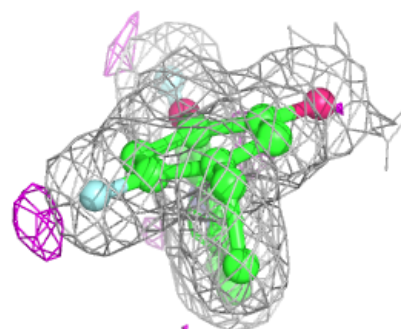
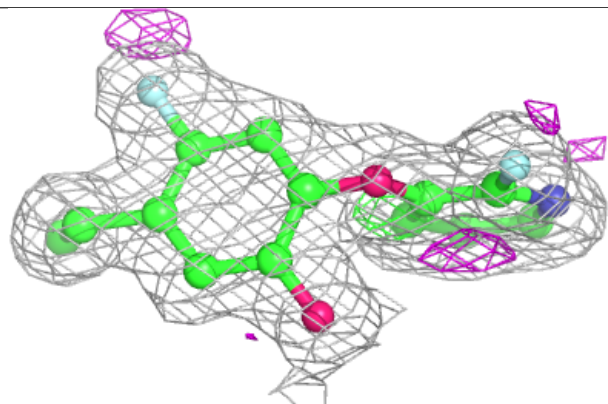
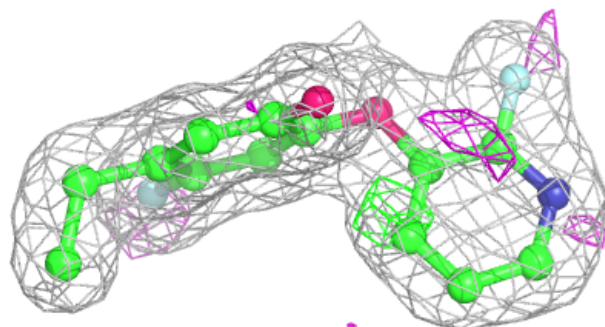


**Electron density around JA3 B 1257:**

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

**Electron density around JA3 G 1257:**

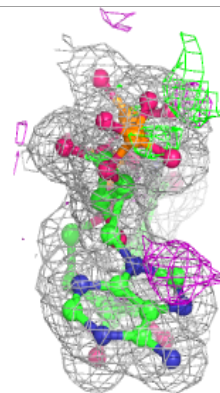
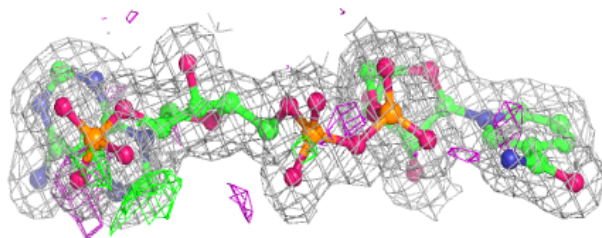
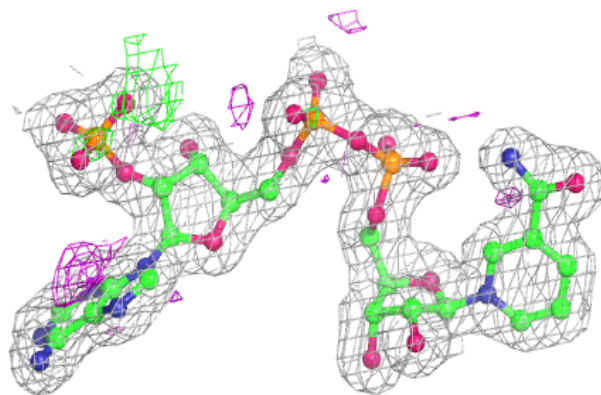
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



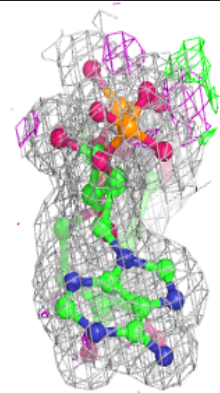
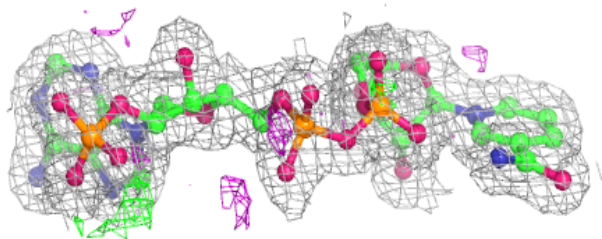
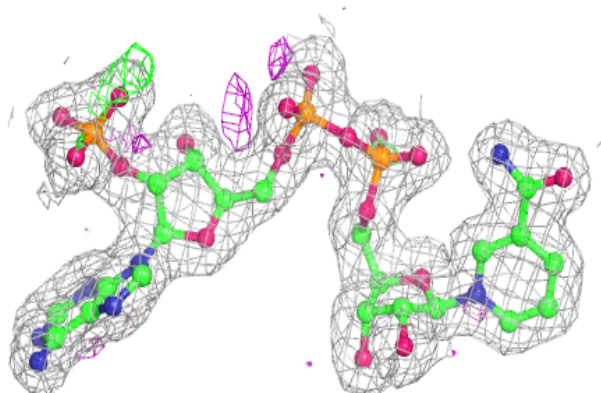


**Electron density around NAP B 400:**

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

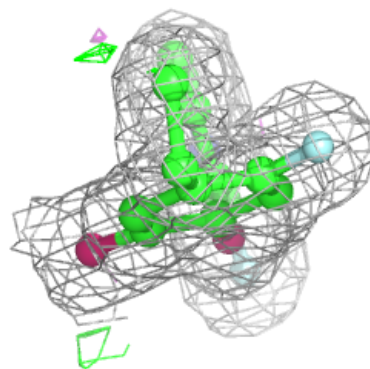
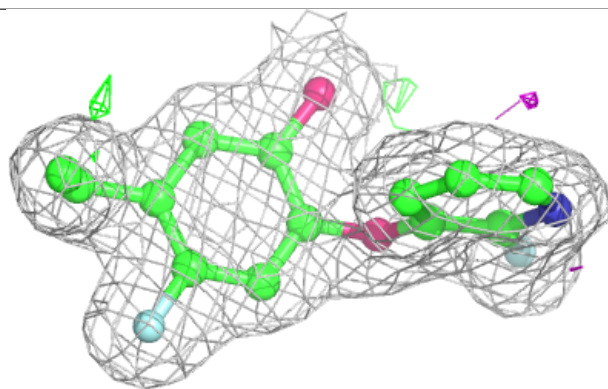
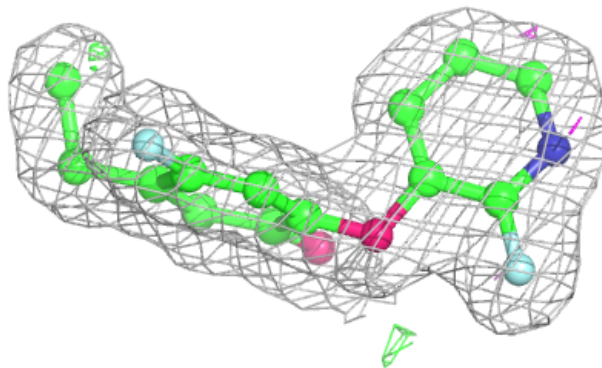
**Electron density around NAP C 400:**

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

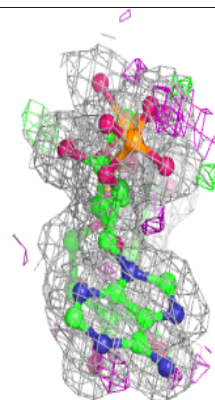
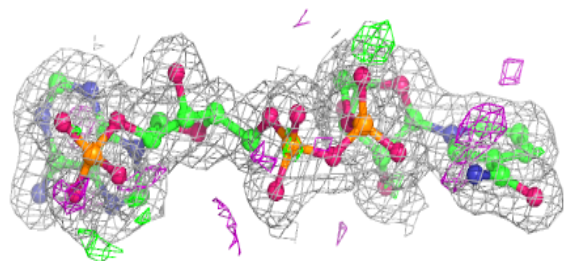
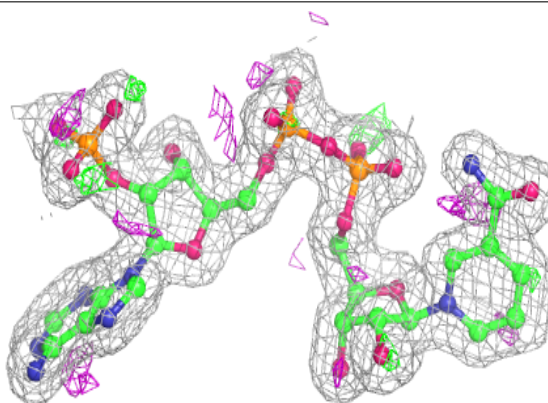


**Electron density around JA3 E 1257:**

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

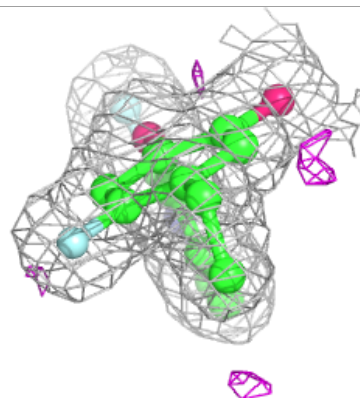
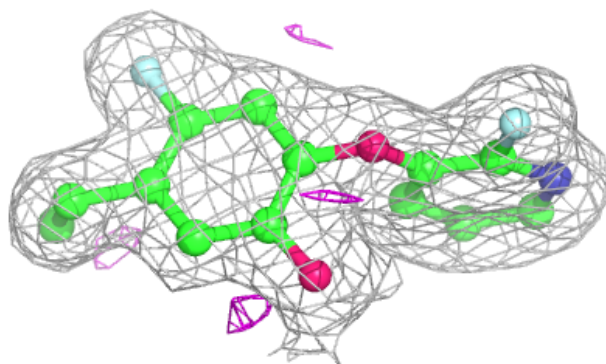
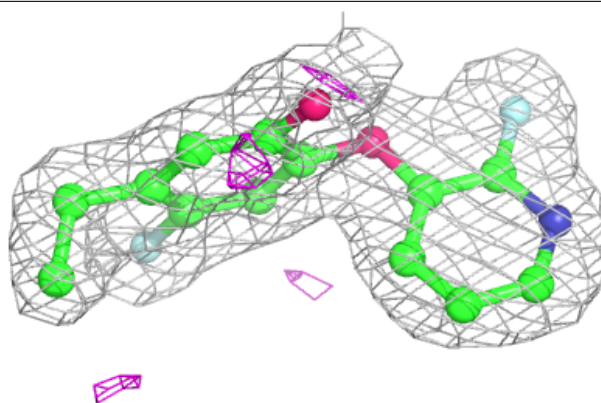
**Electron density around NAP E 400:**

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

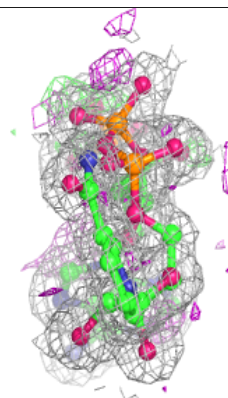
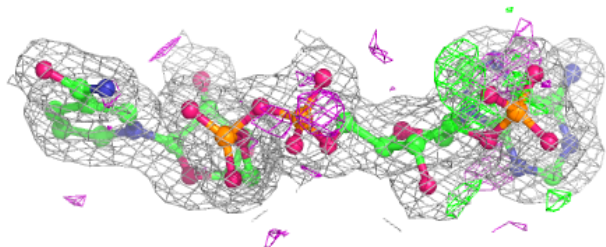
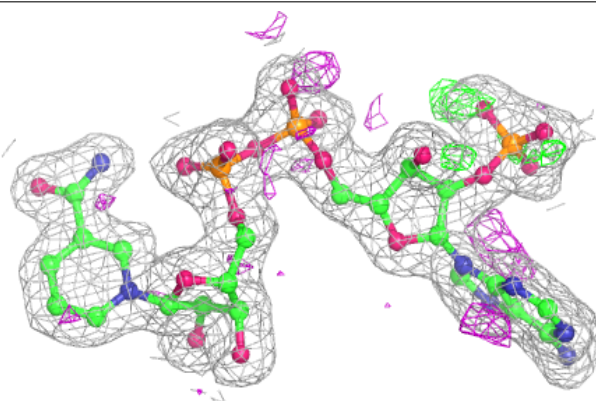


**Electron density around JA3 E 1258:**

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

**Electron density around NAP F 400:**

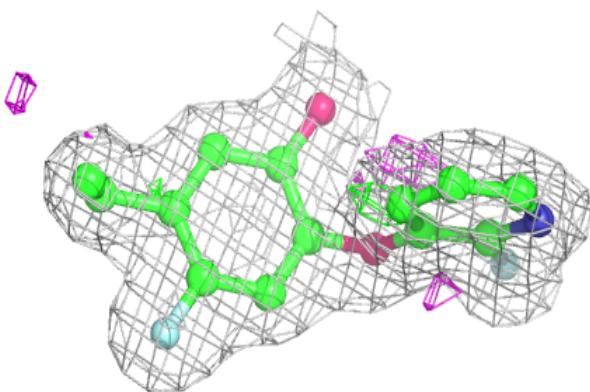
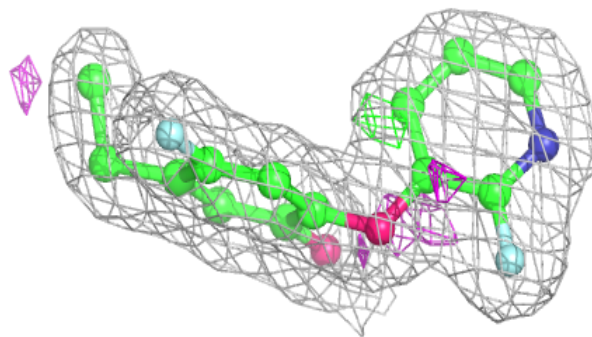
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



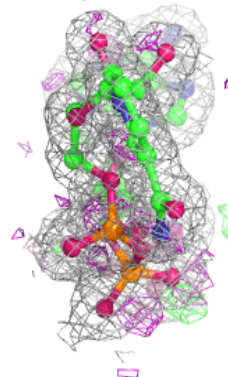
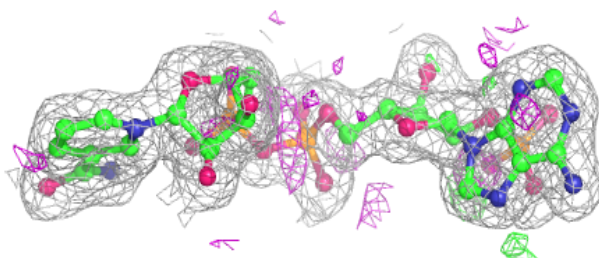
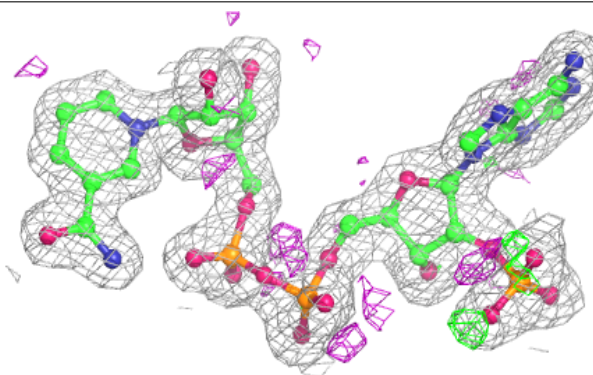


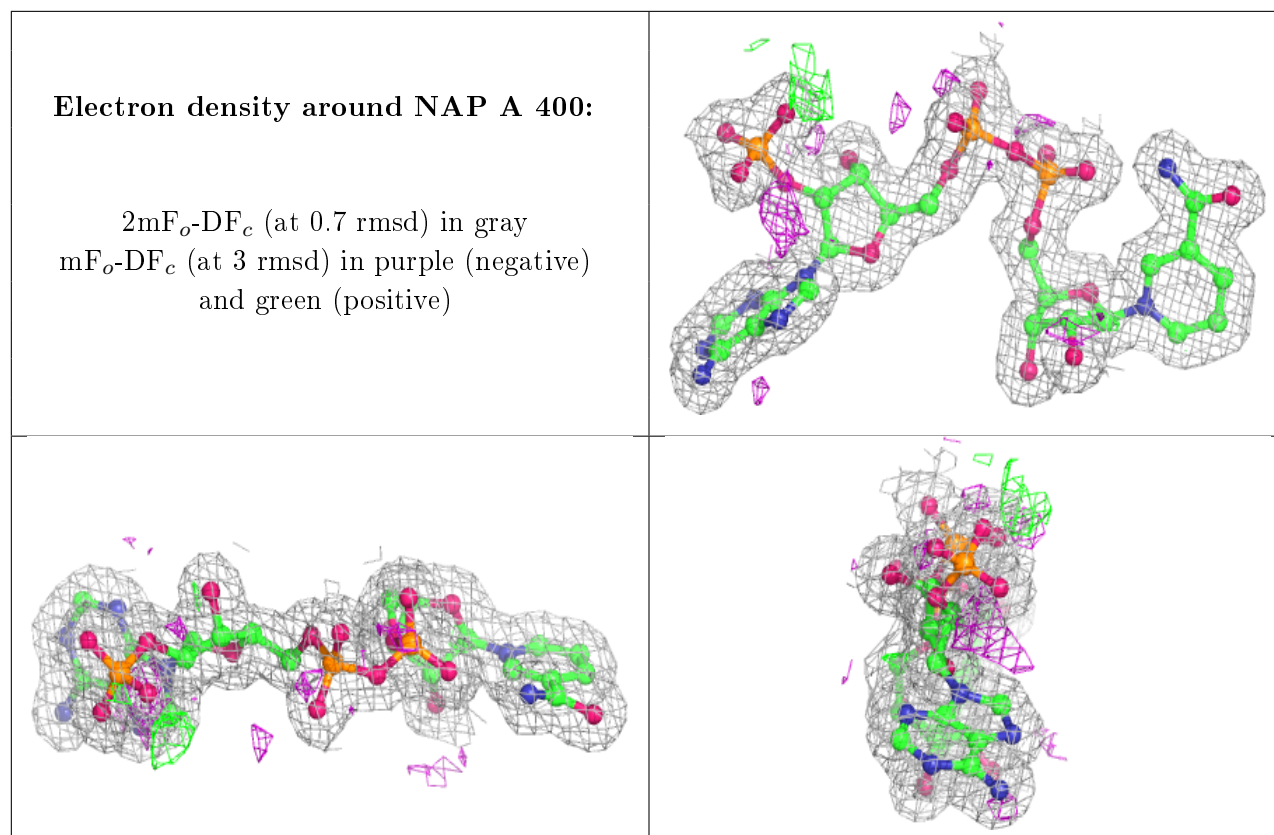
**Electron density around JA3 A 1259:**

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

**Electron density around NAP G 400:**

$2mF_o-DF_c$  (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.