



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:29 AM UTC

PDB ID : 9PL0 / pdb_00009pl0
Title : The structure of the Fusobacterium nucleatum Enoyl-Acyl Carrier Protein Reductase (FabK) bound to an inhibitor
Authors : Alaidi, O.; Avad, K.; Hevener, K.
Deposited on : 2025-07-15
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

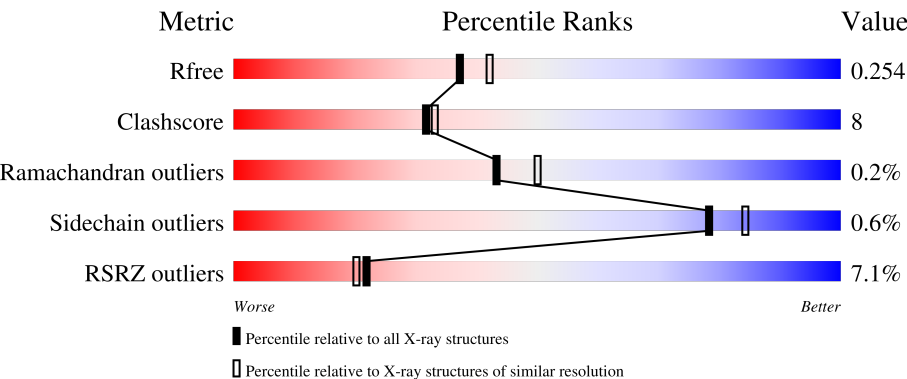
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	338	3% 77% 17% 7%
1	B	338	4% 80% 14% 7%
1	C	338	5% 77% 15% 7%
1	D	338	4% 75% 18% 7%
1	E	338	4% 78% 15% 7%

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Mol	Chain	Length	Quality of chain
1	F	338	
1	G	338	
1	H	338	
1	I	338	
1	J	338	
1	K	338	
1	L	338	

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
5	DMS	A	405	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30074 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	2	0
			2361	1486	409	448	18			
1	B	316	Total	C	N	O	S	0	1	0
			2369	1493	411	447	18			
1	C	315	Total	C	N	O	S	0	2	0
			2363	1486	411	448	18			
1	D	316	Total	C	N	O	S	0	2	0
			2377	1498	414	447	18			
1	E	314	Total	C	N	O	S	0	1	0
			2347	1477	408	445	17			
1	F	315	Total	C	N	O	S	0	0	0
			2344	1476	405	445	18			
1	J	314	Total	C	N	O	S	0	0	0
			2336	1471	404	444	17			
1	G	315	Total	C	N	O	S	0	0	0
			2344	1476	405	445	18			
1	H	315	Total	C	N	O	S	0	0	0
			2344	1476	405	445	18			
1	I	314	Total	C	N	O	S	0	0	0
			2336	1471	404	444	17			
1	K	314	Total	C	N	O	S	0	1	0
			2345	1477	406	445	17			
1	L	314	Total	C	N	O	S	0	1	0
			2345	1477	406	445	17			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8RGV3
A	-18	GLY	-	expression tag	UNP Q8RGV3
A	-17	SER	-	expression tag	UNP Q8RGV3
A	-16	SER	-	expression tag	UNP Q8RGV3
A	-15	HIS	-	expression tag	UNP Q8RGV3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q8RGV3
A	-13	HIS	-	expression tag	UNP Q8RGV3
A	-12	HIS	-	expression tag	UNP Q8RGV3
A	-11	HIS	-	expression tag	UNP Q8RGV3
A	-10	HIS	-	expression tag	UNP Q8RGV3
A	-9	SER	-	expression tag	UNP Q8RGV3
A	-8	SER	-	expression tag	UNP Q8RGV3
A	-7	GLY	-	expression tag	UNP Q8RGV3
A	-6	LEU	-	expression tag	UNP Q8RGV3
A	-5	VAL	-	expression tag	UNP Q8RGV3
A	-4	PRO	-	expression tag	UNP Q8RGV3
A	-3	ARG	-	expression tag	UNP Q8RGV3
A	-2	GLY	-	expression tag	UNP Q8RGV3
A	-1	SER	-	expression tag	UNP Q8RGV3
A	0	HIS	-	expression tag	UNP Q8RGV3
B	-19	MET	-	expression tag	UNP Q8RGV3
B	-18	GLY	-	expression tag	UNP Q8RGV3
B	-17	SER	-	expression tag	UNP Q8RGV3
B	-16	SER	-	expression tag	UNP Q8RGV3
B	-15	HIS	-	expression tag	UNP Q8RGV3
B	-14	HIS	-	expression tag	UNP Q8RGV3
B	-13	HIS	-	expression tag	UNP Q8RGV3
B	-12	HIS	-	expression tag	UNP Q8RGV3
B	-11	HIS	-	expression tag	UNP Q8RGV3
B	-10	HIS	-	expression tag	UNP Q8RGV3
B	-9	SER	-	expression tag	UNP Q8RGV3
B	-8	SER	-	expression tag	UNP Q8RGV3
B	-7	GLY	-	expression tag	UNP Q8RGV3
B	-6	LEU	-	expression tag	UNP Q8RGV3
B	-5	VAL	-	expression tag	UNP Q8RGV3
B	-4	PRO	-	expression tag	UNP Q8RGV3
B	-3	ARG	-	expression tag	UNP Q8RGV3
B	-2	GLY	-	expression tag	UNP Q8RGV3
B	-1	SER	-	expression tag	UNP Q8RGV3
B	0	HIS	-	expression tag	UNP Q8RGV3
C	-19	MET	-	expression tag	UNP Q8RGV3
C	-18	GLY	-	expression tag	UNP Q8RGV3
C	-17	SER	-	expression tag	UNP Q8RGV3
C	-16	SER	-	expression tag	UNP Q8RGV3
C	-15	HIS	-	expression tag	UNP Q8RGV3
C	-14	HIS	-	expression tag	UNP Q8RGV3
C	-13	HIS	-	expression tag	UNP Q8RGV3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q8RGV3
C	-11	HIS	-	expression tag	UNP Q8RGV3
C	-10	HIS	-	expression tag	UNP Q8RGV3
C	-9	SER	-	expression tag	UNP Q8RGV3
C	-8	SER	-	expression tag	UNP Q8RGV3
C	-7	GLY	-	expression tag	UNP Q8RGV3
C	-6	LEU	-	expression tag	UNP Q8RGV3
C	-5	VAL	-	expression tag	UNP Q8RGV3
C	-4	PRO	-	expression tag	UNP Q8RGV3
C	-3	ARG	-	expression tag	UNP Q8RGV3
C	-2	GLY	-	expression tag	UNP Q8RGV3
C	-1	SER	-	expression tag	UNP Q8RGV3
C	0	HIS	-	expression tag	UNP Q8RGV3
D	-19	MET	-	expression tag	UNP Q8RGV3
D	-18	GLY	-	expression tag	UNP Q8RGV3
D	-17	SER	-	expression tag	UNP Q8RGV3
D	-16	SER	-	expression tag	UNP Q8RGV3
D	-15	HIS	-	expression tag	UNP Q8RGV3
D	-14	HIS	-	expression tag	UNP Q8RGV3
D	-13	HIS	-	expression tag	UNP Q8RGV3
D	-12	HIS	-	expression tag	UNP Q8RGV3
D	-11	HIS	-	expression tag	UNP Q8RGV3
D	-10	HIS	-	expression tag	UNP Q8RGV3
D	-9	SER	-	expression tag	UNP Q8RGV3
D	-8	SER	-	expression tag	UNP Q8RGV3
D	-7	GLY	-	expression tag	UNP Q8RGV3
D	-6	LEU	-	expression tag	UNP Q8RGV3
D	-5	VAL	-	expression tag	UNP Q8RGV3
D	-4	PRO	-	expression tag	UNP Q8RGV3
D	-3	ARG	-	expression tag	UNP Q8RGV3
D	-2	GLY	-	expression tag	UNP Q8RGV3
D	-1	SER	-	expression tag	UNP Q8RGV3
D	0	HIS	-	expression tag	UNP Q8RGV3
E	-19	MET	-	expression tag	UNP Q8RGV3
E	-18	GLY	-	expression tag	UNP Q8RGV3
E	-17	SER	-	expression tag	UNP Q8RGV3
E	-16	SER	-	expression tag	UNP Q8RGV3
E	-15	HIS	-	expression tag	UNP Q8RGV3
E	-14	HIS	-	expression tag	UNP Q8RGV3
E	-13	HIS	-	expression tag	UNP Q8RGV3
E	-12	HIS	-	expression tag	UNP Q8RGV3
E	-11	HIS	-	expression tag	UNP Q8RGV3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP Q8RGV3
E	-9	SER	-	expression tag	UNP Q8RGV3
E	-8	SER	-	expression tag	UNP Q8RGV3
E	-7	GLY	-	expression tag	UNP Q8RGV3
E	-6	LEU	-	expression tag	UNP Q8RGV3
E	-5	VAL	-	expression tag	UNP Q8RGV3
E	-4	PRO	-	expression tag	UNP Q8RGV3
E	-3	ARG	-	expression tag	UNP Q8RGV3
E	-2	GLY	-	expression tag	UNP Q8RGV3
E	-1	SER	-	expression tag	UNP Q8RGV3
E	0	HIS	-	expression tag	UNP Q8RGV3
F	-19	MET	-	expression tag	UNP Q8RGV3
F	-18	GLY	-	expression tag	UNP Q8RGV3
F	-17	SER	-	expression tag	UNP Q8RGV3
F	-16	SER	-	expression tag	UNP Q8RGV3
F	-15	HIS	-	expression tag	UNP Q8RGV3
F	-14	HIS	-	expression tag	UNP Q8RGV3
F	-13	HIS	-	expression tag	UNP Q8RGV3
F	-12	HIS	-	expression tag	UNP Q8RGV3
F	-11	HIS	-	expression tag	UNP Q8RGV3
F	-10	HIS	-	expression tag	UNP Q8RGV3
F	-9	SER	-	expression tag	UNP Q8RGV3
F	-8	SER	-	expression tag	UNP Q8RGV3
F	-7	GLY	-	expression tag	UNP Q8RGV3
F	-6	LEU	-	expression tag	UNP Q8RGV3
F	-5	VAL	-	expression tag	UNP Q8RGV3
F	-4	PRO	-	expression tag	UNP Q8RGV3
F	-3	ARG	-	expression tag	UNP Q8RGV3
F	-2	GLY	-	expression tag	UNP Q8RGV3
F	-1	SER	-	expression tag	UNP Q8RGV3
F	0	HIS	-	expression tag	UNP Q8RGV3
J	-19	MET	-	expression tag	UNP Q8RGV3
J	-18	GLY	-	expression tag	UNP Q8RGV3
J	-17	SER	-	expression tag	UNP Q8RGV3
J	-16	SER	-	expression tag	UNP Q8RGV3
J	-15	HIS	-	expression tag	UNP Q8RGV3
J	-14	HIS	-	expression tag	UNP Q8RGV3
J	-13	HIS	-	expression tag	UNP Q8RGV3
J	-12	HIS	-	expression tag	UNP Q8RGV3
J	-11	HIS	-	expression tag	UNP Q8RGV3
J	-10	HIS	-	expression tag	UNP Q8RGV3
J	-9	SER	-	expression tag	UNP Q8RGV3

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	SER	-	expression tag	UNP Q8RGV3
J	-7	GLY	-	expression tag	UNP Q8RGV3
J	-6	LEU	-	expression tag	UNP Q8RGV3
J	-5	VAL	-	expression tag	UNP Q8RGV3
J	-4	PRO	-	expression tag	UNP Q8RGV3
J	-3	ARG	-	expression tag	UNP Q8RGV3
J	-2	GLY	-	expression tag	UNP Q8RGV3
J	-1	SER	-	expression tag	UNP Q8RGV3
J	0	HIS	-	expression tag	UNP Q8RGV3
G	-19	MET	-	expression tag	UNP Q8RGV3
G	-18	GLY	-	expression tag	UNP Q8RGV3
G	-17	SER	-	expression tag	UNP Q8RGV3
G	-16	SER	-	expression tag	UNP Q8RGV3
G	-15	HIS	-	expression tag	UNP Q8RGV3
G	-14	HIS	-	expression tag	UNP Q8RGV3
G	-13	HIS	-	expression tag	UNP Q8RGV3
G	-12	HIS	-	expression tag	UNP Q8RGV3
G	-11	HIS	-	expression tag	UNP Q8RGV3
G	-10	HIS	-	expression tag	UNP Q8RGV3
G	-9	SER	-	expression tag	UNP Q8RGV3
G	-8	SER	-	expression tag	UNP Q8RGV3
G	-7	GLY	-	expression tag	UNP Q8RGV3
G	-6	LEU	-	expression tag	UNP Q8RGV3
G	-5	VAL	-	expression tag	UNP Q8RGV3
G	-4	PRO	-	expression tag	UNP Q8RGV3
G	-3	ARG	-	expression tag	UNP Q8RGV3
G	-2	GLY	-	expression tag	UNP Q8RGV3
G	-1	SER	-	expression tag	UNP Q8RGV3
G	0	HIS	-	expression tag	UNP Q8RGV3
H	-19	MET	-	expression tag	UNP Q8RGV3
H	-18	GLY	-	expression tag	UNP Q8RGV3
H	-17	SER	-	expression tag	UNP Q8RGV3
H	-16	SER	-	expression tag	UNP Q8RGV3
H	-15	HIS	-	expression tag	UNP Q8RGV3
H	-14	HIS	-	expression tag	UNP Q8RGV3
H	-13	HIS	-	expression tag	UNP Q8RGV3
H	-12	HIS	-	expression tag	UNP Q8RGV3
H	-11	HIS	-	expression tag	UNP Q8RGV3
H	-10	HIS	-	expression tag	UNP Q8RGV3
H	-9	SER	-	expression tag	UNP Q8RGV3
H	-8	SER	-	expression tag	UNP Q8RGV3
H	-7	GLY	-	expression tag	UNP Q8RGV3

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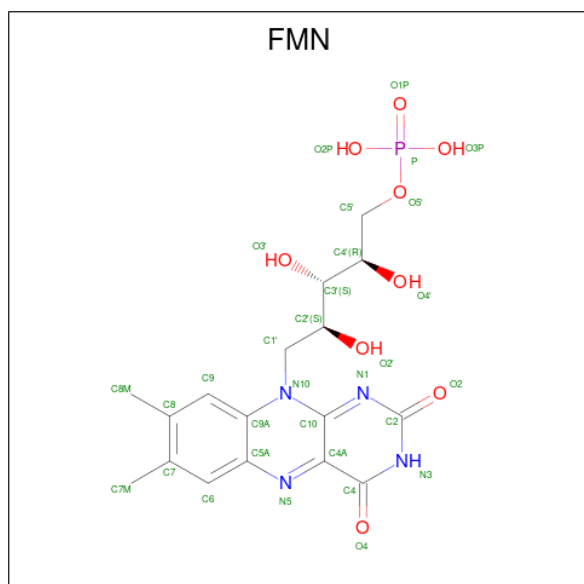
Chain	Residue	Modelled	Actual	Comment	Reference
H	-6	LEU	-	expression tag	UNP Q8RGV3
H	-5	VAL	-	expression tag	UNP Q8RGV3
H	-4	PRO	-	expression tag	UNP Q8RGV3
H	-3	ARG	-	expression tag	UNP Q8RGV3
H	-2	GLY	-	expression tag	UNP Q8RGV3
H	-1	SER	-	expression tag	UNP Q8RGV3
H	0	HIS	-	expression tag	UNP Q8RGV3
I	-19	MET	-	expression tag	UNP Q8RGV3
I	-18	GLY	-	expression tag	UNP Q8RGV3
I	-17	SER	-	expression tag	UNP Q8RGV3
I	-16	SER	-	expression tag	UNP Q8RGV3
I	-15	HIS	-	expression tag	UNP Q8RGV3
I	-14	HIS	-	expression tag	UNP Q8RGV3
I	-13	HIS	-	expression tag	UNP Q8RGV3
I	-12	HIS	-	expression tag	UNP Q8RGV3
I	-11	HIS	-	expression tag	UNP Q8RGV3
I	-10	HIS	-	expression tag	UNP Q8RGV3
I	-9	SER	-	expression tag	UNP Q8RGV3
I	-8	SER	-	expression tag	UNP Q8RGV3
I	-7	GLY	-	expression tag	UNP Q8RGV3
I	-6	LEU	-	expression tag	UNP Q8RGV3
I	-5	VAL	-	expression tag	UNP Q8RGV3
I	-4	PRO	-	expression tag	UNP Q8RGV3
I	-3	ARG	-	expression tag	UNP Q8RGV3
I	-2	GLY	-	expression tag	UNP Q8RGV3
I	-1	SER	-	expression tag	UNP Q8RGV3
I	0	HIS	-	expression tag	UNP Q8RGV3
K	-19	MET	-	expression tag	UNP Q8RGV3
K	-18	GLY	-	expression tag	UNP Q8RGV3
K	-17	SER	-	expression tag	UNP Q8RGV3
K	-16	SER	-	expression tag	UNP Q8RGV3
K	-15	HIS	-	expression tag	UNP Q8RGV3
K	-14	HIS	-	expression tag	UNP Q8RGV3
K	-13	HIS	-	expression tag	UNP Q8RGV3
K	-12	HIS	-	expression tag	UNP Q8RGV3
K	-11	HIS	-	expression tag	UNP Q8RGV3
K	-10	HIS	-	expression tag	UNP Q8RGV3
K	-9	SER	-	expression tag	UNP Q8RGV3
K	-8	SER	-	expression tag	UNP Q8RGV3
K	-7	GLY	-	expression tag	UNP Q8RGV3
K	-6	LEU	-	expression tag	UNP Q8RGV3
K	-5	VAL	-	expression tag	UNP Q8RGV3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP Q8RGV3
K	-3	ARG	-	expression tag	UNP Q8RGV3
K	-2	GLY	-	expression tag	UNP Q8RGV3
K	-1	SER	-	expression tag	UNP Q8RGV3
K	0	HIS	-	expression tag	UNP Q8RGV3
L	-19	MET	-	expression tag	UNP Q8RGV3
L	-18	GLY	-	expression tag	UNP Q8RGV3
L	-17	SER	-	expression tag	UNP Q8RGV3
L	-16	SER	-	expression tag	UNP Q8RGV3
L	-15	HIS	-	expression tag	UNP Q8RGV3
L	-14	HIS	-	expression tag	UNP Q8RGV3
L	-13	HIS	-	expression tag	UNP Q8RGV3
L	-12	HIS	-	expression tag	UNP Q8RGV3
L	-11	HIS	-	expression tag	UNP Q8RGV3
L	-10	HIS	-	expression tag	UNP Q8RGV3
L	-9	SER	-	expression tag	UNP Q8RGV3
L	-8	SER	-	expression tag	UNP Q8RGV3
L	-7	GLY	-	expression tag	UNP Q8RGV3
L	-6	LEU	-	expression tag	UNP Q8RGV3
L	-5	VAL	-	expression tag	UNP Q8RGV3
L	-4	PRO	-	expression tag	UNP Q8RGV3
L	-3	ARG	-	expression tag	UNP Q8RGV3
L	-2	GLY	-	expression tag	UNP Q8RGV3
L	-1	SER	-	expression tag	UNP Q8RGV3
L	0	HIS	-	expression tag	UNP Q8RGV3

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

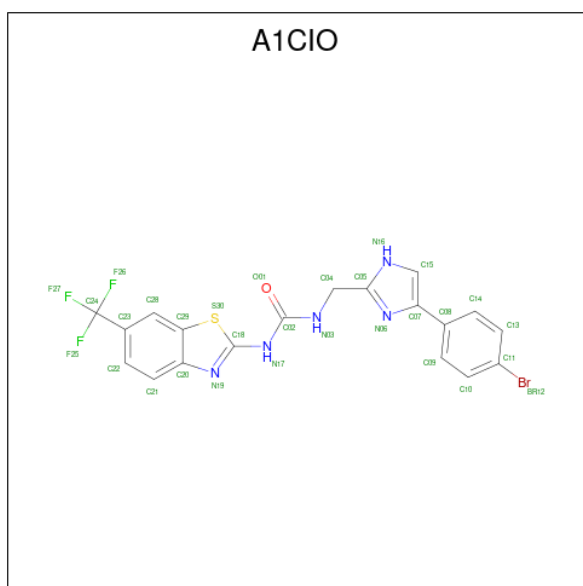
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		
3	D	2	Total	Na	0	0
			2	2		
3	E	2	Total	Na	0	0
			2	2		
3	F	2	Total	Na	0	0
			2	2		
3	J	2	Total	Na	0	0
			2	2		
3	G	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	2	Total	Na	0	0
			2	2		
3	I	2	Total	Na	0	0
			2	2		
3	K	2	Total	Na	0	0
			2	2		
3	L	2	Total	Na	0	0
			2	2		

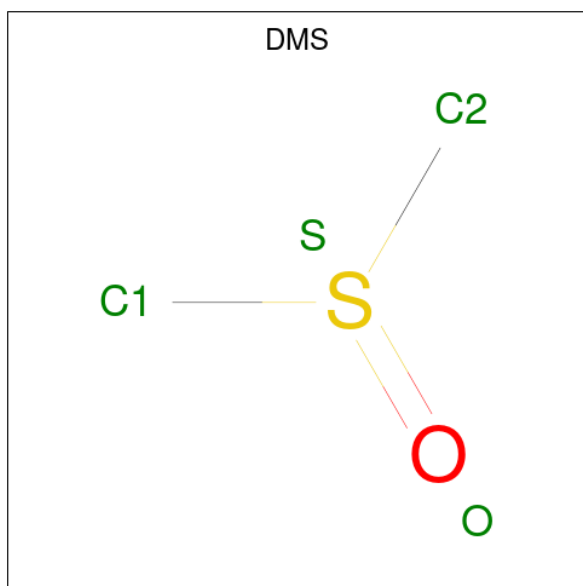
- Molecule 4 is N-{[4-(4-bromophenyl)-1H-imidazol-2-yl]methyl}-N'-[6-(trifluoromethyl)-1,3-benzothiazol-2-yl]urea (CCD ID: A1CIO) (formula: C₁₉H₁₃BrF₃N₅OS) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	J	1	Total	Br	C	F	N	O	S	0	0
			30	1	19	3	5	1	1		
4	G	1	Total	Br	C	F	N	O	S	0	0
			30	1	19	3	5	1	1		
4	H	1	Total	Br	C	F	N	O	S	0	0
			30	1	19	3	5	1	1		
4	I	1	Total	Br	C	F	N	O	S	0	0
			30	1	19	3	5	1	1		
4	K	1	Total	Br	C	F	N	O	S	0	0
			30	1	19	3	5	1	1		
4	L	1	Total	Br	C	F	N	O	S	0	0
			30	1	19	3	5	1	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



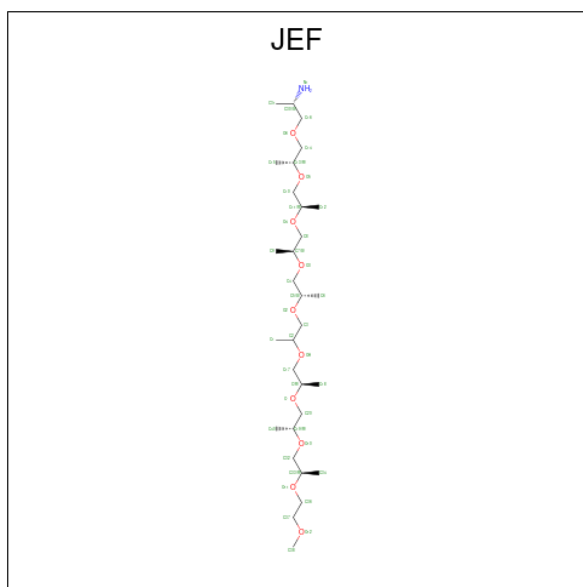
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	O	S	0	0
			4	2	1	1		
5	F	1	Total	C	O	S	0	0
			4	2	1	1		
5	F	1	Total	C	O	S	0	0
			4	2	1	1		
5	J	1	Total	C	O	S	0	0
			4	2	1	1		
5	J	1	Total	C	O	S	0	0
			4	2	1	1		
5	H	1	Total	C	O	S	0	0
			4	2	1	1		
5	I	1	Total	C	O	S	0	0
			4	2	1	1		
5	K	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is O-(O-(2-AMINOPROPYL)-O'-(2-METHOXYETHYL)POLYPROPYLENE GLYCOL 500) (CCD ID: JEF) (formula: C₃₀H₆₃NO₁₀).



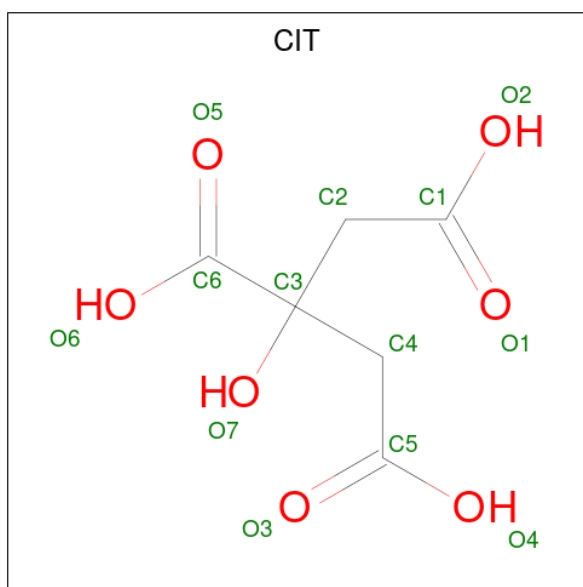
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	A	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			16	11	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	9	3		
6	C	1	Total	C	O	0	0
			6	4	2		
6	D	1	Total	C	O	0	0
			10	7	3		
6	D	1	Total	C	O	0	0
			8	6	2		
6	E	1	Total	C	O	0	0
			16	11	5		
6	E	1	Total	C	O	0	0
			10	7	3		
6	E	1	Total	C	O	0	0
			7	5	2		
6	F	1	Total	C	O	0	0
			10	7	3		
6	J	1	Total	C	O	0	0
			12	9	3		
6	G	1	Total	C	O	0	0
			8	5	3		
6	H	1	Total	C	O	0	0
			7	4	3		
6	I	1	Total	C	O	0	0
			8	5	3		
6	K	1	Total	C	O	0	0
			9	6	3		

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	80	Total	O	0	1
			80	80		
8	B	99	Total	O	0	1
			99	99		
8	C	70	Total	O	0	0
			70	70		
8	D	66	Total	O	0	1
			66	66		
8	E	82	Total	O	0	1
			82	82		
8	F	73	Total	O	0	1
			73	73		
8	J	78	Total	O	0	0
			78	78		
8	G	55	Total	O	0	1
			55	55		
8	H	72	Total	O	0	0
			72	72		
8	I	78	Total	O	0	1
			78	78		
8	K	76	Total	O	0	1
			76	76		

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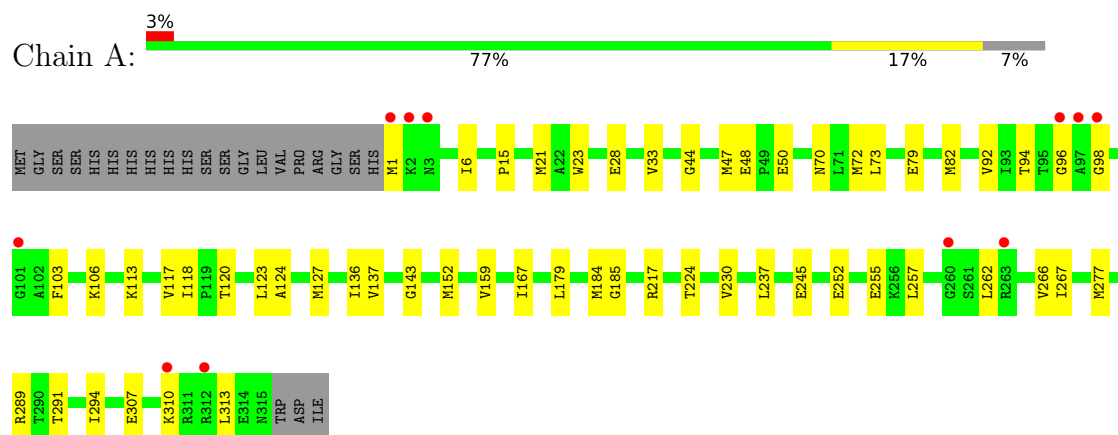
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	59	Total	O	0	0
			59	59		

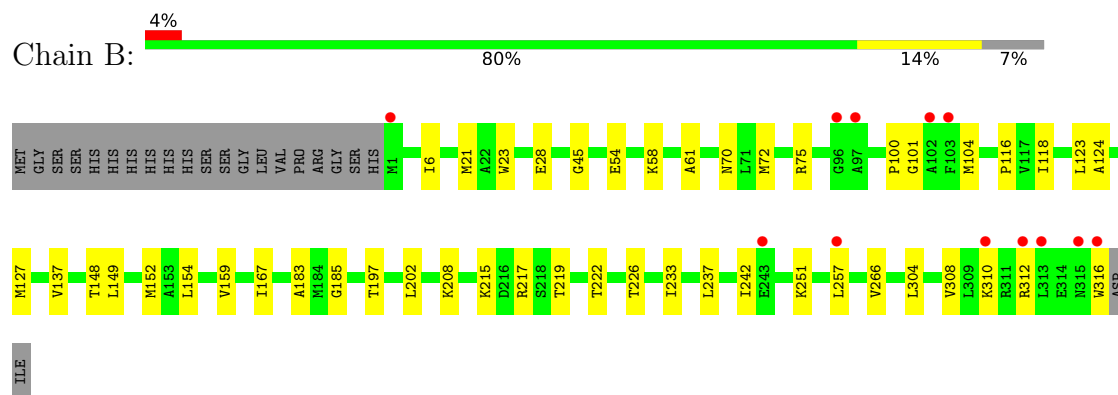
3 Residue-property plots [i](#)

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.

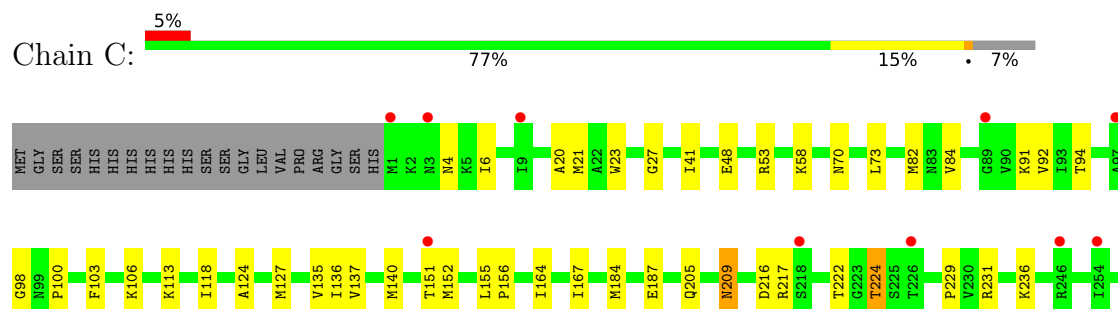
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase

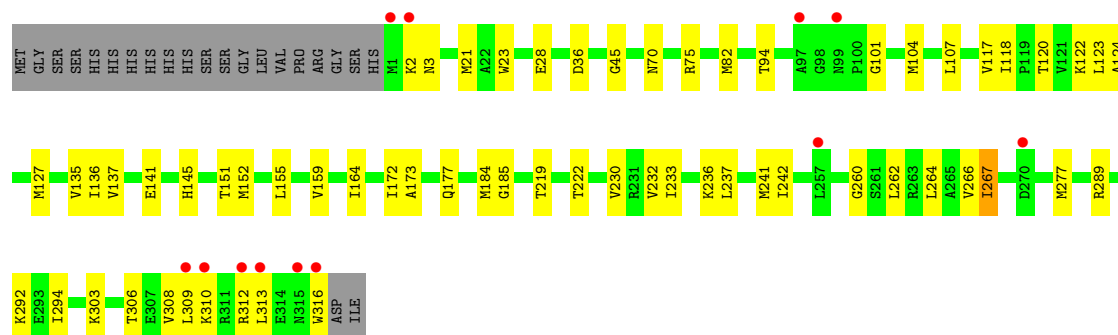
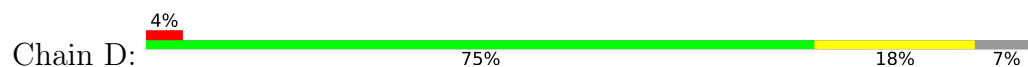


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase

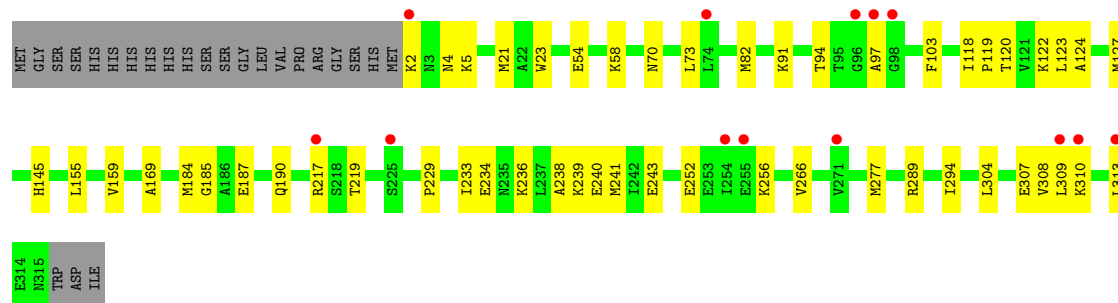
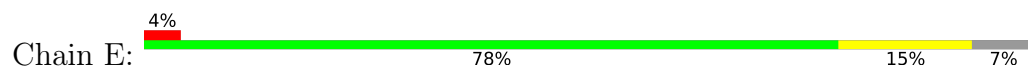




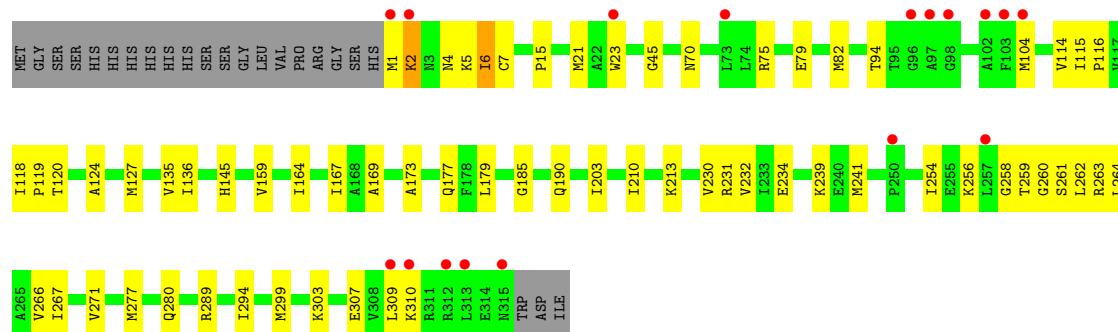
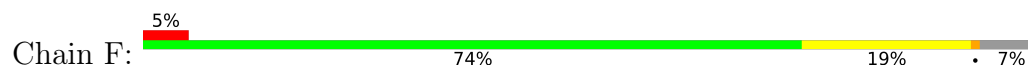
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase



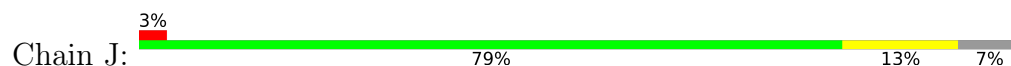
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase

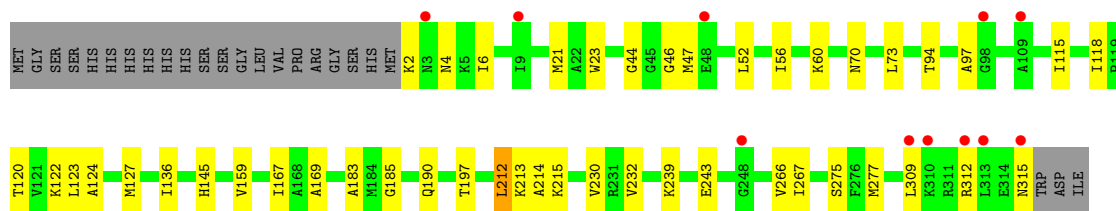


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase

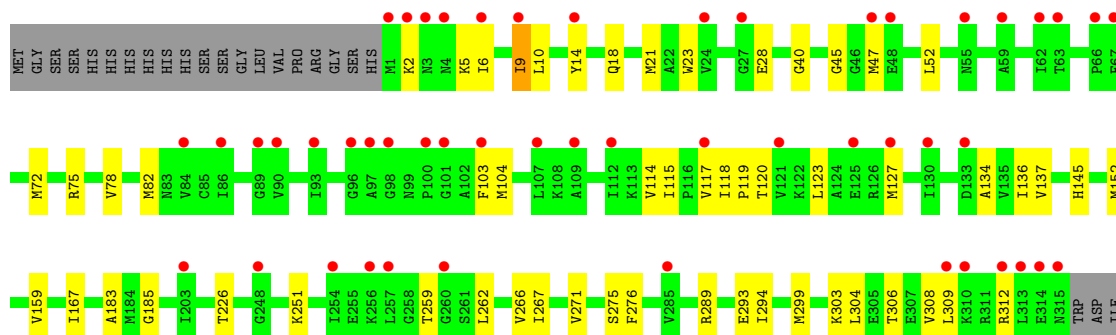
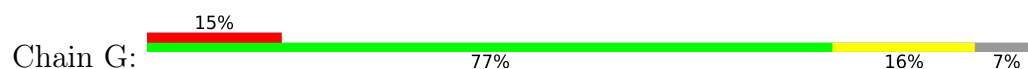


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase

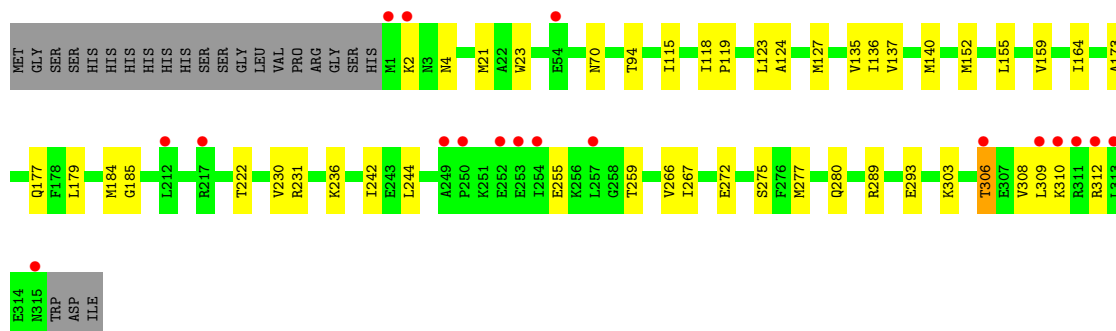
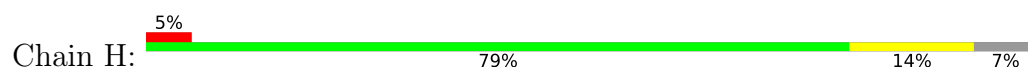




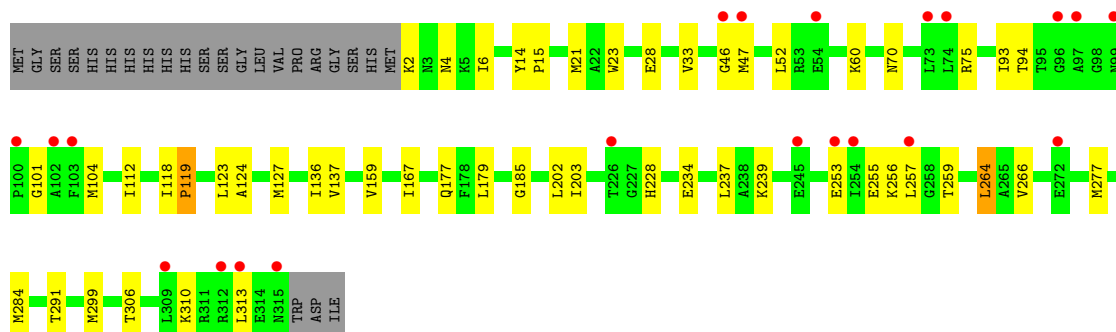
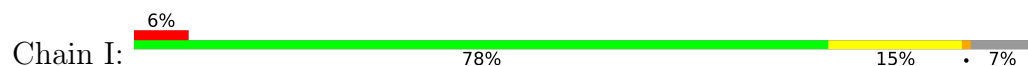
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase



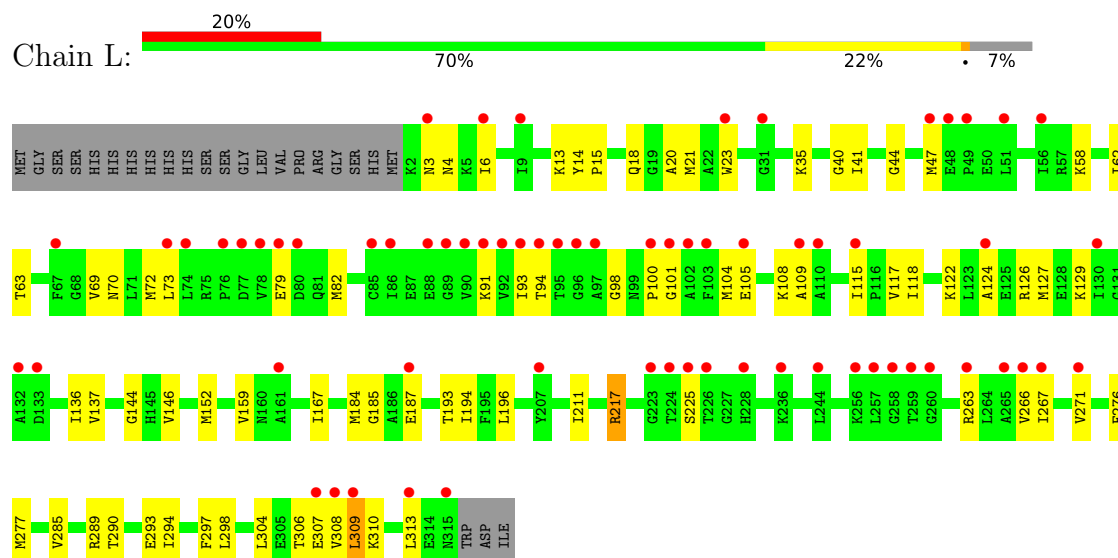
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.27Å 194.08Å 166.82Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	52.27 – 2.25 52.27 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (52.27-2.25) 94.9 (52.27-2.25)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.213 , 0.254 0.214 , 0.254	Depositor DCC
R_{free} test set	1985 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30074	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0454e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1CIO, JEF, NA, DMS, FMN, CIT

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	0.14	0/2388	0.30	0/3214
1	B	0.12	0/2395	0.31	0/3225
1	C	0.26	3/2387 (0.1%)	0.31	1/3213 (0.0%)
1	D	0.12	0/2406	0.28	0/3239
1	E	0.16	0/2371	0.30	0/3192
1	F	0.12	0/2368	0.29	0/3188
1	G	0.13	0/2368	0.29	0/3188
1	H	0.14	0/2368	0.31	0/3188
1	I	0.11	0/2360	0.30	0/3178
1	J	0.10	0/2360	0.28	0/3178
1	K	0.12	0/2369	0.30	0/3189
1	L	0.12	0/2369	0.30	0/3189
All	All	0.14	3/28509 (0.0%)	0.30	1/38381 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	209	ASN	CA-C	7.35	1.62	1.52
1	C	209	ASN	N-CA	6.70	1.54	1.46
1	C	209	ASN	C-O	5.92	1.31	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	ASN	CA-C-O	5.31	126.10	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	217	ARG	Sidechain

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	2361	0	2474	46	0
1	B	2369	0	2478	37	0
1	C	2363	0	2473	41	0
1	D	2377	0	2491	46	0
1	E	2347	0	2456	33	0
1	F	2344	0	2457	48	0
1	G	2344	0	2457	41	0
1	H	2344	0	2456	32	0
1	I	2336	0	2445	40	0
1	J	2336	0	2444	38	0
1	K	2345	0	2456	46	0
1	L	2345	0	2457	54	0
2	A	31	0	19	3	0
2	B	31	0	19	2	0
2	C	31	0	19	1	0
2	D	31	0	19	1	0
2	E	31	0	19	4	0
2	F	31	0	19	1	0
2	G	31	0	19	2	0
2	H	31	0	19	1	0
2	I	31	0	19	1	0
2	J	31	0	19	2	0
2	K	31	0	19	1	0
2	L	31	0	19	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
4	C	30	0	0	0	0
4	D	30	0	0	2	0
4	E	30	0	0	1	0
4	F	30	0	0	2	0
4	G	30	0	0	6	0
4	H	30	0	0	0	0
4	I	30	0	0	3	0
4	J	30	0	0	2	0
4	K	30	0	0	1	0
4	L	30	0	0	0	0
5	A	8	0	12	4	0
5	C	8	0	12	0	0
5	D	4	0	6	2	0
5	E	4	0	6	0	0
5	F	8	0	12	3	0
5	H	4	0	6	1	0
5	I	4	0	6	1	0
5	J	8	0	12	3	0
5	K	4	0	6	0	0
6	A	15	0	17	1	0
6	B	28	0	33	2	0
6	C	6	0	7	2	0
6	D	18	0	19	0	0
6	E	33	0	34	0	0
6	F	10	0	10	3	0
6	G	8	0	9	2	0
6	H	7	0	6	1	0
6	I	8	0	6	0	0
6	J	12	0	17	1	0
6	K	9	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	13	0	5	0	0
8	A	80	0	0	1	0
8	B	99	0	0	1	0
8	C	70	0	0	3	0
8	D	66	0	0	3	0
8	E	82	0	0	2	0
8	F	73	0	0	3	0
8	G	55	0	0	8	0
8	H	72	0	0	0	0
8	I	78	0	0	4	0
8	J	78	0	0	1	0
8	K	76	0	0	5	0
8	L	59	0	0	2	0
All	All	30074	0	30022	482	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 8.

All (482) 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)
5:D:406:DMS:H13	8:D:552:HOH:O	1.65	0.95
1:A:230:VAL:HG21	5:A:405:DMS:H22	1.51	0.91
4:G:404:A1CIO:C28	8:G:502[A]:HOH:O	2.20	0.90
1:A:266:VAL:HG23	1:A:267:ILE:HD12	1.55	0.86
1:J:312:ARG:HH22	1:I:179:LEU:HD12	1.43	0.83
1:J:183:ALA:HB1	1:I:179:LEU:HG	1.60	0.83
1:J:312:ARG:HH11	1:I:306:THR:HG23	1.44	0.81
1:F:213:LYS:NZ	8:F:501:HOH:O	2.15	0.79
1:L:72:MET:HG3	8:L:554:HOH:O	1.82	0.79
1:F:258:GLY:HA3	5:F:406:DMS:H22	1.67	0.76
1:D:312[A]:ARG:HG3	8:D:505:HOH:O	1.86	0.76
1:I:228:HIS:HE1	8:I:545[A]:HOH:O	1.66	0.76
1:F:116:PRO:HG3	1:F:127:MET:HE2	1.66	0.75
1:I:33:VAL:HA	1:I:291:THR:HG21	1.68	0.75
1:A:82:MET:HE1	1:A:103:PHE:HB3	1.69	0.74
1:D:266:VAL:HG23	1:D:267:ILE:HD12	1.70	0.73
1:L:101:GLY:HA2	1:L:104:MET:HB2	1.70	0.73
1:I:264:LEU:HD22	8:I:526:HOH:O	1.87	0.73
1:A:184:MET:HE1	1:B:152:MET:HE1	1.70	0.72
1:G:82:MET:HE1	1:G:103:PHE:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:GLY:HA2	1:L:47:MET:HE2	1.71	0.72
1:J:309:LEU:HD22	1:J:312:ARG:HE	1.53	0.72
1:I:277:MET:HE3	5:I:405:DMS:H21	1.71	0.71
1:F:210:ILE:HD11	1:F:271:VAL:HG13	1.73	0.71
1:C:184:MET:HE1	1:D:152:MET:HE1	1.74	0.69
1:F:6:ILE:HD13	1:F:167:ILE:HD11	1.74	0.69
1:K:312:ARG:HD3	1:L:306:THR:HG21	1.75	0.68
1:A:277:MET:HE3	5:A:405:DMS:H21	1.75	0.68
1:J:44:GLY:HA2	1:J:47:MET:HE2	1.76	0.68
1:J:312:ARG:HH22	1:I:179:LEU:CD1	2.06	0.68
1:L:100:PRO:HD2	1:L:127:MET:HE1	1.76	0.68
1:K:122[A]:LYS:HD3	8:K:556:HOH:O	1.93	0.68
1:J:275:SER:OG	5:J:406:DMS:H13	1.93	0.68
1:C:6:ILE:HG12	1:C:167:ILE:HD11	1.76	0.67
1:D:23:TRP:HB3	1:D:266:VAL:HG21	1.77	0.67
1:A:33:VAL:HA	1:A:291:THR:HG21	1.77	0.67
1:L:4:ASN:HD21	1:L:15:PRO:HB3	1.60	0.66
1:H:2:LYS:HD2	1:H:4:ASN:HB2	1.77	0.66
1:L:118:ILE:HD11	1:L:137:VAL:HG12	1.76	0.66
1:I:310:LYS:HA	1:I:313:LEU:HD13	1.78	0.65
1:K:152:MET:HG2	1:L:152:MET:HG2	1.78	0.64
1:I:177:GLN:HE22	1:I:284:MET:HE1	1.62	0.64
1:L:4:ASN:ND2	1:L:15:PRO:HB3	2.11	0.64
1:E:82:MET:HE1	1:E:103:PHE:HB3	1.80	0.64
1:K:122[B]:LYS:HD3	8:K:556:HOH:O	1.98	0.63
1:E:310:LYS:HD3	1:E:313:LEU:HD12	1.80	0.63
1:G:23:TRP:HB3	1:G:266:VAL:HG21	1.80	0.63
1:F:203:ILE:HG22	1:F:266:VAL:HG23	1.80	0.62
1:H:23:TRP:HB3	1:H:266:VAL:HG21	1.80	0.62
1:I:6:ILE:HG13	1:I:167:ILE:HD11	1.82	0.62
1:C:82:MET:HE1	1:C:103:PHE:HB3	1.82	0.61
1:A:1:MET:HG3	1:A:15:PRO:HG3	1.83	0.61
1:G:226:THR:HA	1:G:251:LYS:HE2	1.83	0.61
1:G:152:MET:HG2	1:H:152:MET:HG2	1.83	0.61
1:A:230:VAL:HG21	5:A:405:DMS:C2	2.27	0.61
1:K:69:VAL:HG23	1:K:90:VAL:HG11	1.82	0.61
4:G:404:A1CIO:C07	8:G:503:HOH:O	2.49	0.60
1:G:303:LYS:HE2	1:H:312:ARG:HH21	1.66	0.60
1:B:100:PRO:HD2	1:B:127:MET:HE1	1.82	0.60
1:F:262:LEU:HB3	6:F:407:JEF:H401	1.82	0.60
1:C:307:GLU:O	1:C:310:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:ILE:HD11	1:H:137:VAL:HG22	1.82	0.60
1:F:258:GLY:HA3	5:F:406:DMS:C2	2.32	0.59
1:C:209:ASN:OD1	8:C:501:HOH:O	2.16	0.59
1:A:1:MET:HE1	1:B:312:ARG:HH21	1.67	0.59
1:B:308:VAL:HG22	1:C:205:GLN:HG2	1.85	0.59
1:A:44:GLY:HA2	1:A:47:MET:HE2	1.84	0.58
1:D:262:LEU:HB3	5:D:406:DMS:H23	1.85	0.58
1:G:183:ALA:HB1	1:H:179:LEU:HG	1.85	0.58
1:F:104:MET:HE2	1:F:104:MET:HA	1.85	0.58
1:L:310:LYS:HD3	1:L:313:LEU:HD12	1.85	0.58
1:G:262:LEU:HB2	6:G:405:JEF:H321	1.86	0.58
1:A:23:TRP:HB3	1:A:266:VAL:HG21	1.86	0.58
1:B:118:ILE:HD11	1:B:137:VAL:HG22	1.85	0.58
4:G:404:A1CIO:C23	8:G:502[A]:HOH:O	2.49	0.57
1:C:118:ILE:HD11	1:C:137:VAL:HG12	1.86	0.57
1:K:6:ILE:HG13	1:K:167:ILE:HD11	1.87	0.57
1:K:226:THR:HA	1:K:251:LYS:HZ1	1.70	0.57
1:L:193:THR:HA	1:L:196:LEU:HD13	1.85	0.57
1:K:23:TRP:HB3	1:K:266:VAL:HG21	1.87	0.57
1:G:289:ARG:HH11	1:G:294:ILE:HG12	1.68	0.56
1:H:222:THR:HG22	1:H:242:ILE:HG13	1.85	0.56
1:G:72:MET:HG3	8:G:549:HOH:O	2.04	0.56
1:A:217:ARG:NH2	1:B:148:THR:H	2.03	0.56
1:C:23:TRP:HB3	1:C:266:VAL:HG21	1.87	0.56
1:F:230:VAL:HG11	1:F:277:MET:HE2	1.88	0.56
1:K:244:LEU:HD21	1:K:253:GLU:HG2	1.86	0.56
1:L:136:ILE:HG12	1:L:167:ILE:HB	1.87	0.56
1:D:101:GLY:HA2	1:D:104:MET:HG2	1.87	0.56
1:H:230:VAL:HG11	1:H:277:MET:HE2	1.86	0.56
1:B:6:ILE:HG13	1:B:167:ILE:HD11	1.88	0.56
1:I:118:ILE:HD11	1:I:137:VAL:HG12	1.87	0.56
1:I:203:ILE:HG22	1:I:266:VAL:HG13	1.87	0.56
1:E:123:LEU:O	1:E:127:MET:HG2	2.05	0.55
1:D:122:LYS:NZ	1:L:109:ALA:HB1	2.22	0.55
1:G:145:HIS:HB2	8:G:502[A]:HOH:O	2.04	0.55
1:B:61:ALA:HB1	1:I:23:TRP:HZ3	1.72	0.55
1:B:222:THR:HG22	1:B:242:ILE:HG13	1.89	0.55
1:I:123:LEU:O	1:I:127:MET:HG2	2.07	0.55
1:F:104:MET:HE1	1:F:114:VAL:HG11	1.88	0.55
1:C:136:ILE:HG12	1:C:167:ILE:HB	1.88	0.55
1:D:173:ALA:H	1:D:177:GLN:HG3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:VAL:HG13	1:F:267:ILE:HG13	1.89	0.55
1:K:226:THR:HA	1:K:251:LYS:NZ	2.22	0.55
1:C:151:THR:HG22	1:D:152:MET:HE3	1.88	0.54
1:L:159:VAL:HG11	1:L:185:GLY:HA3	1.89	0.54
1:G:47:MET:HE3	1:G:52:LEU:HA	1.89	0.54
1:A:6:ILE:HG13	1:A:167:ILE:HD11	1.89	0.54
1:A:123:LEU:O	1:A:127:MET:HG2	2.08	0.54
1:E:155:LEU:HD23	1:E:184:MET:HE3	1.89	0.54
1:D:309:LEU:HD22	1:D:312[B]:ARG:HE	1.72	0.54
1:B:237:LEU:HD11	1:B:257:LEU:HB3	1.89	0.54
1:J:73:LEU:HB2	1:J:97:ALA:O	2.07	0.54
1:H:179:LEU:HD21	1:H:309:LEU:HD22	1.90	0.54
1:J:123:LEU:O	1:J:127:MET:HG2	2.08	0.54
1:H:159:VAL:HG11	1:H:185:GLY:HA3	1.89	0.54
1:A:159:VAL:HG11	1:A:185:GLY:HA3	1.90	0.53
1:C:152:MET:HG2	1:D:152:MET:HE2	1.89	0.53
1:K:21:MET:HA	2:K:401:FMN:C5A	2.38	0.53
1:E:21:MET:HA	2:E:401:FMN:C5A	2.38	0.53
1:J:6:ILE:HG13	1:J:167:ILE:HD11	1.90	0.53
1:G:312:ARG:HH11	1:G:312:ARG:HG2	1.73	0.53
1:F:2:LYS:HE3	1:F:7:CYS:HB3	1.90	0.53
1:G:289:ARG:HB3	1:G:293:GLU:HB2	1.91	0.53
1:I:15:PRO:HD2	1:I:299:MET:HE1	1.90	0.53
1:F:289:ARG:HB2	1:F:294:ILE:HG13	1.89	0.53
1:C:48:GLU:CD	1:C:48:GLU:H	2.17	0.53
1:J:230:VAL:HG11	1:J:277:MET:HE2	1.90	0.53
1:I:136:ILE:HG12	1:I:167:ILE:HB	1.90	0.53
1:I:253:GLU:HA	1:I:256:LYS:HE2	1.91	0.53
1:D:21:MET:HA	2:D:401:FMN:C5A	2.39	0.52
1:H:173:ALA:H	1:H:177:GLN:HG3	1.74	0.52
1:H:303:LYS:HA	1:H:306:THR:OG1	2.10	0.52
1:D:310:LYS:HA	1:D:313:LEU:HD13	1.91	0.52
1:J:118:ILE:HD13	1:J:124:ALA:HB2	1.91	0.52
1:G:159:VAL:HG11	1:G:185:GLY:HA3	1.91	0.52
1:B:21:MET:HA	2:B:401:FMN:C5A	2.39	0.52
1:H:275:SER:OG	5:H:405:DMS:H23	2.09	0.52
1:D:36:ASP:HB3	1:D:292:LYS:HD2	1.90	0.52
1:A:277:MET:CE	5:A:405:DMS:H21	2.37	0.52
1:I:21:MET:HA	2:I:401:FMN:C5A	2.40	0.52
1:C:21:MET:HA	2:C:401:FMN:C5A	2.40	0.52
1:C:73:LEU:HB2	1:C:98:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:LYS:HA	1:F:259:THR:HG23	1.92	0.52
1:L:23:TRP:HB3	1:L:266:VAL:HG21	1.91	0.52
1:L:122:LYS:HD2	1:L:126:ARG:NH1	2.25	0.51
1:L:263:ARG:HG3	1:L:267:ILE:HD12	1.92	0.51
1:G:104:MET:HE1	1:G:114:VAL:HB	1.91	0.51
1:B:159:VAL:HG11	1:B:185:GLY:HA3	1.92	0.51
1:H:123:LEU:O	1:H:127:MET:HG2	2.10	0.51
1:K:159:VAL:HG11	1:K:185:GLY:HA3	1.92	0.51
1:G:118:ILE:HD11	1:G:137:VAL:HG22	1.92	0.51
1:A:136:ILE:HG12	1:A:167:ILE:HB	1.92	0.51
1:F:241:MET:HE3	1:F:254:ILE:HG23	1.91	0.51
4:J:405:A1CIO:C28	8:J:574:HOH:O	2.59	0.51
1:F:21:MET:HA	2:F:402:FMN:C5A	2.41	0.51
1:L:58:LYS:O	1:L:62:ILE:HG12	2.11	0.51
1:C:275:SER:OG	6:C:405:JEF:H383	2.10	0.51
1:D:118:ILE:HD11	1:D:137:VAL:HG22	1.93	0.50
1:F:23:TRP:O	1:F:266:VAL:HG21	2.11	0.50
1:L:117:VAL:HG22	1:L:136:ILE:HB	1.93	0.50
4:E:404:A1CIO:S30	4:E:404:A1CIO:N03	2.85	0.50
1:I:23:TRP:O	1:I:266:VAL:HG11	2.11	0.50
1:I:93:ILE:HD12	1:I:112:ILE:HG21	1.93	0.50
1:A:1:MET:CE	1:B:312:ARG:HH21	2.25	0.50
1:G:6:ILE:HD13	1:G:9:ILE:HD11	1.92	0.50
1:G:306:THR:HG21	1:H:312:ARG:HD2	1.93	0.50
1:A:73:LEU:HB2	1:A:98:GLY:HA3	1.94	0.50
1:G:120:THR:HG22	1:G:123:LEU:HB2	1.94	0.50
1:B:101:GLY:HA2	1:B:104:MET:HG2	1.93	0.50
1:I:237:LEU:HD11	1:I:257:LEU:HB3	1.92	0.50
1:F:259:THR:HA	6:F:407:JEF:O11	2.11	0.50
1:L:21:MET:HA	2:L:401:FMN:N5	2.25	0.50
1:A:21:MET:HA	2:A:401:FMN:C5A	2.42	0.49
1:G:136:ILE:HG12	1:G:167:ILE:HB	1.93	0.49
1:C:224:THR:HG22	1:C:229:PRO:HB3	1.93	0.49
1:K:73:LEU:HB2	1:K:97:ALA:O	2.12	0.49
1:K:242:ILE:O	1:K:246:ARG:HG3	2.12	0.49
1:A:289:ARG:HB2	1:A:294:ILE:HG13	1.94	0.49
1:E:308:VAL:C	1:E:310:LYS:H	2.19	0.49
1:G:45:GLY:O	1:G:75:ARG:HD2	2.12	0.49
1:H:21:MET:HA	2:H:401:FMN:C5A	2.42	0.49
1:C:4:ASN:OD1	1:C:6:ILE:HG22	2.13	0.49
1:A:310:LYS:HB2	1:A:313:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LYS:O	1:E:243:GLU:HG3	2.12	0.49
1:J:266:VAL:HG23	1:J:267:ILE:HG12	1.95	0.49
1:A:82:MET:HE2	1:A:106:LYS:HE2	1.94	0.49
1:D:222:THR:HG22	1:D:242:ILE:HG13	1.93	0.49
1:F:260:GLY:HA3	1:F:263:ARG:NH2	2.27	0.49
1:K:5:LYS:HB2	1:K:187:GLU:HG2	1.94	0.49
4:I:404:A1CIO:C20	8:I:545[A]:HOH:O	2.61	0.49
1:K:219:THR:HG22	1:K:233:ILE:HD13	1.95	0.49
1:K:289:ARG:HB3	1:K:293:GLU:HB2	1.93	0.49
1:B:116:PRO:CG	1:B:127:MET:HE2	2.43	0.48
1:F:135:VAL:HG13	1:F:164:ILE:HD11	1.93	0.48
1:K:26:GLY:HA2	1:K:42:ILE:HG23	1.95	0.48
1:L:196:LEU:HD23	1:L:211:ILE:HG13	1.94	0.48
1:K:314:GLU:HB3	1:L:3:ASN:ND2	2.28	0.48
1:K:155:LEU:HD23	1:K:184:MET:HE3	1.94	0.48
1:J:159:VAL:HG11	1:J:185:GLY:HA3	1.95	0.48
4:G:404:A1CIO:C29	8:G:502[A]:HOH:O	2.57	0.48
1:E:5:LYS:HB2	1:E:187:GLU:HG2	1.96	0.48
1:J:21:MET:HA	2:J:402:FMN:N5	2.29	0.48
1:L:306:THR:O	1:L:309:LEU:HB3	2.13	0.48
1:B:70:ASN:OD1	1:B:72:MET:HE2	2.13	0.48
1:C:100:PRO:HD2	1:C:127:MET:HE1	1.95	0.48
1:E:217:ARG:HD3	1:F:120:THR:HG21	1.94	0.48
1:C:27:GLY:HA3	1:C:58:LYS:HB2	1.95	0.48
1:J:145:HIS:HB3	4:J:405:A1CIO:C18	2.44	0.48
1:G:312:ARG:HG2	1:G:312:ARG:NH1	2.26	0.48
1:B:118:ILE:HD13	1:B:124:ALA:HB2	1.95	0.48
1:F:307:GLU:O	1:F:310:LYS:HD2	2.14	0.48
1:J:312:ARG:HH11	1:I:306:THR:CG2	2.20	0.48
1:A:120:THR:HG22	1:B:217[A]:ARG:HD2	1.94	0.48
1:A:152:MET:HG2	1:B:152:MET:HE2	1.95	0.48
4:D:404:A1CIO:C29	8:D:503:HOH:O	2.61	0.48
1:B:116:PRO:HG2	1:B:127:MET:HE2	1.96	0.48
1:E:54:GLU:HG2	1:E:58:LYS:HD2	1.96	0.48
1:D:145:HIS:HB3	4:D:404:A1CIO:C02	2.44	0.47
1:E:2:LYS:HG3	1:E:4:ASN:HB3	1.96	0.47
1:K:149:LEU:HD23	1:K:154:LEU:HD13	1.95	0.47
1:F:173:ALA:H	1:F:177:GLN:HG3	1.79	0.47
1:B:316:TRP:CE3	8:B:577:HOH:O	2.56	0.47
1:C:118:ILE:HD13	1:C:124:ALA:HB2	1.97	0.47
1:I:101:GLY:HA2	1:I:104:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:ASN:HA	1:L:94:THR:O	2.15	0.47
1:G:5:LYS:O	1:G:9:ILE:HG13	2.13	0.47
1:G:119:PRO:HB3	4:G:404:A1CIO:C15	2.44	0.47
1:K:145:HIS:CD2	4:K:404:A1CIO:N06	2.82	0.47
1:B:23:TRP:O	1:B:266:VAL:HG11	2.15	0.47
1:K:260:GLY:H	6:K:406:JEF:H372	1.79	0.47
1:L:73:LEU:HB2	1:L:98:GLY:HA3	1.95	0.47
1:L:304:LEU:O	1:L:308:VAL:HG23	2.14	0.47
1:A:143:GLY:HA3	2:A:401:FMN:HM82	1.97	0.47
1:B:21:MET:HA	2:B:401:FMN:N5	2.29	0.47
1:E:145:HIS:HE1	1:E:229:PRO:HD2	1.79	0.47
1:F:79:GLU:HA	1:F:82:MET:HE2	1.97	0.47
1:F:104:MET:HE1	1:F:114:VAL:HG21	1.96	0.47
1:I:47:MET:HE3	1:I:52:LEU:HA	1.95	0.47
1:K:135:VAL:HG13	1:K:164:ILE:HD11	1.97	0.47
1:B:123:LEU:O	1:B:127:MET:HG2	2.15	0.47
1:E:236:LYS:O	1:E:240:GLU:HG3	2.15	0.47
1:L:289:ARG:HB3	1:L:293:GLU:HB2	1.96	0.47
1:B:197:THR:HA	1:B:208:LYS:HD2	1.97	0.47
1:A:159:VAL:O	6:A:407:JEF:H33	2.15	0.46
1:C:4:ASN:HD21	1:C:187:GLU:HG3	1.81	0.46
1:L:4:ASN:OD1	1:L:187:GLU:HG3	2.15	0.46
1:E:289:ARG:NH2	8:E:501:HOH:O	2.48	0.46
1:A:70:ASN:HA	1:A:94:THR:O	2.16	0.46
1:D:152:MET:HE2	1:D:152:MET:HB2	1.81	0.46
1:J:2:LYS:C	1:J:4:ASN:H	2.24	0.46
1:G:21:MET:HA	2:G:401:FMN:C5A	2.46	0.46
1:L:118:ILE:HD13	1:L:124:ALA:HB2	1.96	0.46
1:L:307:GLU:C	1:L:309:LEU:H	2.24	0.46
1:D:312[B]:ARG:H	1:D:312[B]:ARG:HG2	1.51	0.46
1:E:73:LEU:HB2	1:E:97:ALA:O	2.16	0.46
1:J:56:ILE:O	1:J:60:LYS:HG2	2.15	0.46
1:K:72:MET:HB3	8:K:552:HOH:O	2.15	0.46
1:J:23:TRP:HB3	1:J:266:VAL:HG21	1.97	0.46
1:G:6:ILE:HG13	1:G:167:ILE:HD11	1.97	0.46
1:H:236:LYS:HD2	1:H:272:GLU:HG2	1.96	0.46
1:G:28:GLU:HG2	8:G:533:HOH:O	2.16	0.46
1:I:15:PRO:HD2	1:I:299:MET:CE	2.46	0.46
1:A:118:ILE:HD13	1:A:124:ALA:HB2	1.98	0.46
1:F:118:ILE:HD13	1:F:124:ALA:HB2	1.97	0.46
1:H:266:VAL:HG23	1:H:267:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:GLN:HB3	1:L:40:GLY:HA2	1.98	0.46
1:B:226:THR:HB	1:B:251:LYS:HZ3	1.79	0.46
1:C:53:ARG:NH2	1:C:84:VAL:HG22	2.30	0.46
1:E:234:GLU:HG2	1:E:239:LYS:HG3	1.98	0.46
1:I:119:PRO:HB3	4:I:404:A1CIO:C15	2.45	0.46
1:D:155:LEU:HD23	1:D:184:MET:HE3	1.98	0.46
1:D:237:LEU:HG	1:D:241:MET:HE2	1.98	0.46
1:L:126:ARG:HA	1:L:129:LYS:HE2	1.96	0.46
1:D:159:VAL:HG11	1:D:185:GLY:HA3	1.97	0.46
1:E:70:ASN:HA	1:E:94:THR:O	2.16	0.46
1:F:261:SER:HA	1:F:264:LEU:HD12	1.97	0.46
1:B:215:LYS:HA	1:B:215:LYS:HD3	1.74	0.45
1:E:304:LEU:O	1:E:308:VAL:HG23	2.17	0.45
1:J:21:MET:HA	2:J:402:FMN:C5A	2.46	0.45
1:I:14:TYR:HB3	1:I:299:MET:HE3	1.98	0.45
1:L:271:VAL:HA	1:L:276:PHE:CZ	2.51	0.45
1:C:152:MET:HB2	1:D:141:GLU:OE2	2.16	0.45
1:F:115:ILE:HG22	1:F:136:ILE:HG13	1.99	0.45
1:B:45:GLY:O	1:B:75:ARG:HD2	2.16	0.45
1:E:118:ILE:HD13	1:E:124:ALA:HB2	1.99	0.45
1:F:1:MET:HE3	1:F:4:ASN:HD22	1.82	0.45
1:F:116:PRO:HG3	1:F:127:MET:CE	2.43	0.45
1:F:169:ALA:HB2	1:F:190:GLN:HB3	1.98	0.45
1:K:82:MET:HE2	1:K:107:LEU:HD11	1.98	0.45
1:J:214:ALA:C	1:J:215:LYS:HD2	2.41	0.45
1:J:230:VAL:HG21	5:J:406:DMS:H23	1.98	0.45
1:K:2:LYS:HE3	1:K:2:LYS:HB2	1.77	0.45
1:H:231:ARG:NH1	1:H:280:GLN:HE21	2.15	0.45
1:L:289:ARG:HE	1:L:294:ILE:HD13	1.82	0.45
1:A:21:MET:HA	2:A:401:FMN:N5	2.31	0.45
4:I:404:A1CIO:C29	8:I:545[A]:HOH:O	2.63	0.45
1:L:115:ILE:HG22	1:L:136:ILE:HG13	1.99	0.45
1:L:225:SER:HB2	8:L:501:HOH:O	2.16	0.45
1:L:290:THR:O	1:L:294:ILE:HG12	2.17	0.45
1:C:70[A]:ASN:HA	1:C:94:THR:O	2.16	0.45
1:G:21:MET:HA	2:G:401:FMN:N5	2.32	0.45
1:I:159:VAL:HG11	1:I:185:GLY:HA3	1.99	0.45
1:H:118:ILE:HD13	1:H:124:ALA:HB2	1.98	0.45
1:I:46:GLY:HA2	1:I:75:ARG:HH21	1.82	0.45
1:L:20:ALA:HB2	1:L:41:ILE:HG22	1.99	0.45
1:D:303:LYS:HB3	1:D:303:LYS:HE3	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:HIS:HB2	8:F:503[A]:HOH:O	2.17	0.45
1:I:118:ILE:HD13	1:I:124:ALA:HB2	1.98	0.45
1:E:277:MET:HB2	2:E:401:FMN:C7M	2.47	0.44
1:F:258:GLY:CA	5:F:406:DMS:H22	2.40	0.44
1:J:315:ASN:ND2	1:I:2:LYS:HD2	2.31	0.44
1:L:35:LYS:HB2	1:L:63:THR:HB	1.98	0.44
6:B:406:JEF:H342	6:B:406:JEF:H362	1.60	0.44
1:J:70:ASN:HA	1:J:94:THR:O	2.16	0.44
1:A:96:GLY:HA2	1:A:117:VAL:O	2.18	0.44
1:D:236:LYS:HB2	1:D:236:LYS:HE3	1.78	0.44
1:F:230:VAL:HG12	1:F:232:VAL:HG13	1.99	0.44
1:J:309:LEU:HD23	1:J:309:LEU:HA	1.87	0.44
1:K:74:LEU:HB2	8:K:552:HOH:O	2.17	0.44
1:A:262:LEU:O	1:A:266:VAL:HG22	2.18	0.44
1:G:266:VAL:HG23	1:G:267:ILE:HG12	1.99	0.44
1:J:47:MET:HE3	1:J:52:LEU:HA	1.99	0.44
1:H:123:LEU:HD23	1:H:123:LEU:HA	1.85	0.44
1:A:117:VAL:HG22	1:A:136:ILE:HB	2.00	0.44
1:E:159:VAL:HG11	1:E:185:GLY:HA3	2.00	0.44
1:E:238:ALA:HA	1:E:241:MET:HE2	1.99	0.44
1:F:70:ASN:HA	1:F:94:THR:O	2.18	0.44
1:D:219:THR:HG22	1:D:233:ILE:HD13	1.99	0.44
1:F:263:ARG:HG3	6:F:407:JEF:H402	2.00	0.44
1:A:48:GLU:OE2	1:A:50:GLU:HB2	2.18	0.44
1:A:72:MET:HB3	8:A:549:HOH:O	2.18	0.44
1:C:217:ARG:HD3	1:D:120:THR:HG22	2.00	0.44
1:F:15:PRO:HD2	1:F:299:MET:HE1	1.98	0.44
1:A:237:LEU:HD11	1:A:257:LEU:HB3	2.00	0.44
1:C:70[B]:ASN:HA	1:C:94:THR:O	2.17	0.44
1:I:70:ASN:HA	1:I:94:THR:O	2.17	0.44
1:K:145:HIS:HB2	8:K:504[A]:HOH:O	2.17	0.44
1:C:224:THR:CG2	1:C:229:PRO:HB3	2.47	0.43
1:D:230:VAL:HG11	1:D:277:MET:HE2	1.99	0.43
1:J:46:GLY:O	6:J:407:JEF:O10	2.36	0.43
1:G:123:LEU:O	1:G:127:MET:HG2	2.18	0.43
1:H:308:VAL:C	1:H:310:LYS:H	2.26	0.43
1:L:21:MET:HA	2:L:401:FMN:C5A	2.48	0.43
1:L:105:GLU:HA	1:L:108:LYS:HB2	1.99	0.43
1:B:308:VAL:C	1:B:310:LYS:H	2.26	0.43
1:C:152:MET:HG3	1:D:151:THR:HB	2.00	0.43
1:E:289:ARG:HB2	1:E:294:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:213:LYS:HB3	1:J:213:LYS:HE2	1.67	0.43
1:G:18:GLN:HB3	1:G:40:GLY:HA2	2.00	0.43
1:B:219:THR:HG22	1:B:233:ILE:HD13	2.01	0.43
1:E:219:THR:HG22	1:E:233:ILE:HD13	2.00	0.43
1:J:120:THR:HG22	1:J:122:LYS:H	1.83	0.43
1:G:14:TYR:CE1	1:G:299:MET:HG3	2.53	0.43
1:H:155:LEU:HD23	1:H:184:MET:HE3	2.00	0.43
1:J:239:LYS:O	1:J:243:GLU:HG3	2.18	0.43
1:K:237:LEU:HD11	1:K:257:LEU:HB3	1.99	0.43
1:L:277:MET:O	2:L:401:FMN:HM73	2.19	0.43
6:B:406:JEF:H403	6:B:406:JEF:H322	1.52	0.43
1:L:263:ARG:HA	1:L:266:VAL:HG22	1.99	0.43
1:A:307:GLU:O	1:A:310:LYS:HG2	2.19	0.43
1:D:70:ASN:HA	1:D:94:THR:O	2.19	0.43
1:I:255:GLU:O	1:I:259:THR:HG23	2.18	0.43
1:K:194:ILE:HD13	1:K:298:LEU:HD11	2.00	0.43
4:F:405:A1CIO:C29	8:F:503[A]:HOH:O	2.66	0.43
1:C:82:MET:HE2	1:C:106:LYS:HD3	2.00	0.43
1:E:23:TRP:O	1:E:266:VAL:HG11	2.18	0.43
1:J:169:ALA:HB2	1:J:190:GLN:HB3	2.01	0.43
1:D:289:ARG:HB2	1:D:294:ILE:HG13	2.01	0.43
1:I:234:GLU:HG2	1:I:239:LYS:HG3	2.01	0.43
1:K:201:CYS:HB3	1:K:208:LYS:HZ1	1.83	0.43
1:C:92:VAL:HG22	1:C:113:LYS:HB2	2.00	0.42
1:E:252:GLU:O	1:E:256:LYS:HG3	2.18	0.42
1:E:277:MET:HB2	2:E:401:FMN:HM73	2.00	0.42
1:F:45:GLY:O	1:F:75:ARG:HD2	2.18	0.42
1:H:2:LYS:HB2	1:H:4:ASN:N	2.33	0.42
1:L:144:GLY:O	1:L:146:VAL:HG13	2.19	0.42
1:C:91:LYS:HE3	1:C:91:LYS:HB3	1.74	0.42
1:F:5:LYS:HE3	1:F:5:LYS:HB2	1.93	0.42
1:F:262:LEU:O	1:F:266:VAL:HG12	2.20	0.42
1:H:244:LEU:HD12	1:H:244:LEU:HA	1.84	0.42
1:L:79:GLU:HA	1:L:82:MET:HE3	2.02	0.42
1:A:118:ILE:HD11	1:A:137:VAL:HG12	2.00	0.42
1:D:45:GLY:O	1:D:75:ARG:HD2	2.20	0.42
1:F:234:GLU:HG2	1:F:239:LYS:HG3	2.01	0.42
1:J:120:THR:HG22	1:J:122:LYS:N	2.34	0.42
1:C:155:LEU:N	8:C:503:HOH:O	2.51	0.42
1:C:222:THR:HG21	6:C:405:JEF:H381	2.01	0.42
1:I:28:GLU:HG3	1:I:202:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:ILE:HD11	1:K:298:LEU:HD23	2.01	0.42
1:L:6:ILE:HG12	1:L:167:ILE:HD11	2.01	0.42
1:A:310:LYS:O	1:A:313:LEU:HB2	2.20	0.42
1:D:172:ILE:HG23	1:D:177:GLN:HB2	2.00	0.42
1:E:91:LYS:HE3	8:E:510:HOH:O	2.20	0.42
1:J:230:VAL:HG21	5:J:406:DMS:C2	2.50	0.42
1:I:2:LYS:C	1:I:4:ASN:H	2.28	0.42
1:C:135:VAL:HG13	1:C:164:ILE:HD11	2.00	0.42
1:C:155:LEU:HB3	1:C:156:PRO:HD3	2.01	0.42
1:F:159:VAL:HG11	1:F:185:GLY:HA3	2.02	0.42
1:K:120:THR:CG2	1:L:217:ARG:HD3	2.50	0.42
1:K:225:SER:OG	1:K:245:GLU:HG3	2.20	0.42
1:B:304:LEU:O	1:B:308:VAL:HG23	2.19	0.41
1:E:120:THR:HG22	1:E:122:LYS:H	1.85	0.41
1:K:28:GLU:HG2	1:K:29:LEU:N	2.34	0.41
1:K:120:THR:HG22	1:L:217:ARG:HD3	2.01	0.41
1:L:194:ILE:HD12	1:L:285:VAL:HG22	2.01	0.41
1:C:231:ARG:NH1	1:C:280:GLN:HE21	2.18	0.41
1:E:119:PRO:HD2	1:E:123:LEU:HD12	2.02	0.41
1:F:179:LEU:HD21	1:F:309:LEU:HD22	2.02	0.41
4:G:404:A1CIO:C05	8:G:503:HOH:O	2.67	0.41
1:A:28:GLU:H	1:A:28:GLU:CD	2.28	0.41
1:D:309:LEU:HD22	1:D:312[B]:ARG:NE	2.35	0.41
1:E:169:ALA:HB2	1:E:190:GLN:HB3	2.01	0.41
1:L:13:LYS:HD2	1:L:14:TYR:CE1	2.55	0.41
1:F:23:TRP:HB3	1:F:266:VAL:HG11	2.01	0.41
1:G:9:ILE:HD12	1:G:10:LEU:HG	2.02	0.41
1:G:289:ARG:HB2	1:G:294:ILE:HG13	2.02	0.41
1:K:207:TYR:CE2	1:K:266:VAL:HG12	2.55	0.41
1:K:312:ARG:C	1:K:315:ASN:H	2.28	0.41
1:C:236:LYS:HD3	1:C:272:GLU:CG	2.50	0.41
1:G:78:VAL:O	1:G:82:MET:HG3	2.20	0.41
6:H:406:JEF:H362	6:H:406:JEF:H322	1.70	0.41
1:K:100:PRO:HG2	1:K:130:ILE:HD11	2.02	0.41
1:B:28:GLU:HG3	1:B:202:LEU:HG	2.03	0.41
1:D:230:VAL:HG12	1:D:232:VAL:HG13	2.03	0.41
1:J:115:ILE:HG22	1:J:136:ILE:HG13	2.02	0.41
1:J:197:THR:HG21	1:J:212:LEU:HD13	2.02	0.41
1:G:304:LEU:O	1:G:308:VAL:HG23	2.20	0.41
1:I:60:LYS:HA	1:I:60:LYS:HD2	1.77	0.41
1:K:176:LYS:HB3	1:L:184:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HG	1:B:183:ALA:HB1	2.03	0.41
1:C:271:VAL:HA	1:C:276:PHE:CZ	2.56	0.41
1:D:28:GLU:CD	1:D:28:GLU:H	2.29	0.41
1:H:289:ARG:HB3	1:H:293:GLU:HB2	2.02	0.41
1:L:91[B]:LYS:HE3	1:L:91[B]:LYS:HB3	1.89	0.41
1:B:152:MET:HE2	1:B:152:MET:HB2	1.78	0.41
1:H:70:ASN:HA	1:H:94:THR:O	2.21	0.41
1:K:266:VAL:HG23	1:K:267:ILE:HG12	2.02	0.41
1:A:92:VAL:HG22	1:A:113:LYS:HB2	2.03	0.41
1:C:140:MET:HE2	1:C:140:MET:HB2	1.95	0.41
1:D:2:LYS:HE3	1:D:2:LYS:HB2	1.82	0.41
1:E:21:MET:HA	2:E:401:FMN:N5	2.35	0.41
1:G:117:VAL:HG22	1:G:136:ILE:HB	2.03	0.41
1:G:275:SER:OG	6:G:405:JEF:H371	2.20	0.41
1:A:252:GLU:HA	1:A:255:GLU:OE1	2.21	0.41
1:D:82:MET:HE2	1:D:107:LEU:HD11	2.02	0.41
1:D:172:ILE:HA	1:D:177:GLN:CB	2.51	0.41
1:D:306:THR:O	1:D:309:LEU:HB2	2.21	0.41
1:J:232:VAL:HG12	1:J:277:MET:HA	2.02	0.41
1:G:115:ILE:HG12	1:G:134:ALA:HB3	2.03	0.41
1:H:135:VAL:HG13	1:H:164:ILE:HD11	2.02	0.41
1:D:260:GLY:O	1:D:264:LEU:HG	2.21	0.40
1:D:308:VAL:C	1:D:310:LYS:H	2.29	0.40
1:F:119:PRO:HB3	4:F:405:A1CIO:C15	2.51	0.40
1:H:255:GLU:O	1:H:259:THR:HG23	2.20	0.40
1:L:69:VAL:HB	1:L:93:ILE:HD13	2.03	0.40
1:A:79:GLU:HG2	1:A:106:LYS:NZ	2.36	0.40
1:D:117:VAL:HG22	1:D:136:ILE:HB	2.03	0.40
1:D:118:ILE:HD13	1:D:124:ALA:HB2	2.02	0.40
1:D:123:LEU:O	1:D:127:MET:HG2	2.20	0.40
1:E:307:GLU:O	1:E:310:LYS:HG2	2.22	0.40
1:H:2:LYS:HB2	1:H:4:ASN:H	1.87	0.40
1:K:289:ARG:HB2	1:K:294:ILE:HG13	2.04	0.40
1:L:297:PHE:CD2	1:L:298:LEU:HD12	2.56	0.40
1:A:224:THR:HB	1:A:245[A]:GLU:OE2	2.21	0.40
1:B:54:GLU:O	1:B:58:LYS:HG3	2.21	0.40
1:B:149:LEU:HD12	1:B:154:LEU:HD13	2.02	0.40
1:F:231:ARG:NH1	1:F:280:GLN:HE21	2.20	0.40
1:J:312:ARG:NH1	1:I:306:THR:HG23	2.24	0.40
1:G:309:LEU:HD23	1:G:309:LEU:HA	1.93	0.40
1:K:30:ALA:HA	1:K:40:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:LYS:HD2	1:K:290:THR:HG22	2.04	0.40
1:K:231:ARG:NH1	1:K:280:GLN:HE21	2.19	0.40
1:C:216:ASP:HA	8:C:505:HOH:O	2.21	0.40
1:G:271:VAL:HA	1:G:276:PHE:CZ	2.56	0.40
1:H:115:ILE:HG22	1:H:136:ILE:HG13	2.04	0.40
1:A:217:ARG:HH21	1:B:148:THR:H	1.66	0.40
1:C:20:ALA:HB2	1:C:41:ILE:HG22	2.02	0.40
1:D:135:VAL:HG13	1:D:164:ILE:HD11	2.03	0.40
1:F:303:LYS:HA	1:F:303:LYS:HD2	1.94	0.40
1:H:140:MET:HE2	1:H:140:MET:HB2	1.97	0.40
1:I:177:GLN:NE2	1:I:284:MET:HE1	2.33	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	315/338 (93%)	303 (96%)	12 (4%)	0	100	100
1	B	315/338 (93%)	303 (96%)	12 (4%)	0	100	100
1	C	315/338 (93%)	301 (96%)	14 (4%)	0	100	100
1	D	316/338 (94%)	303 (96%)	13 (4%)	0	100	100
1	E	313/338 (93%)	303 (97%)	9 (3%)	1 (0%)	36	40
1	F	313/338 (93%)	301 (96%)	12 (4%)	0	100	100
1	G	313/338 (93%)	299 (96%)	13 (4%)	1 (0%)	36	40
1	H	313/338 (93%)	299 (96%)	12 (4%)	2 (1%)	21	21
1	I	312/338 (92%)	299 (96%)	12 (4%)	1 (0%)	36	40
1	J	312/338 (92%)	298 (96%)	14 (4%)	0	100	100
1	K	313/338 (93%)	304 (97%)	8 (3%)	1 (0%)	36	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	313/338 (93%)	300 (96%)	13 (4%)	0	100	100
All	All	3763/4056 (93%)	3613 (96%)	144 (4%)	6 (0%)	43	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	2	LYS
1	E	309	LEU
1	H	306	THR
1	K	119	PRO
1	H	119	PRO
1	I	119	PRO

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	252/270 (93%)	252 (100%)	0	100	100
1	B	252/270 (93%)	252 (100%)	0	100	100
1	C	252/270 (93%)	251 (100%)	1 (0%)	84	89
1	D	253/270 (94%)	250 (99%)	3 (1%)	63	74
1	E	250/270 (93%)	250 (100%)	0	100	100
1	F	250/270 (93%)	248 (99%)	2 (1%)	73	80
1	G	250/270 (93%)	248 (99%)	2 (1%)	73	80
1	H	250/270 (93%)	250 (100%)	0	100	100
1	I	249/270 (92%)	248 (100%)	1 (0%)	84	89
1	J	249/270 (92%)	248 (100%)	1 (0%)	84	89
1	K	250/270 (93%)	244 (98%)	6 (2%)	43	54
1	L	250/270 (93%)	249 (100%)	1 (0%)	84	89
All	All	3007/3240 (93%)	2990 (99%)	17 (1%)	78	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	224	THR
1	D	3	ASN
1	D	267	ILE
1	D	316	TRP
1	F	2	LYS
1	F	6	ILE
1	J	212	LEU
1	G	9	ILE
1	G	259	THR
1	I	264	LEU
1	K	2	LYS
1	K	73	LEU
1	K	118	ILE
1	K	212	LEU
1	K	255	GLU
1	K	310	LYS
1	L	309	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	157	GLN
1	B	157	GLN
1	B	315	ASN
1	C	3	ASN
1	C	157	GLN
1	D	70	ASN
1	D	157	GLN
1	D	205	GLN
1	D	209	ASN
1	D	286	ASN
1	E	70	ASN
1	E	157	GLN
1	E	205	GLN
1	E	228	HIS
1	E	286	ASN
1	F	157	GLN
1	J	157	GLN
1	J	315	ASN
1	H	157	GLN

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Mol	Chain	Res	Type
1	I	157	GLN
1	I	163	ASN
1	K	65	ASN
1	K	157	GLN
1	K	190	GLN
1	K	315	ASN
1	L	4	ASN
1	L	157	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 24 are monoatomic - leaving 54 for Mogul analysis.

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	$\# Z > 2$
6	JEF	I	406	-	7,7,40	0.34	0	6,6,48	0.14	0
2	FMN	C	401	-	33,33,33	1.05	2 (6%)	48,50,50	1.19	6 (12%)
5	DMS	F	401	-	3,3,3	0.19	0	3,3,3	0.08	0
4	A1CIO	G	404	-	32,33,33	2.71	13 (40%)	43,48,48	2.40	8 (18%)
2	FMN	I	401	-	33,33,33	1.04	2 (6%)	48,50,50	1.18	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	F	406	-	3,3,3	0.15	0	3,3,3	0.06	0
6	JEF	E	408	-	6,6,40	0.38	0	5,5,48	0.30	0
2	FMN	A	401	-	33,33,33	1.05	2 (6%)	48,50,50	1.19	6 (12%)
5	DMS	E	405	-	3,3,3	0.19	0	3,3,3	0.12	0
4	A1CIO	J	405	3	32,33,33	2.75	13 (40%)	43,48,48	2.44	10 (23%)
2	FMN	E	401	-	33,33,33	1.04	2 (6%)	48,50,50	1.18	6 (12%)
4	A1CIO	F	405	-	32,33,33	2.76	13 (40%)	43,48,48	2.32	8 (18%)
6	JEF	J	407	-	11,11,40	0.38	0	12,12,48	0.47	0
6	JEF	B	405	-	15,15,40	0.32	0	14,14,48	0.37	0
2	FMN	K	401	-	33,33,33	1.04	2 (6%)	48,50,50	1.21	7 (14%)
6	JEF	C	405	-	5,5,40	0.25	0	4,4,48	0.15	0
5	DMS	J	406	-	3,3,3	0.16	0	3,3,3	0.16	0
6	JEF	A	408	-	5,5,40	0.31	0	4,4,48	0.24	0
5	DMS	A	406	-	3,3,3	0.17	0	3,3,3	0.16	0
2	FMN	F	402	-	33,33,33	1.05	2 (6%)	48,50,50	1.21	7 (14%)
5	DMS	H	405	-	3,3,3	0.17	0	3,3,3	0.13	0
4	A1CIO	E	404	3	32,33,33	2.70	11 (34%)	43,48,48	2.73	12 (27%)
2	FMN	L	401	-	33,33,33	1.05	2 (6%)	48,50,50	1.16	6 (12%)
6	JEF	D	408	-	7,7,40	0.36	0	6,6,48	0.28	0
6	JEF	E	406	-	15,15,40	0.36	0	15,15,48	0.39	0
4	A1CIO	D	404	-	32,33,33	2.87	13 (40%)	43,48,48	2.57	11 (25%)
6	JEF	F	407	-	9,9,40	0.30	0	9,9,48	0.45	0
4	A1CIO	H	404	-	32,33,33	2.83	13 (40%)	43,48,48	2.55	8 (18%)
5	DMS	A	405	-	3,3,3	0.14	0	3,3,3	0.19	0
6	JEF	D	407	-	9,9,40	0.29	0	8,8,48	0.30	0
6	JEF	G	405	-	7,7,40	0.26	0	6,6,48	0.28	0
4	A1CIO	L	404	-	32,33,33	2.76	13 (40%)	43,48,48	2.36	8 (18%)
4	A1CIO	B	404	3	32,33,33	2.76	13 (40%)	43,48,48	2.38	8 (18%)
4	A1CIO	C	404	-	32,33,33	2.63	12 (37%)	43,48,48	2.72	12 (27%)
5	DMS	J	401	-	3,3,3	0.20	0	3,3,3	0.14	0
7	CIT	D	405	-	12,12,12	1.14	0	17,17,17	1.12	2 (11%)
4	A1CIO	I	404	3	32,33,33	2.74	13 (40%)	43,48,48	2.35	6 (13%)
6	JEF	K	406	-	8,8,40	0.33	0	7,7,48	0.23	0
5	DMS	K	405	-	3,3,3	0.18	0	3,3,3	0.13	0
6	JEF	E	407	-	9,9,40	0.31	0	9,9,48	0.39	0
4	A1CIO	A	404	-	32,33,33	2.77	13 (40%)	43,48,48	2.32	7 (16%)
2	FMN	H	401	-	33,33,33	1.04	2 (6%)	48,50,50	1.21	6 (12%)
2	FMN	G	401	-	33,33,33	1.04	2 (6%)	48,50,50	1.19	7 (14%)
6	JEF	H	406	-	6,6,40	0.29	0	5,5,48	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	D	401	-	33,33,33	1.04	2 (6%)	48,50,50	1.21	8 (16%)
6	JEF	A	407	-	8,8,40	0.15	0	8,8,48	0.34	0
6	JEF	B	406	-	11,11,40	0.36	0	12,12,48	0.51	0
5	DMS	C	407	-	3,3,3	0.18	0	3,3,3	0.12	0
5	DMS	C	406	-	3,3,3	0.16	0	3,3,3	0.13	0
2	FMN	B	401	-	33,33,33	1.05	2 (6%)	48,50,50	1.20	7 (14%)
5	DMS	D	406	-	3,3,3	0.19	0	3,3,3	0.09	0
4	A1CIO	K	404	3	32,33,33	2.71	13 (40%)	43,48,48	3.43	12 (27%)
2	FMN	J	402	-	33,33,33	1.04	2 (6%)	48,50,50	1.20	6 (12%)
5	DMS	I	405	-	3,3,3	0.21	0	3,3,3	0.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	JEF	I	406	-	-	3/5/5/46	-
2	FMN	C	401	-	-	4/18/18/18	0/3/3/3
4	A1CIO	G	404	-	-	4/19/19/19	0/4/4/4
2	FMN	I	401	-	-	4/18/18/18	0/3/3/3
6	JEF	E	408	-	-	3/4/4/46	-
2	FMN	A	401	-	-	4/18/18/18	0/3/3/3
4	A1CIO	J	405	3	-	4/19/19/19	0/4/4/4
2	FMN	E	401	-	-	7/18/18/18	0/3/3/3
4	A1CIO	F	405	-	-	6/19/19/19	0/4/4/4
6	JEF	J	407	-	-	7/10/10/46	-
6	JEF	B	405	-	-	9/13/13/46	-
2	FMN	K	401	-	-	4/18/18/18	0/3/3/3
6	JEF	C	405	-	-	3/3/3/46	-
6	JEF	A	408	-	-	1/3/3/46	-
2	FMN	F	402	-	-	4/18/18/18	0/3/3/3
4	A1CIO	E	404	3	-	1/19/19/19	0/4/4/4
2	FMN	L	401	-	-	4/18/18/18	0/3/3/3
6	JEF	D	408	-	-	5/5/5/46	-
6	JEF	E	406	-	-	7/14/14/46	-
4	A1CIO	D	404	-	-	5/19/19/19	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	JEF	F	407	-	-	6/7/7/46	-
4	A1CIO	H	404	-	-	3/19/19/19	0/4/4/4
6	JEF	D	407	-	-	4/7/7/46	-
6	JEF	G	405	-	-	3/5/5/46	-
4	A1CIO	L	404	-	-	6/19/19/19	0/4/4/4
4	A1CIO	B	404	3	-	7/19/19/19	0/4/4/4
4	A1CIO	C	404	-	-	2/19/19/19	0/4/4/4
7	CIT	D	405	-	-	11/16/16/16	-
4	A1CIO	I	404	3	-	5/19/19/19	0/4/4/4
6	JEF	K	406	-	-	2/6/6/46	-
6	JEF	E	407	-	-	3/8/8/46	-
4	A1CIO	A	404	-	-	6/19/19/19	0/4/4/4
2	FMN	H	401	-	-	4/18/18/18	0/3/3/3
2	FMN	G	401	-	-	4/18/18/18	0/3/3/3
6	JEF	H	406	-	-	3/4/4/46	-
2	FMN	D	401	-	-	4/18/18/18	0/3/3/3
6	JEF	A	407	-	-	4/7/7/46	-
6	JEF	B	406	-	-	6/10/10/46	-
2	FMN	B	401	-	-	4/18/18/18	0/3/3/3
4	A1CIO	K	404	3	-	6/19/19/19	0/4/4/4
2	FMN	J	402	-	-	4/18/18/18	0/3/3/3

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	404	A1CIO	C04-C05	7.28	1.53	1.49
4	J	405	A1CIO	C04-C05	7.25	1.53	1.49
4	D	404	A1CIO	C04-C05	7.11	1.53	1.49
4	H	404	A1CIO	C04-C05	7.04	1.53	1.49
4	K	404	A1CIO	C04-C05	6.92	1.53	1.49
4	F	405	A1CIO	C04-C05	6.86	1.53	1.49
4	B	404	A1CIO	C18-S30	-6.52	1.67	1.75
4	I	404	A1CIO	C04-C05	6.50	1.53	1.49
4	A	404	A1CIO	C04-C05	6.50	1.53	1.49
4	G	404	A1CIO	C04-C05	6.49	1.53	1.49
4	D	404	A1CIO	C18-S30	-6.37	1.67	1.75
4	A	404	A1CIO	C18-S30	-6.08	1.68	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	404	A1CIO	C18-N17	6.04	1.47	1.38
4	H	404	A1CIO	C18-S30	-5.95	1.68	1.75
4	L	404	A1CIO	C18-S30	-5.94	1.68	1.75
4	I	404	A1CIO	C18-S30	-5.89	1.68	1.75
4	E	404	A1CIO	C18-S30	-5.86	1.68	1.75
4	C	404	A1CIO	C04-C05	5.78	1.53	1.49
4	F	405	A1CIO	C18-S30	-5.76	1.68	1.75
4	E	404	A1CIO	C02-N03	5.67	1.46	1.35
4	B	404	A1CIO	C04-C05	5.66	1.52	1.49
4	G	404	A1CIO	C18-S30	-5.64	1.68	1.75
4	J	405	A1CIO	C18-N17	5.64	1.46	1.38
4	K	404	A1CIO	C18-N17	5.62	1.46	1.38
4	C	404	A1CIO	C18-S30	-5.51	1.68	1.75
4	H	404	A1CIO	C18-N17	5.49	1.46	1.38
4	A	404	A1CIO	C18-N17	5.47	1.46	1.38
4	D	404	A1CIO	C02-N03	5.46	1.46	1.35
4	D	404	A1CIO	C18-N17	5.45	1.46	1.38
4	B	404	A1CIO	C18-N17	5.43	1.46	1.38
4	H	404	A1CIO	C02-N03	5.42	1.46	1.35
4	G	404	A1CIO	C18-N17	5.41	1.46	1.38
4	K	404	A1CIO	C02-N03	5.41	1.46	1.35
4	G	404	A1CIO	C02-N03	5.37	1.46	1.35
4	F	405	A1CIO	C18-N17	5.37	1.46	1.38
4	A	404	A1CIO	C02-N03	5.37	1.46	1.35
4	J	405	A1CIO	C18-S30	-5.36	1.69	1.75
4	F	405	A1CIO	C02-N03	5.35	1.46	1.35
4	J	405	A1CIO	C02-N03	5.33	1.46	1.35
4	C	404	A1CIO	C18-N17	5.33	1.46	1.38
4	I	404	A1CIO	C18-N17	5.27	1.46	1.38
4	K	404	A1CIO	C18-S30	-5.26	1.69	1.75
4	C	404	A1CIO	C02-N03	5.25	1.45	1.35
4	I	404	A1CIO	C02-N03	5.25	1.45	1.35
4	B	404	A1CIO	C02-N03	5.25	1.45	1.35
4	L	404	A1CIO	C02-N03	4.94	1.45	1.35
4	L	404	A1CIO	C18-N17	4.94	1.45	1.38
4	E	404	A1CIO	C29-S30	-4.79	1.64	1.74
4	L	404	A1CIO	C29-S30	-4.77	1.64	1.74
4	C	404	A1CIO	C07-N06	-4.77	1.30	1.39
4	D	404	A1CIO	C29-S30	-4.56	1.65	1.74
4	H	404	A1CIO	C29-S30	-4.50	1.65	1.74
4	B	404	A1CIO	C29-S30	-4.49	1.65	1.74
4	I	404	A1CIO	C29-S30	-4.37	1.65	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	A1CIO	C29-S30	-4.33	1.65	1.74
4	D	404	A1CIO	C18-N19	4.33	1.39	1.30
4	B	404	A1CIO	C07-N06	-4.32	1.31	1.39
4	E	404	A1CIO	C18-N19	4.26	1.39	1.30
4	F	405	A1CIO	C29-S30	-4.23	1.66	1.74
4	H	404	A1CIO	C18-N19	4.19	1.39	1.30
4	B	404	A1CIO	C18-N19	4.19	1.39	1.30
4	G	404	A1CIO	C29-S30	-4.17	1.66	1.74
4	E	404	A1CIO	C07-N06	-4.14	1.32	1.39
4	H	404	A1CIO	C08-C07	4.13	1.53	1.47
4	L	404	A1CIO	C07-N06	-4.12	1.32	1.39
4	A	404	A1CIO	C07-N06	-4.11	1.32	1.39
4	A	404	A1CIO	C18-N19	4.09	1.38	1.30
4	E	404	A1CIO	C04-C05	4.06	1.51	1.49
4	I	404	A1CIO	C07-N06	-4.05	1.32	1.39
4	F	405	A1CIO	C07-N06	-4.05	1.32	1.39
4	C	404	A1CIO	C29-S30	-4.03	1.66	1.74
4	F	405	A1CIO	C18-N19	4.03	1.38	1.30
4	I	404	A1CIO	C18-N19	4.03	1.38	1.30
4	G	404	A1CIO	C18-N19	4.03	1.38	1.30
4	D	404	A1CIO	C08-C07	3.97	1.53	1.47
4	J	405	A1CIO	C29-S30	-3.97	1.66	1.74
4	J	405	A1CIO	C08-C07	3.95	1.53	1.47
4	I	404	A1CIO	C08-C07	3.95	1.53	1.47
4	J	405	A1CIO	C07-N06	-3.90	1.32	1.39
4	J	405	A1CIO	C18-N19	3.87	1.38	1.30
4	G	404	A1CIO	C07-N06	-3.84	1.32	1.39
4	F	405	A1CIO	C08-C07	3.83	1.53	1.47
4	D	404	A1CIO	C07-N06	-3.83	1.32	1.39
4	K	404	A1CIO	C07-N06	-3.82	1.32	1.39
4	B	404	A1CIO	C08-C07	3.82	1.53	1.47
4	K	404	A1CIO	C08-C07	3.82	1.53	1.47
4	A	404	A1CIO	C08-C07	3.79	1.53	1.47
4	C	404	A1CIO	C18-N19	3.75	1.38	1.30
4	K	404	A1CIO	C18-N19	3.73	1.38	1.30
4	G	404	A1CIO	C08-C07	3.72	1.53	1.47
4	L	404	A1CIO	C08-C07	3.68	1.53	1.47
4	H	404	A1CIO	C07-N06	-3.66	1.32	1.39
4	L	404	A1CIO	C18-N19	3.61	1.38	1.30
4	K	404	A1CIO	C29-S30	-3.57	1.67	1.74
2	G	401	FMN	C4A-N5	3.51	1.38	1.30
4	C	404	A1CIO	C08-C07	3.50	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	402	FMN	C4A-N5	3.49	1.38	1.30
2	C	401	FMN	C4A-N5	3.48	1.38	1.30
2	J	402	FMN	C4A-N5	3.48	1.38	1.30
2	K	401	FMN	C4A-N5	3.47	1.38	1.30
2	L	401	FMN	C4A-N5	3.46	1.38	1.30
2	H	401	FMN	C4A-N5	3.44	1.38	1.30
2	D	401	FMN	C4A-N5	3.43	1.38	1.30
2	A	401	FMN	C4A-N5	3.43	1.38	1.30
2	E	401	FMN	C4A-N5	3.42	1.38	1.30
4	E	404	A1CIO	C02-N17	3.41	1.47	1.39
2	B	401	FMN	C4A-N5	3.41	1.38	1.30
2	I	401	FMN	C4A-N5	3.37	1.38	1.30
4	K	404	A1CIO	C02-N17	3.18	1.46	1.39
4	E	404	A1CIO	C20-N19	3.13	1.46	1.39
4	D	404	A1CIO	C20-N19	3.11	1.46	1.39
4	H	404	A1CIO	C20-N19	3.07	1.46	1.39
4	J	405	A1CIO	C02-N17	3.01	1.46	1.39
4	I	404	A1CIO	C20-N19	2.95	1.45	1.39
4	B	404	A1CIO	C20-N19	2.90	1.45	1.39
4	G	404	A1CIO	C20-N19	2.87	1.45	1.39
4	F	405	A1CIO	C20-N19	2.85	1.45	1.39
4	E	404	A1CIO	C08-C07	2.83	1.51	1.47
4	G	404	A1CIO	C02-N17	2.81	1.45	1.39
4	A	404	A1CIO	C20-N19	2.80	1.45	1.39
4	F	405	A1CIO	C02-N17	2.80	1.45	1.39
4	C	404	A1CIO	C02-N17	2.77	1.45	1.39
4	A	404	A1CIO	C02-N17	2.76	1.45	1.39
4	H	404	A1CIO	C02-N17	2.76	1.45	1.39
4	I	404	A1CIO	C02-N17	2.71	1.45	1.39
4	E	404	A1CIO	C15-N16	-2.69	1.30	1.36
4	L	404	A1CIO	C20-N19	2.67	1.45	1.39
2	C	401	FMN	C10-N1	2.64	1.38	1.33
4	C	404	A1CIO	C20-N19	2.63	1.45	1.39
4	D	404	A1CIO	C02-N17	2.62	1.45	1.39
2	B	401	FMN	C10-N1	2.59	1.38	1.33
2	J	402	FMN	C10-N1	2.59	1.38	1.33
2	F	402	FMN	C10-N1	2.58	1.38	1.33
4	B	404	A1CIO	C02-N17	2.57	1.45	1.39
2	E	401	FMN	C10-N1	2.57	1.38	1.33
2	L	401	FMN	C10-N1	2.57	1.38	1.33
2	A	401	FMN	C10-N1	2.56	1.38	1.33
2	I	401	FMN	C10-N1	2.56	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	405	A1CIO	C20-N19	2.56	1.45	1.39
2	G	401	FMN	C10-N1	2.55	1.38	1.33
2	D	401	FMN	C10-N1	2.53	1.38	1.33
2	H	401	FMN	C10-N1	2.49	1.38	1.33
2	K	401	FMN	C10-N1	2.48	1.38	1.33
4	L	404	A1CIO	C15-N16	-2.48	1.31	1.36
4	H	404	A1CIO	C15-N16	-2.43	1.31	1.36
4	K	404	A1CIO	O01-C02	-2.41	1.18	1.23
4	L	404	A1CIO	BR12-C11	2.41	1.95	1.90
4	L	404	A1CIO	C02-N17	2.35	1.44	1.39
4	D	404	A1CIO	C15-N16	-2.31	1.31	1.36
4	G	404	A1CIO	C15-N16	-2.30	1.31	1.36
4	K	404	A1CIO	C15-N16	-2.29	1.31	1.36
4	K	404	A1CIO	C20-N19	2.26	1.44	1.39
4	B	404	A1CIO	O01-C02	-2.19	1.18	1.23
4	H	404	A1CIO	BR12-C11	2.15	1.94	1.90
4	B	404	A1CIO	C15-N16	-2.15	1.31	1.36
4	F	405	A1CIO	BR12-C11	2.14	1.94	1.90
4	J	405	A1CIO	BR12-C11	2.14	1.94	1.90
4	J	405	A1CIO	C15-N16	-2.14	1.31	1.36
4	I	404	A1CIO	BR12-C11	2.13	1.94	1.90
4	B	404	A1CIO	BR12-C11	2.13	1.94	1.90
4	A	404	A1CIO	BR12-C11	2.12	1.94	1.90
4	F	405	A1CIO	C15-N16	-2.12	1.31	1.36
4	K	404	A1CIO	BR12-C11	2.12	1.94	1.90
4	I	404	A1CIO	C15-N16	-2.11	1.31	1.36
4	D	404	A1CIO	BR12-C11	2.11	1.94	1.90
4	A	404	A1CIO	O01-C02	-2.10	1.18	1.23
4	A	404	A1CIO	C15-N16	-2.10	1.31	1.36
4	F	405	A1CIO	O01-C02	-2.10	1.18	1.23
4	C	404	A1CIO	BR12-C11	2.09	1.94	1.90
4	G	404	A1CIO	O01-C02	-2.08	1.18	1.23
4	G	404	A1CIO	BR12-C11	2.08	1.94	1.90
4	L	404	A1CIO	O01-C02	-2.08	1.18	1.23
4	C	404	A1CIO	O01-C02	-2.07	1.19	1.23
4	D	404	A1CIO	O01-C02	-2.07	1.19	1.23
4	J	405	A1CIO	O01-C02	-2.05	1.19	1.23
4	I	404	A1CIO	O01-C02	-2.03	1.19	1.23
4	H	404	A1CIO	O01-C02	-2.02	1.19	1.23

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	404	A1CIO	C29-S30-C18	11.97	99.41	88.33
4	G	404	A1CIO	C29-S30-C18	10.79	98.32	88.33
4	J	405	A1CIO	C29-S30-C18	10.73	98.26	88.33
4	K	404	A1CIO	C29-S30-C18	10.69	98.23	88.33
4	H	404	A1CIO	C29-S30-C18	10.69	98.22	88.33
4	F	405	A1CIO	C29-S30-C18	10.60	98.14	88.33
4	I	404	A1CIO	C29-S30-C18	10.59	98.13	88.33
4	C	404	A1CIO	C29-S30-C18	10.57	98.11	88.33
4	L	404	A1CIO	C29-S30-C18	10.26	97.82	88.33
4	D	404	A1CIO	C29-S30-C18	10.21	97.78	88.33
4	A	404	A1CIO	C29-S30-C18	10.18	97.75	88.33
4	B	404	A1CIO	C29-S30-C18	9.93	97.52	88.33
4	K	404	A1CIO	N17-C02-N03	8.32	132.43	116.01
4	K	404	A1CIO	C04-N03-C02	7.77	132.82	120.66
4	K	404	A1CIO	C18-N17-C02	7.55	137.18	124.54
4	E	404	A1CIO	S30-C18-N19	-7.41	108.15	117.06
4	K	404	A1CIO	S30-C18-N19	-6.99	108.66	117.06
4	J	405	A1CIO	S30-C18-N19	-6.64	109.08	117.06
4	D	404	A1CIO	N17-C18-N19	6.56	132.07	120.87
4	C	404	A1CIO	S30-C18-N19	-6.40	109.37	117.06
4	G	404	A1CIO	S30-C18-N19	-6.35	109.43	117.06
4	F	405	A1CIO	S30-C18-N19	-6.17	109.64	117.06
4	I	404	A1CIO	S30-C18-N19	-6.09	109.74	117.06
4	A	404	A1CIO	S30-C18-N19	-6.09	109.74	117.06
4	H	404	A1CIO	S30-C18-N19	-6.08	109.75	117.06
4	C	404	A1CIO	C04-C05-N16	6.05	132.44	122.96
4	B	404	A1CIO	S30-C18-N19	-5.83	110.06	117.06
4	K	404	A1CIO	S30-C18-N17	5.78	131.99	121.87
4	D	404	A1CIO	S30-C18-N19	-5.76	110.13	117.06
4	L	404	A1CIO	S30-C18-N19	-5.74	110.16	117.06
4	B	404	A1CIO	N17-C18-N19	5.65	130.52	120.87
4	H	404	A1CIO	N17-C18-N19	5.63	130.49	120.87
4	C	404	A1CIO	C14-C08-C07	-5.42	114.80	120.87
4	K	404	A1CIO	O01-C02-N03	-5.34	113.30	122.47
4	H	404	A1CIO	C08-C07-N06	5.09	127.74	119.95
4	L	404	A1CIO	N17-C18-N19	4.85	129.15	120.87
4	A	404	A1CIO	N17-C18-N19	4.78	129.03	120.87
4	I	404	A1CIO	N17-C18-N19	4.63	128.77	120.87
4	D	404	A1CIO	C18-N17-C02	4.56	132.17	124.54
4	D	404	A1CIO	C08-C07-N06	4.22	126.41	119.95
4	E	404	A1CIO	C04-N03-C02	4.14	127.13	120.66
4	E	404	A1CIO	C08-C07-N06	4.11	126.24	119.95
4	G	404	A1CIO	N17-C18-N19	4.06	127.81	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	404	A1CIO	C08-C07-N06	4.00	126.07	119.95
4	F	405	A1CIO	N17-C18-N19	3.90	127.54	120.87
4	K	404	A1CIO	C28-C29-C20	-3.81	119.16	121.99
4	L	404	A1CIO	C08-C07-N06	3.75	125.70	119.95
4	C	404	A1CIO	C04-C05-N06	-3.69	119.59	124.41
4	A	404	A1CIO	C04-C05-N16	3.67	128.72	122.96
4	B	404	A1CIO	C04-C05-N16	3.65	128.68	122.96
4	C	404	A1CIO	C09-C08-C07	3.55	124.85	120.87
4	K	404	A1CIO	C08-C07-N06	3.55	125.39	119.95
4	K	404	A1CIO	C28-C29-S30	3.43	134.63	126.07
4	I	404	A1CIO	C04-C05-N16	3.43	128.34	122.96
4	B	404	A1CIO	C18-N17-C02	3.42	130.26	124.54
4	E	404	A1CIO	N17-C18-N19	3.36	126.61	120.87
4	I	404	A1CIO	C08-C07-N06	3.25	124.92	119.95
4	E	404	A1CIO	C08-C07-C15	-3.22	124.42	129.06
2	A	401	FMN	C4-N3-C2	-3.19	119.97	125.64
2	K	401	FMN	C4-N3-C2	-3.18	119.99	125.64
4	F	405	A1CIO	C04-C05-N16	3.18	127.94	122.96
2	D	401	FMN	C4-N3-C2	-3.15	120.04	125.64
2	F	402	FMN	C4-N3-C2	-3.14	120.06	125.64
2	C	401	FMN	C4-N3-C2	-3.13	120.09	125.64
2	H	401	FMN	C4-N3-C2	-3.11	120.12	125.64
4	F	405	A1CIO	C08-C07-N06	3.09	124.69	119.95
4	H	404	A1CIO	C08-C07-C15	-3.09	124.61	129.06
4	J	405	A1CIO	C28-C29-S30	3.06	133.72	126.07
2	E	401	FMN	C4-N3-C2	-3.04	120.24	125.64
2	J	402	FMN	C4-N3-C2	-3.02	120.29	125.64
4	J	405	A1CIO	C08-C07-N06	3.00	124.55	119.95
2	B	401	FMN	C4-N3-C2	-2.99	120.33	125.64
4	C	404	A1CIO	C28-C29-S30	2.98	133.50	126.07
4	J	405	A1CIO	N17-C18-N19	2.97	125.94	120.87
2	I	401	FMN	C4-N3-C2	-2.96	120.39	125.64
4	D	404	A1CIO	C04-N03-C02	2.95	125.27	120.66
4	H	404	A1CIO	C18-N17-C02	2.93	129.44	124.54
2	G	401	FMN	C4-N3-C2	-2.93	120.44	125.64
2	L	401	FMN	C4-N3-C2	-2.91	120.47	125.64
4	J	405	A1CIO	C04-C05-N16	2.80	127.35	122.96
4	A	404	A1CIO	C08-C07-N06	2.80	124.24	119.95
4	C	404	A1CIO	C08-C07-C15	2.78	133.07	129.06
4	J	405	A1CIO	C28-C29-C20	-2.74	119.95	121.99
4	G	404	A1CIO	C28-C29-S30	2.73	132.89	126.07
4	K	404	A1CIO	O01-C02-N17	-2.71	114.27	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	404	A1CIO	C04-C05-N16	2.70	127.19	122.96
2	H	401	FMN	C4A-C10-N10	2.66	120.29	116.48
4	F	405	A1CIO	C28-C29-S30	2.66	132.70	126.07
4	C	404	A1CIO	C28-C29-C20	-2.63	120.03	121.99
4	D	404	A1CIO	C04-C05-N16	2.63	127.08	122.96
4	B	404	A1CIO	C08-C07-N06	2.61	123.95	119.95
2	F	402	FMN	C4A-C4-N3	2.60	119.88	113.25
2	I	401	FMN	C4A-C10-N10	2.60	120.20	116.48
4	C	404	A1CIO	N17-C18-N19	2.59	125.30	120.87
2	A	401	FMN	C4A-C4-N3	2.58	119.83	113.25
2	J	402	FMN	C4A-C4-N3	2.58	119.82	113.25
2	K	401	FMN	C4A-C10-N10	2.58	120.17	116.48
2	C	401	FMN	C4A-C4-N3	2.58	119.82	113.25
2	J	402	FMN	C4A-C10-N10	2.58	120.17	116.48
2	D	401	FMN	C4A-C4-N3	2.57	119.81	113.25
2	K	401	FMN	C4A-C4-N3	2.56	119.77	113.25
2	B	401	FMN	C4A-C4-N3	2.54	119.72	113.25
2	D	401	FMN	C4A-C10-N10	2.53	120.11	116.48
2	E	401	FMN	C4A-C4-N3	2.53	119.68	113.25
2	A	401	FMN	C4A-C10-N10	2.52	120.08	116.48
2	G	401	FMN	C4A-C4-N3	2.51	119.65	113.25
2	L	401	FMN	C4A-C4-N3	2.51	119.64	113.25
2	C	401	FMN	C4A-C10-N10	2.50	120.06	116.48
2	H	401	FMN	C4A-C4-N3	2.50	119.61	113.25
2	I	401	FMN	C4A-C4-N3	2.49	119.58	113.25
2	E	401	FMN	C4A-C10-N10	2.49	120.04	116.48
2	L	401	FMN	O4-C4-C4A	-2.46	120.03	126.53
2	L	401	FMN	C4A-C10-N10	2.46	120.01	116.48
4	L	404	A1CIO	C28-C29-S30	2.46	132.21	126.07
2	B	401	FMN	C4A-C10-N10	2.46	120.00	116.48
4	I	404	A1CIO	C28-C29-S30	2.46	132.21	126.07
2	C	401	FMN	O4-C4-C4A	-2.46	120.05	126.53
4	A	404	A1CIO	C28-C29-S30	2.45	132.19	126.07
2	A	401	FMN	O4-C4-C4A	-2.45	120.06	126.53
2	F	402	FMN	C4A-C10-N10	2.45	119.99	116.48
2	E	401	FMN	O4-C4-C4A	-2.44	120.08	126.53
2	D	401	FMN	O4-C4-C4A	-2.44	120.08	126.53
2	G	401	FMN	C4A-C10-N10	2.44	119.98	116.48
2	F	402	FMN	O4-C4-C4A	-2.44	120.09	126.53
2	J	402	FMN	O4-C4-C4A	-2.43	120.12	126.53
2	H	401	FMN	O4-C4-C4A	-2.42	120.15	126.53
2	K	401	FMN	O4-C4-C4A	-2.41	120.17	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	402	FMN	C10-C4A-N5	-2.40	119.91	124.81
2	G	401	FMN	O4-C4-C4A	-2.40	120.21	126.53
4	K	404	A1CIO	C20-C29-S30	-2.40	106.21	109.75
2	B	401	FMN	O4-C4-C4A	-2.39	120.23	126.53
2	G	401	FMN	C10-C4A-N5	-2.38	119.95	124.81
2	I	401	FMN	O4-C4-C4A	-2.37	120.27	126.53
2	E	401	FMN	C10-C4A-N5	-2.36	119.98	124.81
2	K	401	FMN	C10-C4A-N5	-2.36	119.99	124.81
4	H	404	A1CIO	C28-C29-S30	2.36	131.95	126.07
2	H	401	FMN	C10-C4A-N5	-2.35	120.01	124.81
2	F	402	FMN	C10-C4A-N5	-2.34	120.03	124.81
7	D	405	CIT	O5-C6-C3	-2.33	117.57	122.09
4	D	404	A1CIO	S30-C18-N17	-2.33	117.79	121.87
4	E	404	A1CIO	C28-C29-S30	2.32	131.87	126.07
2	G	401	FMN	C4'-C3'-C2'	-2.32	109.70	113.57
4	J	405	A1CIO	C20-C29-S30	-2.31	106.33	109.75
2	A	401	FMN	C10-C4A-N5	-2.31	120.09	124.81
2	C	401	FMN	C10-C4A-N5	-2.31	120.09	124.81
2	I	401	FMN	C10-C4A-N5	-2.30	120.11	124.81
2	D	401	FMN	C10-C4A-N5	-2.30	120.12	124.81
2	L	401	FMN	C10-C4A-N5	-2.30	120.12	124.81
4	B	404	A1CIO	C28-C29-S30	2.26	131.71	126.07
2	B	401	FMN	C10-C4A-N5	-2.25	120.22	124.81
2	B	401	FMN	C9A-C5A-N5	-2.25	120.07	122.45
4	E	404	A1CIO	C14-C08-C09	2.23	121.41	118.57
4	L	404	A1CIO	C14-C08-C07	-2.23	118.38	120.87
7	D	405	CIT	O6-C6-C3	2.22	117.41	113.14
2	F	402	FMN	C9A-C5A-N5	-2.22	120.10	122.45
4	C	404	A1CIO	C20-C29-S30	-2.22	106.47	109.75
4	D	404	A1CIO	C08-C07-C15	-2.22	125.86	129.06
2	B	401	FMN	C5A-C9A-N10	2.22	119.97	117.97
4	G	404	A1CIO	C20-C29-S30	-2.21	106.49	109.75
4	A	404	A1CIO	C28-C29-C20	-2.20	120.35	121.99
4	E	404	A1CIO	C20-C29-S30	-2.20	106.50	109.75
2	D	401	FMN	C9A-C5A-N5	-2.19	120.13	122.45
4	E	404	A1CIO	C29-C28-C23	-2.17	119.61	122.09
2	K	401	FMN	C9A-C5A-N5	-2.17	120.15	122.45
2	D	401	FMN	C5A-C9A-N10	2.16	119.92	117.97
2	K	401	FMN	C5A-C9A-N10	2.16	119.92	117.97
4	D	404	A1CIO	C28-C29-S30	2.15	131.45	126.07
4	B	404	A1CIO	C28-C29-C20	-2.15	120.39	121.99
4	J	405	A1CIO	C18-N17-C02	-2.14	120.96	124.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	402	FMN	C9A-C5A-N5	-2.14	120.19	122.45
4	E	404	A1CIO	N17-C02-N03	2.10	120.15	116.01
2	G	401	FMN	C9A-C5A-N5	-2.08	120.25	122.45
2	H	401	FMN	C9A-C5A-N5	-2.08	120.25	122.45
4	F	405	A1CIO	C20-C29-S30	-2.07	106.69	109.75
4	J	405	A1CIO	N17-C02-N03	2.07	120.09	116.01
4	G	404	A1CIO	C04-C05-N16	2.06	126.20	122.96
4	G	404	A1CIO	C08-C07-C15	-2.06	126.09	129.06
2	D	401	FMN	C4A-C10-N1	-2.05	119.56	124.59
4	E	404	A1CIO	C14-C08-C07	-2.05	118.58	120.87
2	A	401	FMN	C4A-C10-N1	-2.04	119.58	124.59
2	E	401	FMN	C9A-C5A-N5	-2.04	120.29	122.45
2	C	401	FMN	C4A-C10-N1	-2.03	119.61	124.59
4	L	404	A1CIO	C20-C29-S30	-2.03	106.75	109.75
4	H	404	A1CIO	F26-C24-C23	-2.03	108.56	112.90
4	F	405	A1CIO	C29-C28-C23	-2.02	119.79	122.09
2	F	402	FMN	C4A-C10-N1	-2.01	119.66	124.59
2	L	401	FMN	C9A-C5A-N5	-2.01	120.33	122.45
2	I	401	FMN	C4A-C10-N1	-2.01	119.67	124.59
4	C	404	A1CIO	C29-C28-C23	-2.01	119.81	122.09
4	D	404	A1CIO	F26-C24-C23	-2.00	108.61	112.90

There are no chirality outliers.

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FMN	C5'-O5'-P-O1P
2	A	401	FMN	C5'-O5'-P-O2P
2	A	401	FMN	C5'-O5'-P-O3P
2	B	401	FMN	C5'-O5'-P-O2P
2	B	401	FMN	C5'-O5'-P-O3P
2	C	401	FMN	C5'-O5'-P-O2P
2	C	401	FMN	C5'-O5'-P-O3P
2	D	401	FMN	C5'-O5'-P-O2P
2	D	401	FMN	C5'-O5'-P-O3P
2	E	401	FMN	C5'-O5'-P-O1P
2	E	401	FMN	C5'-O5'-P-O2P
2	E	401	FMN	C5'-O5'-P-O3P
2	F	402	FMN	C5'-O5'-P-O2P
2	F	402	FMN	C5'-O5'-P-O3P
2	J	402	FMN	C5'-O5'-P-O1P
2	J	402	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	J	402	FMN	C5'-O5'-P-O3P
2	G	401	FMN	C5'-O5'-P-O1P
2	G	401	FMN	C5'-O5'-P-O2P
2	G	401	FMN	C5'-O5'-P-O3P
2	H	401	FMN	C5'-O5'-P-O2P
2	H	401	FMN	C5'-O5'-P-O3P
2	I	401	FMN	C5'-O5'-P-O2P
2	I	401	FMN	C5'-O5'-P-O3P
2	K	401	FMN	C5'-O5'-P-O1P
2	K	401	FMN	C5'-O5'-P-O2P
2	K	401	FMN	C5'-O5'-P-O3P
2	L	401	FMN	C5'-O5'-P-O1P
2	L	401	FMN	C5'-O5'-P-O2P
2	L	401	FMN	C5'-O5'-P-O3P
4	A	404	A1CIO	N19-C18-N17-C02
4	A	404	A1CIO	S30-C18-N17-C02
4	B	404	A1CIO	N19-C18-N17-C02
4	B	404	A1CIO	S30-C18-N17-C02
4	C	404	A1CIO	N19-C18-N17-C02
4	C	404	A1CIO	S30-C18-N17-C02
4	F	405	A1CIO	N19-C18-N17-C02
4	F	405	A1CIO	S30-C18-N17-C02
4	G	404	A1CIO	N19-C18-N17-C02
4	G	404	A1CIO	S30-C18-N17-C02
4	H	404	A1CIO	S30-C18-N17-C02
4	I	404	A1CIO	C15-C07-C08-C09
4	I	404	A1CIO	C15-C07-C08-C14
4	I	404	A1CIO	N06-C07-C08-C09
4	I	404	A1CIO	N06-C07-C08-C14
4	K	404	A1CIO	C15-C07-C08-C09
4	K	404	A1CIO	C15-C07-C08-C14
4	K	404	A1CIO	N06-C07-C08-C09
4	K	404	A1CIO	N06-C07-C08-C14
4	L	404	A1CIO	N19-C18-N17-C02
4	L	404	A1CIO	S30-C18-N17-C02
6	A	407	JEF	O10-C32-C33-O11
6	B	406	JEF	C34-C33-O11-C36
6	J	407	JEF	C34-C33-O11-C36
6	J	407	JEF	O10-C32-C33-O11
7	D	405	CIT	C2-C3-C4-C5
7	D	405	CIT	O7-C3-C4-C5
7	D	405	CIT	C2-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
7	D	405	CIT	C2-C3-C6-O6
7	D	405	CIT	O7-C3-C6-O5
7	D	405	CIT	O7-C3-C6-O6
4	L	404	A1CIO	C15-C07-C08-C14
6	D	407	JEF	C37-C36-O11-C33
4	L	404	A1CIO	N06-C07-C08-C09
4	L	404	A1CIO	C15-C07-C08-C09
4	L	404	A1CIO	N06-C07-C08-C14
6	B	405	JEF	O10-C19-C20-O
6	J	407	JEF	O11-C36-C37-O12
6	E	406	JEF	C20-C19-O10-C32
4	D	404	A1CIO	C15-C07-C08-C09
4	H	404	A1CIO	N19-C18-N17-C02
6	A	407	JEF	O11-C36-C37-O12
6	D	407	JEF	O11-C36-C37-O12
6	E	407	JEF	C33-C32-O10-C19
4	D	404	A1CIO	N06-C07-C08-C09
6	B	406	JEF	O11-C36-C37-O12
6	D	408	JEF	O10-C32-C33-O11
6	C	405	JEF	C37-C36-O11-C33
4	J	405	A1CIO	O01-C02-N03-C04
4	K	404	A1CIO	O01-C02-N03-C04
4	J	405	A1CIO	N17-C02-N03-C04
4	K	404	A1CIO	N17-C02-N03-C04
6	E	406	JEF	O-C-C17-OH
6	E	406	JEF	O10-C19-C20-O
4	D	404	A1CIO	C15-C07-C08-C14
4	D	404	A1CIO	N06-C07-C08-C14
6	J	407	JEF	C36-C37-O12-C38
4	J	405	A1CIO	N19-C18-N17-C02
6	B	405	JEF	O11-C36-C37-O12
6	K	406	JEF	O11-C36-C37-O12
6	D	408	JEF	C40-C19-O10-C32
6	E	408	JEF	O10-C32-C33-O11
6	G	405	JEF	O10-C32-C33-O11
6	B	405	JEF	C1-C2-OH-C17
4	B	404	A1CIO	C15-C07-C08-C09
6	H	406	JEF	O10-C32-C33-O11
6	I	406	JEF	O11-C36-C37-O12
7	D	405	CIT	C6-C3-C4-C5
6	B	406	JEF	C40-C19-O10-C32
6	B	405	JEF	C20-C19-O10-C32

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Mol	Chain	Res	Type	Atoms
6	F	407	JEF	O11-C36-C37-O12
4	B	404	A1CIO	C15-C07-C08-C14
4	A	404	A1CIO	C15-C07-C08-C09
4	B	404	A1CIO	N06-C07-C08-C09
6	H	406	JEF	C32-C33-O11-C36
6	E	406	JEF	C1-C2-OH-C17
2	B	401	FMN	C5'-O5'-P-O1P
2	H	401	FMN	C5'-O5'-P-O1P
6	E	408	JEF	C37-C36-O11-C33
6	D	408	JEF	C37-C36-O11-C33
4	A	404	A1CIO	C15-C07-C08-C14
7	D	405	CIT	C1-C2-C3-C4
4	I	404	A1CIO	N19-C18-N17-C02
4	E	404	A1CIO	C05-C04-N03-C02
6	B	406	JEF	C33-C32-O10-C19
4	B	404	A1CIO	N06-C07-C08-C14
6	J	407	JEF	O10-C32-C33-C34
7	D	405	CIT	C1-C2-C3-C6
4	D	404	A1CIO	N19-C18-N17-C02
6	B	405	JEF	C36-C37-O12-C38
4	A	404	A1CIO	N06-C07-C08-C09
6	F	407	JEF	C32-C33-O11-C36
6	I	406	JEF	C32-C33-O11-C36
4	J	405	A1CIO	S30-C18-N17-C02
6	E	408	JEF	C32-C33-O11-C36
4	A	404	A1CIO	N06-C07-C08-C14
6	A	408	JEF	C37-C36-O11-C33
6	I	406	JEF	C37-C36-O11-C33
6	B	405	JEF	C37-C36-O11-C33
6	E	407	JEF	C37-C36-O11-C33
6	E	406	JEF	O11-C36-C37-O12
6	D	408	JEF	C33-C32-O10-C19
6	C	405	JEF	C36-C37-O12-C38
6	C	405	JEF	O11-C36-C37-O12
6	A	407	JEF	O10-C32-C33-C34
6	E	407	JEF	O11-C36-C37-O12
6	F	407	JEF	C40-C19-O10-C32
6	F	407	JEF	C20-C19-O10-C32
2	C	401	FMN	C4'-C5'-O5'-P
2	J	402	FMN	C4'-C5'-O5'-P
2	G	401	FMN	C4'-C5'-O5'-P
2	H	401	FMN	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	I	401	FMN	C4'-C5'-O5'-P
2	K	401	FMN	C4'-C5'-O5'-P
6	B	405	JEF	O-C-C17-OH
6	B	406	JEF	C36-C37-O12-C38
6	E	406	JEF	C33-C32-O10-C19
2	B	401	FMN	C4'-C5'-O5'-P
2	F	402	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C2'-C3'-C4'-O4'
6	G	405	JEF	C32-C33-O11-C36
2	L	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C4'-C5'-O5'-P
2	D	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C4'-C5'-O5'-P
6	D	407	JEF	C36-C37-O12-C38
6	K	406	JEF	C36-C37-O12-C38
4	F	405	A1CIO	C15-C07-C08-C09
6	G	405	JEF	C37-C36-O11-C33
4	F	405	A1CIO	C15-C07-C08-C14
6	D	407	JEF	O10-C32-C33-O11
6	B	405	JEF	C17-C-O-C20
7	D	405	CIT	C4-C3-C6-O6
2	E	401	FMN	O3'-C3'-C4'-C5'
6	A	407	JEF	C37-C36-O11-C33
6	F	407	JEF	C33-C32-O10-C19
6	J	407	JEF	C37-C36-O11-C33
6	B	405	JEF	C19-C20-O-C
6	H	406	JEF	C37-C36-O11-C33
4	F	405	A1CIO	N06-C07-C08-C09
2	C	401	FMN	C5'-O5'-P-O1P
2	D	401	FMN	C5'-O5'-P-O1P
2	F	402	FMN	C5'-O5'-P-O1P
2	I	401	FMN	C5'-O5'-P-O1P
4	F	405	A1CIO	N06-C07-C08-C14
6	B	406	JEF	C20-C19-O10-C32
6	J	407	JEF	C33-C32-O10-C19
6	D	408	JEF	C32-C33-O11-C36
4	G	404	A1CIO	N06-C07-C08-C09
2	E	401	FMN	O3'-C3'-C4'-O4'
6	E	406	JEF	C34-C33-O11-C36
4	B	404	A1CIO	N03-C04-C05-N16
4	H	404	A1CIO	N03-C04-C05-N16
6	F	407	JEF	O10-C32-C33-O11

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Mol	Chain	Res	Type	Atoms
7	D	405	CIT	C1-C2-C3-O7
4	G	404	A1CIO	N06-C07-C08-C14

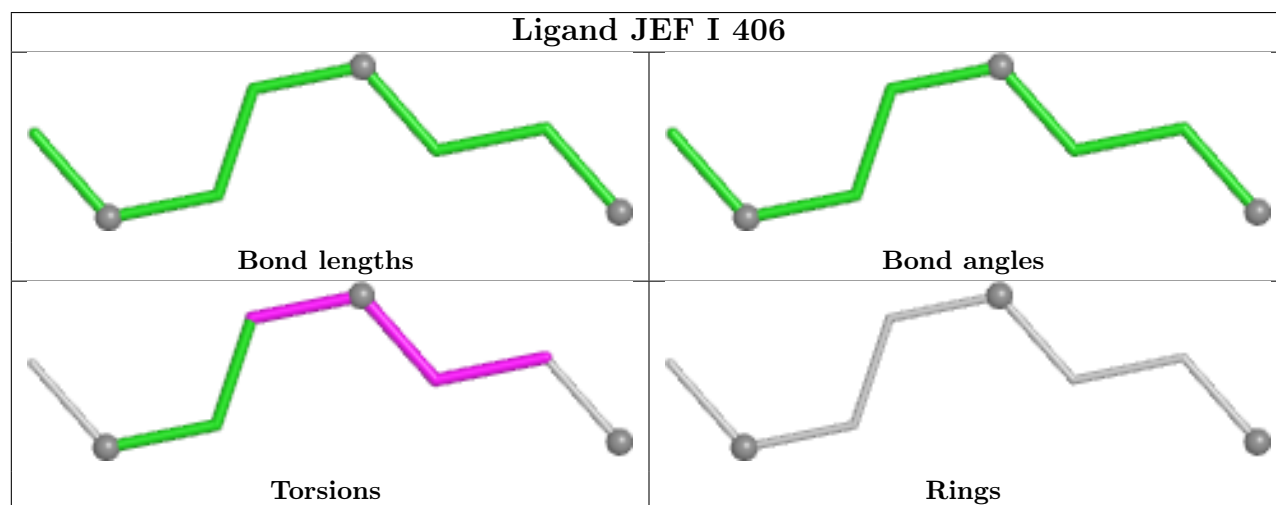
There are no ring outliers.

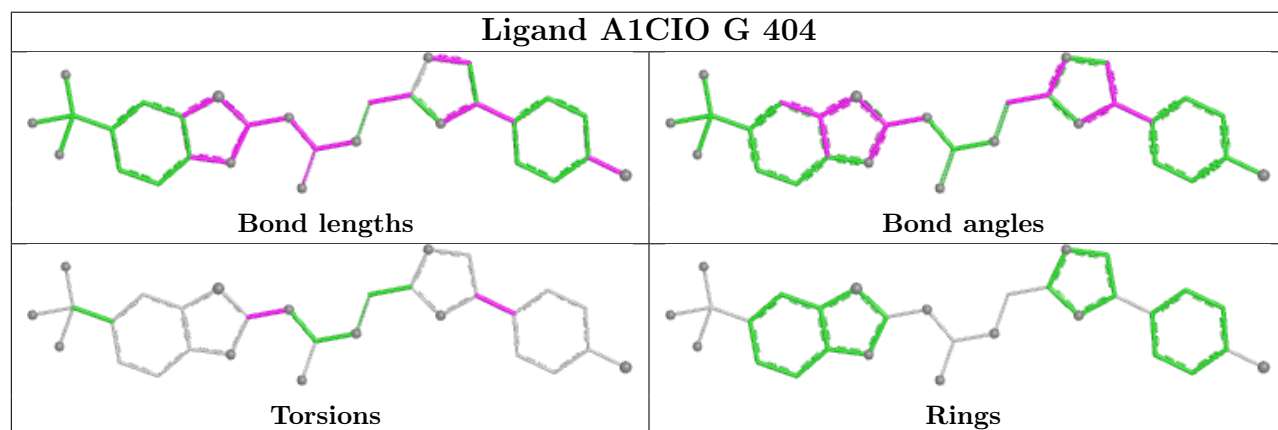
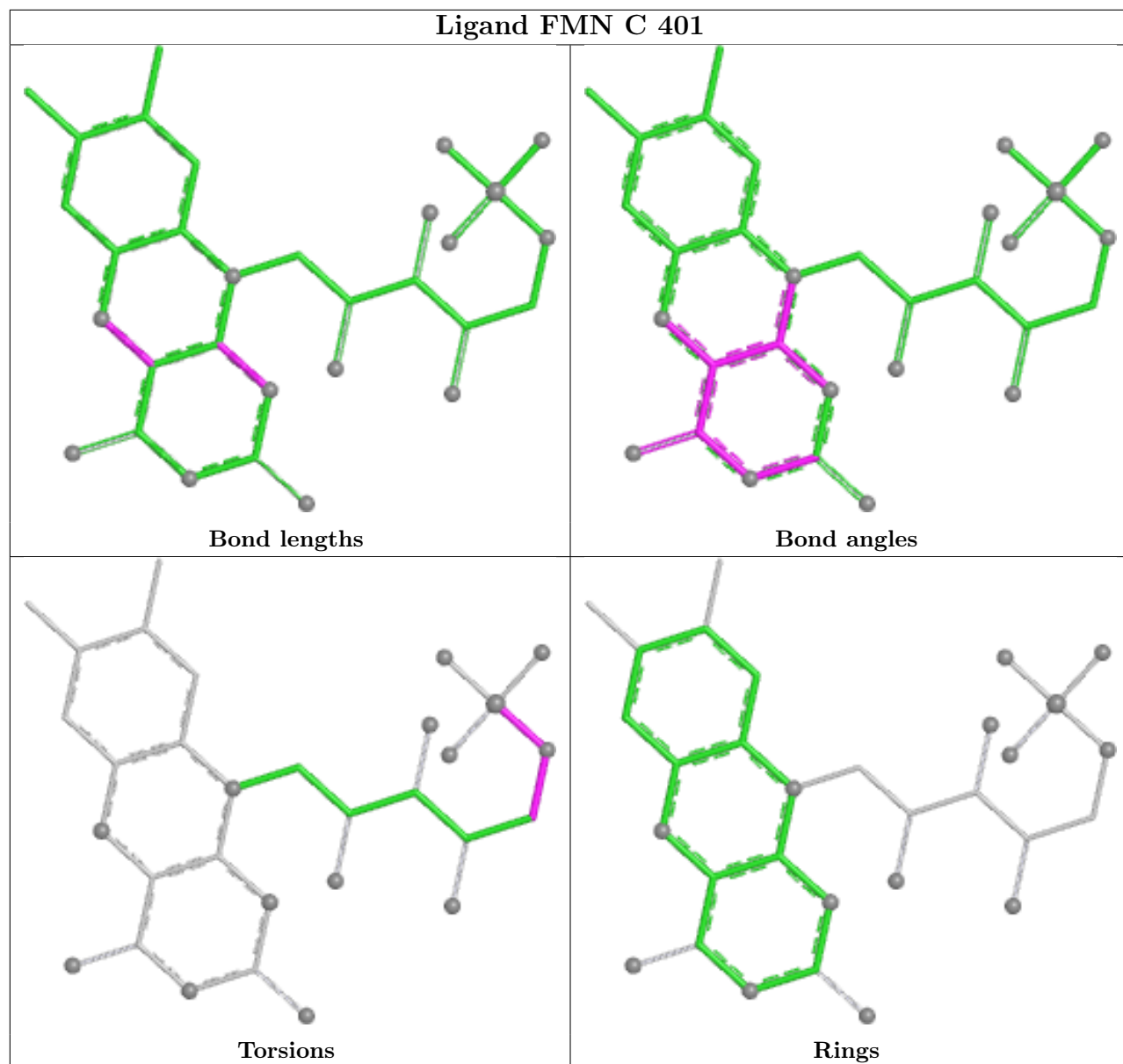
33 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	FMN	1	0
4	G	404	A1CIO	6	0
2	I	401	FMN	1	0
5	F	406	DMS	3	0
2	A	401	FMN	3	0
4	J	405	A1CIO	2	0
2	E	401	FMN	4	0
4	F	405	A1CIO	2	0
6	J	407	JEF	1	0
2	K	401	FMN	1	0
6	C	405	JEF	2	0
5	J	406	DMS	3	0
2	F	402	FMN	1	0
5	H	405	DMS	1	0
4	E	404	A1CIO	1	0
2	L	401	FMN	3	0
4	D	404	A1CIO	2	0
6	F	407	JEF	3	0
5	A	405	DMS	4	0
6	G	405	JEF	2	0
4	I	404	A1CIO	3	0
6	K	406	JEF	1	0
2	H	401	FMN	1	0
2	G	401	FMN	2	0
6	H	406	JEF	1	0
2	D	401	FMN	1	0
6	A	407	JEF	1	0
6	B	406	JEF	2	0
2	B	401	FMN	2	0
5	D	406	DMS	2	0
4	K	404	A1CIO	1	0
2	J	402	FMN	2	0
5	I	405	DMS	1	0

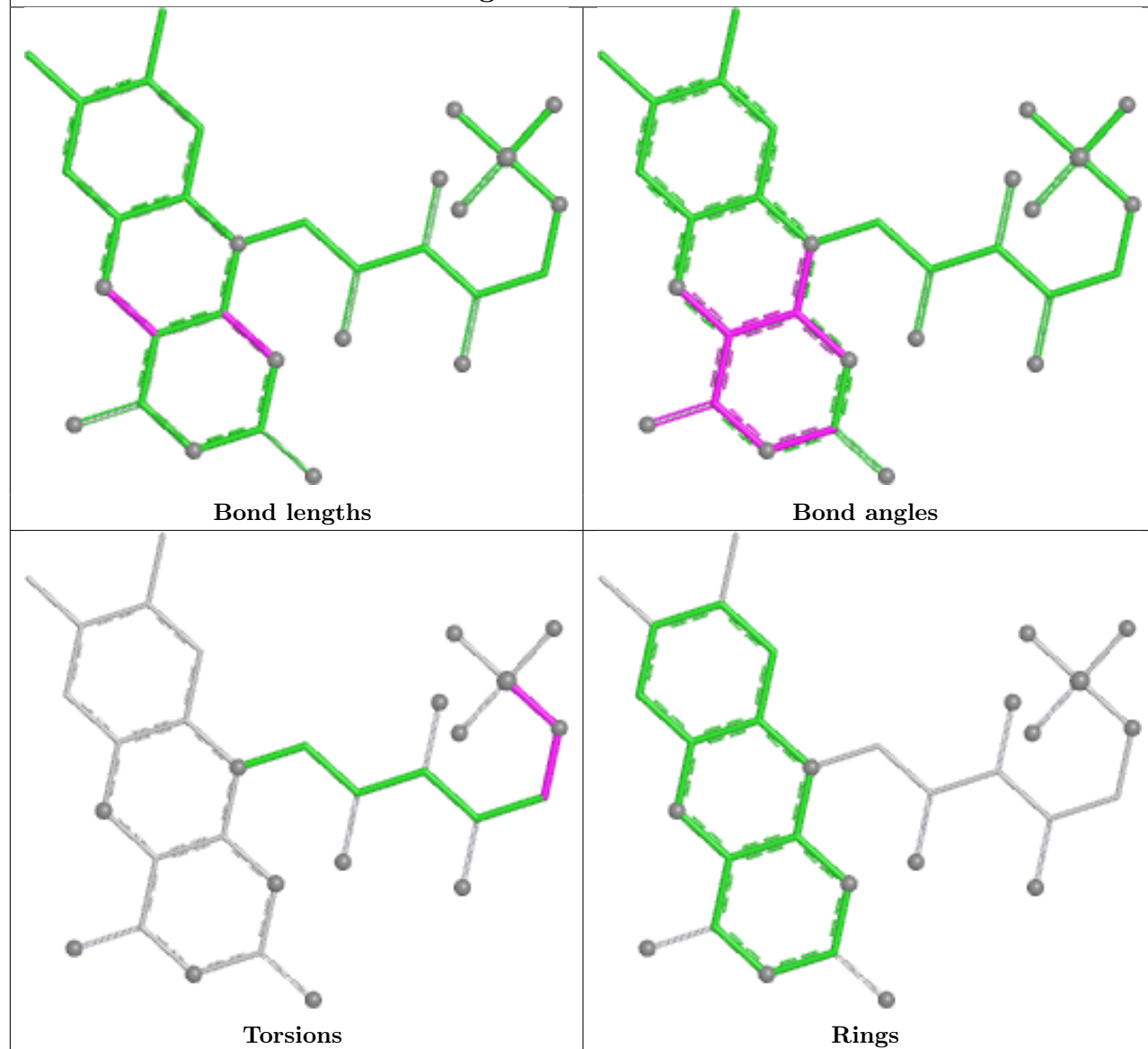
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

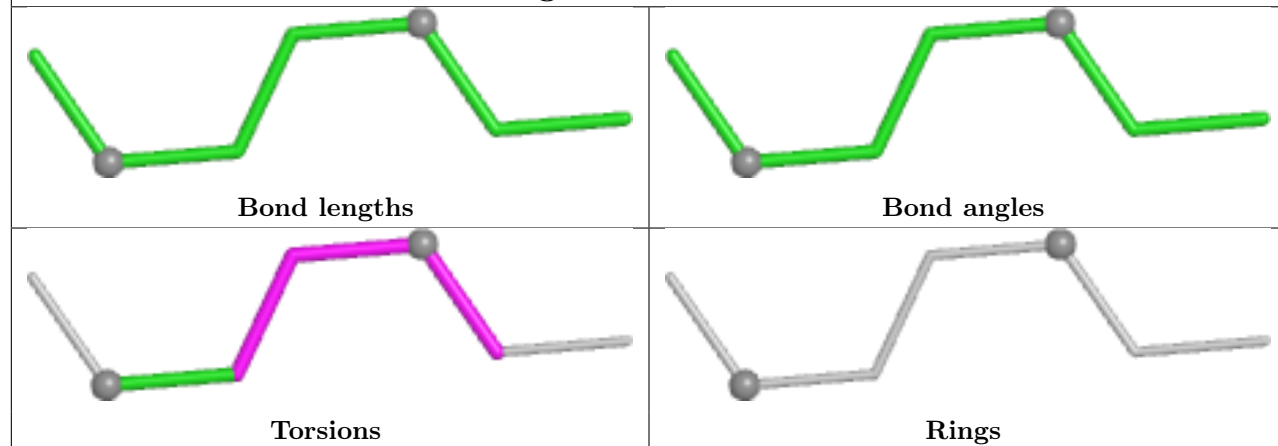


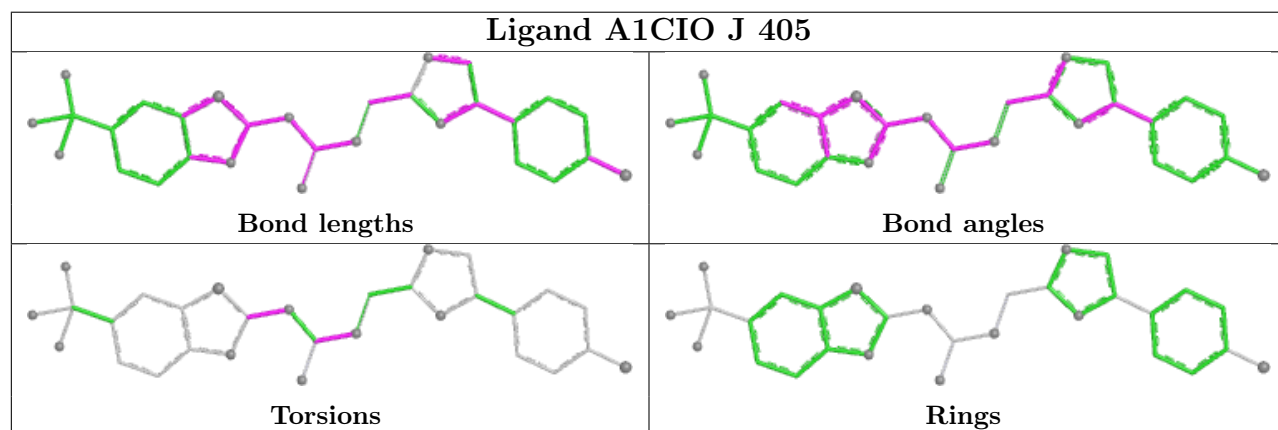
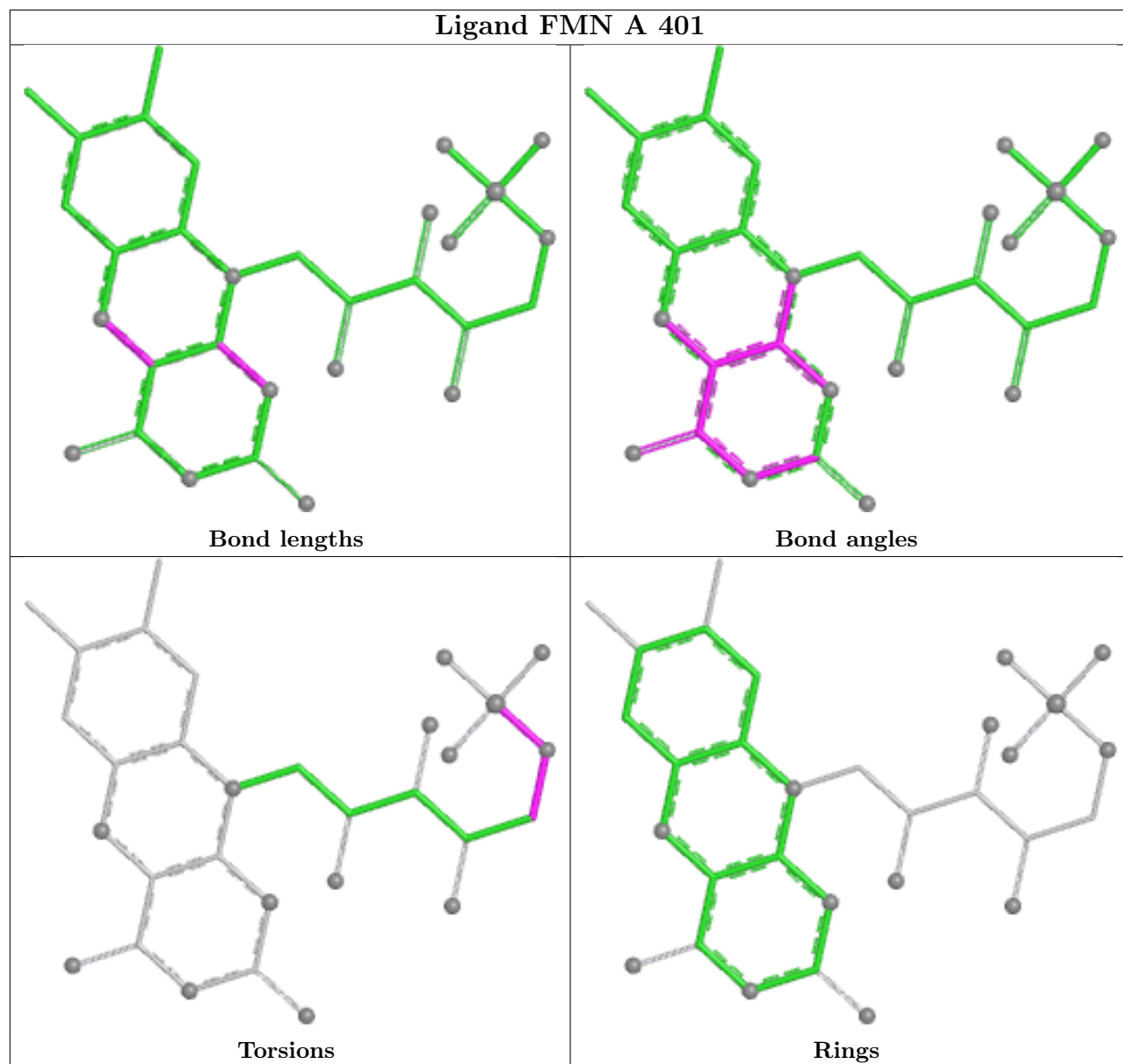


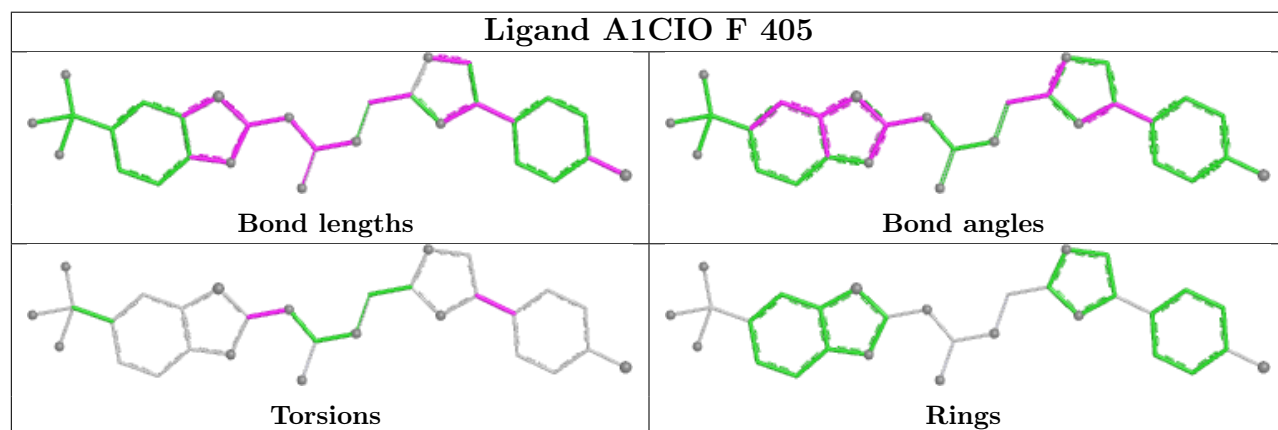
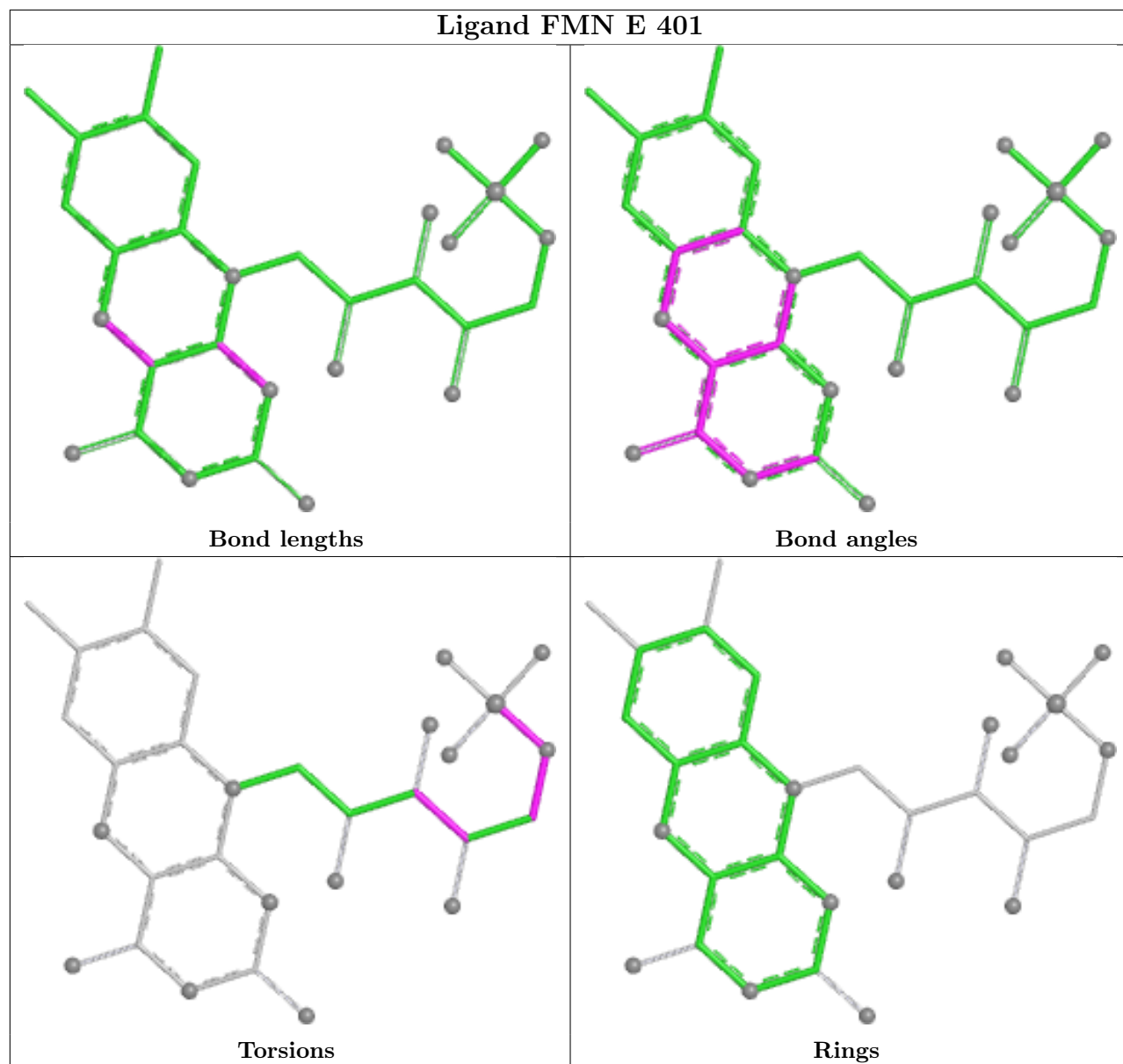
Ligand FMN I 401



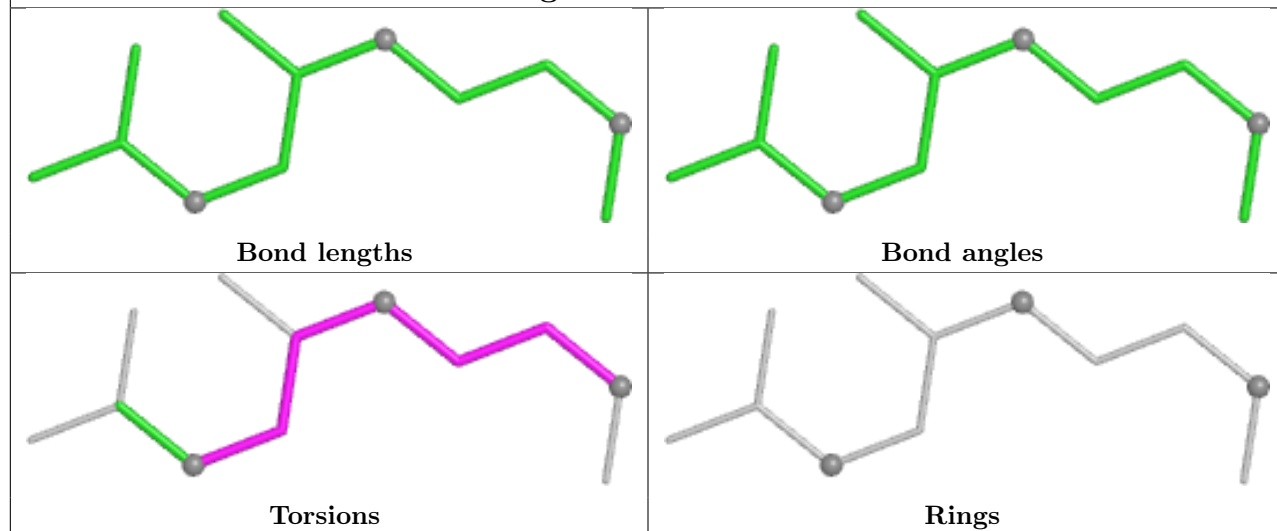
Ligand JEF E 408



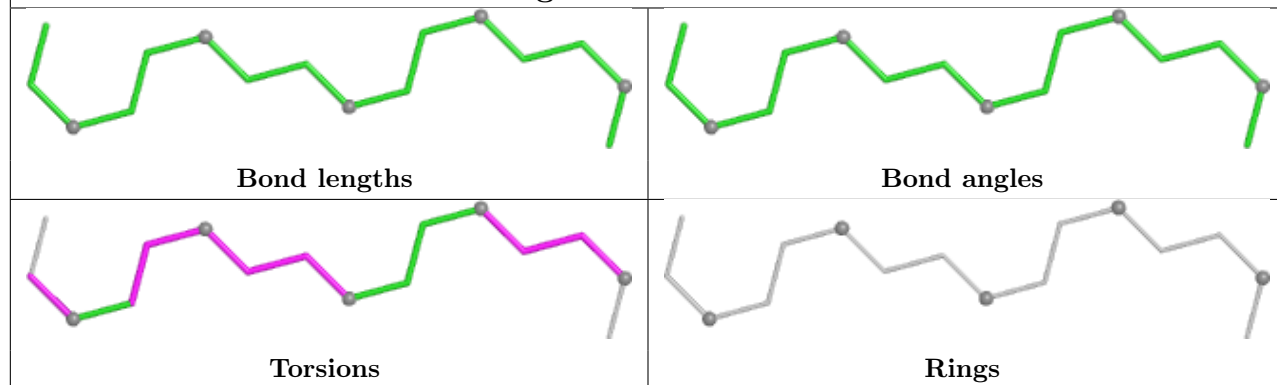


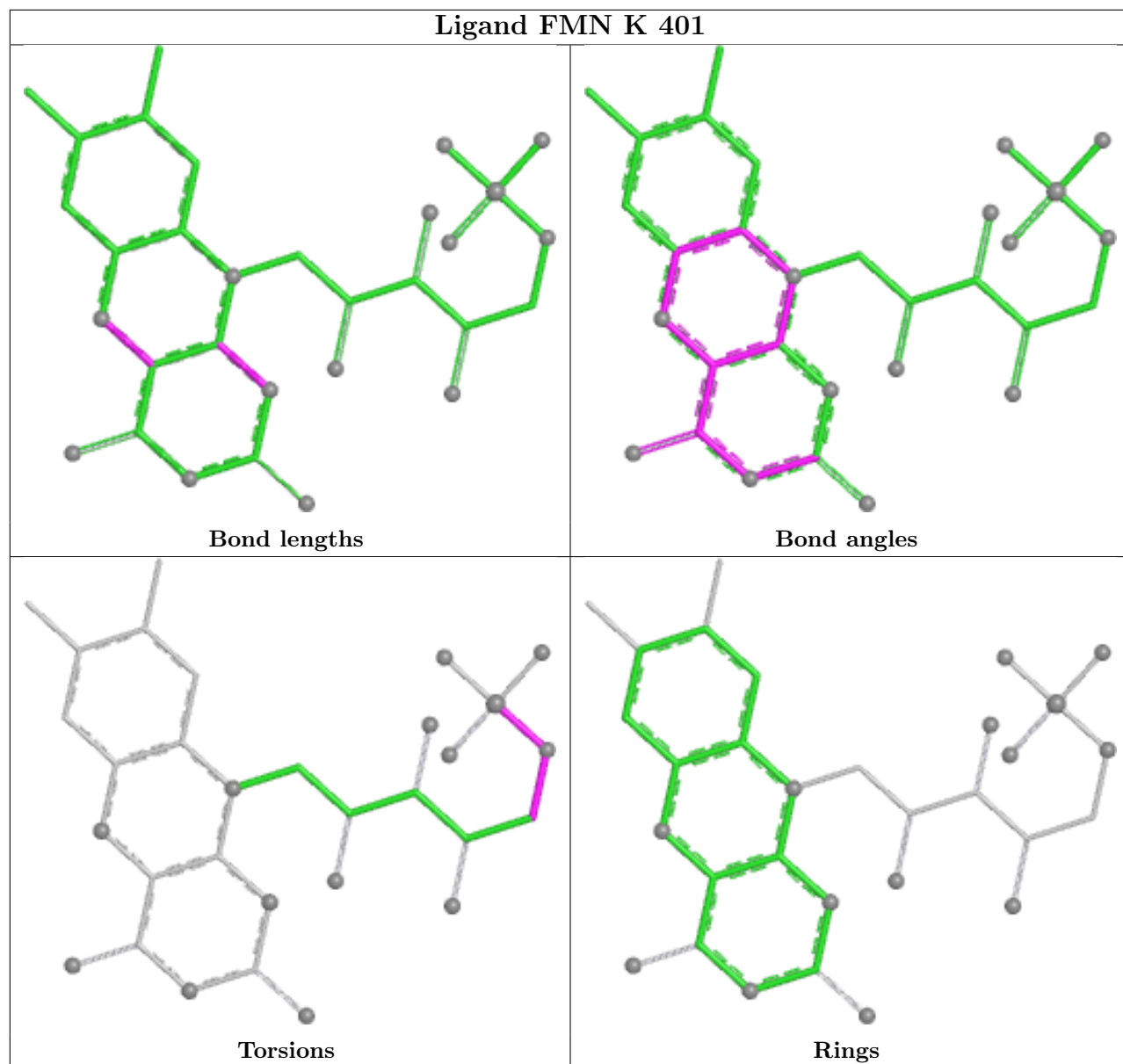


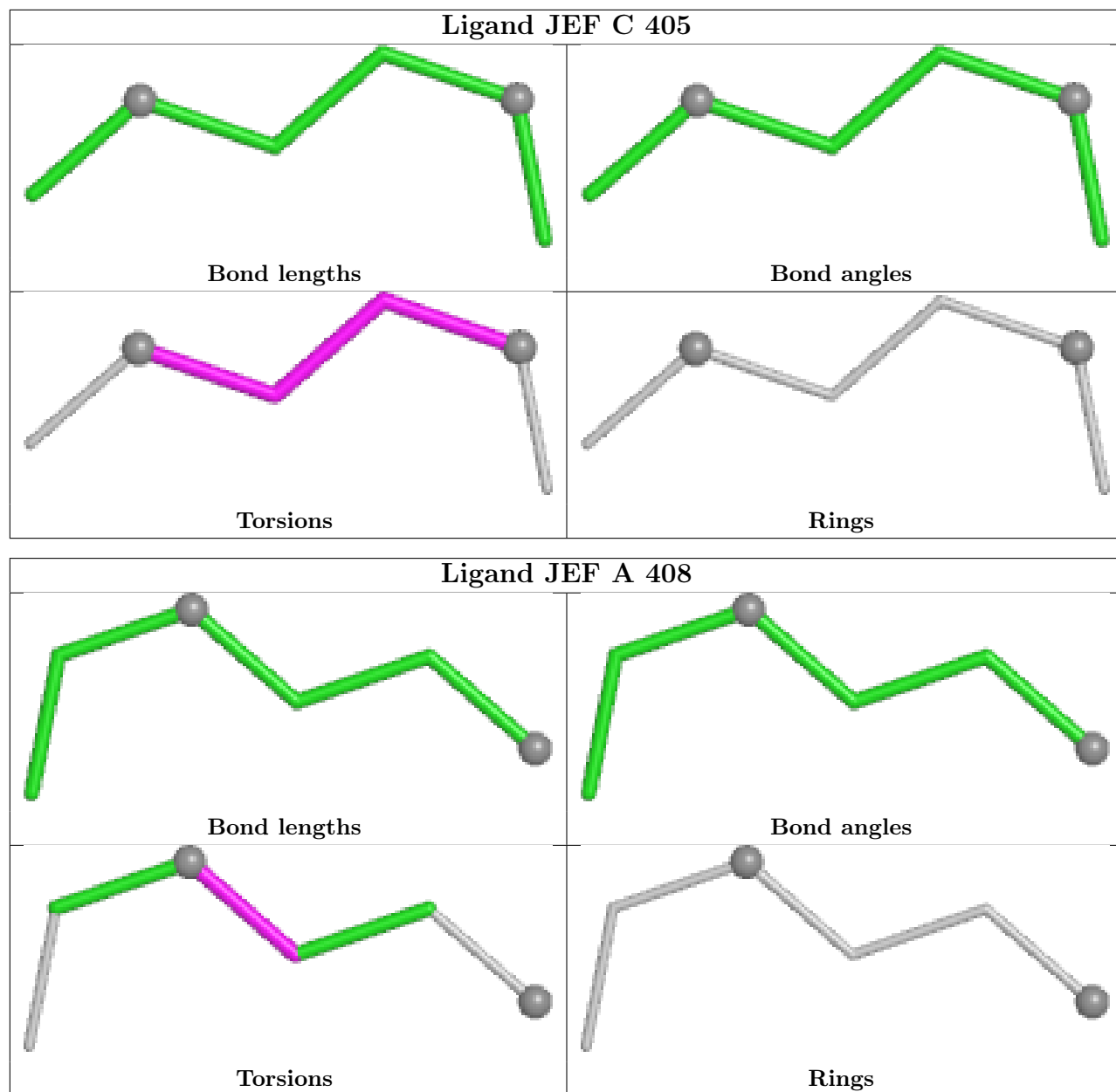
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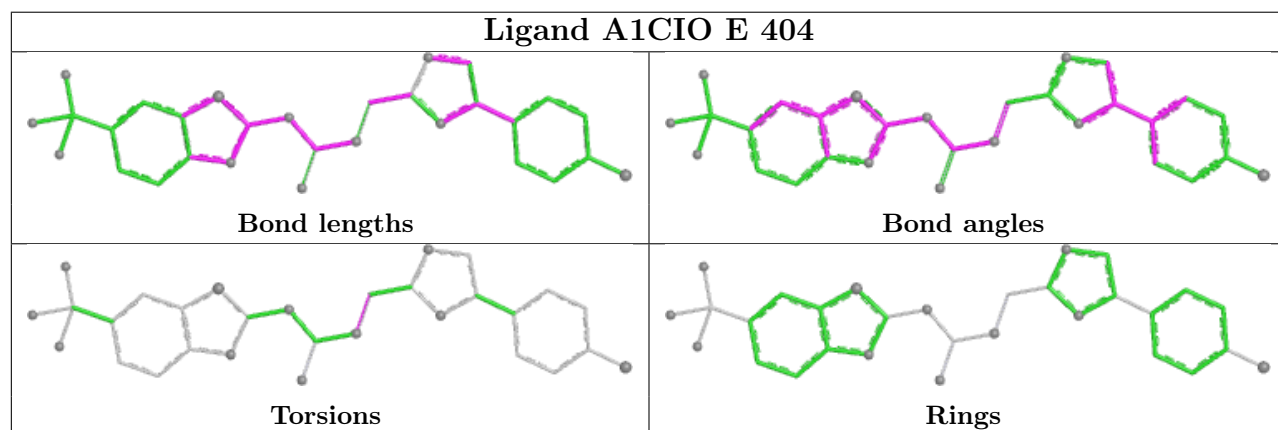
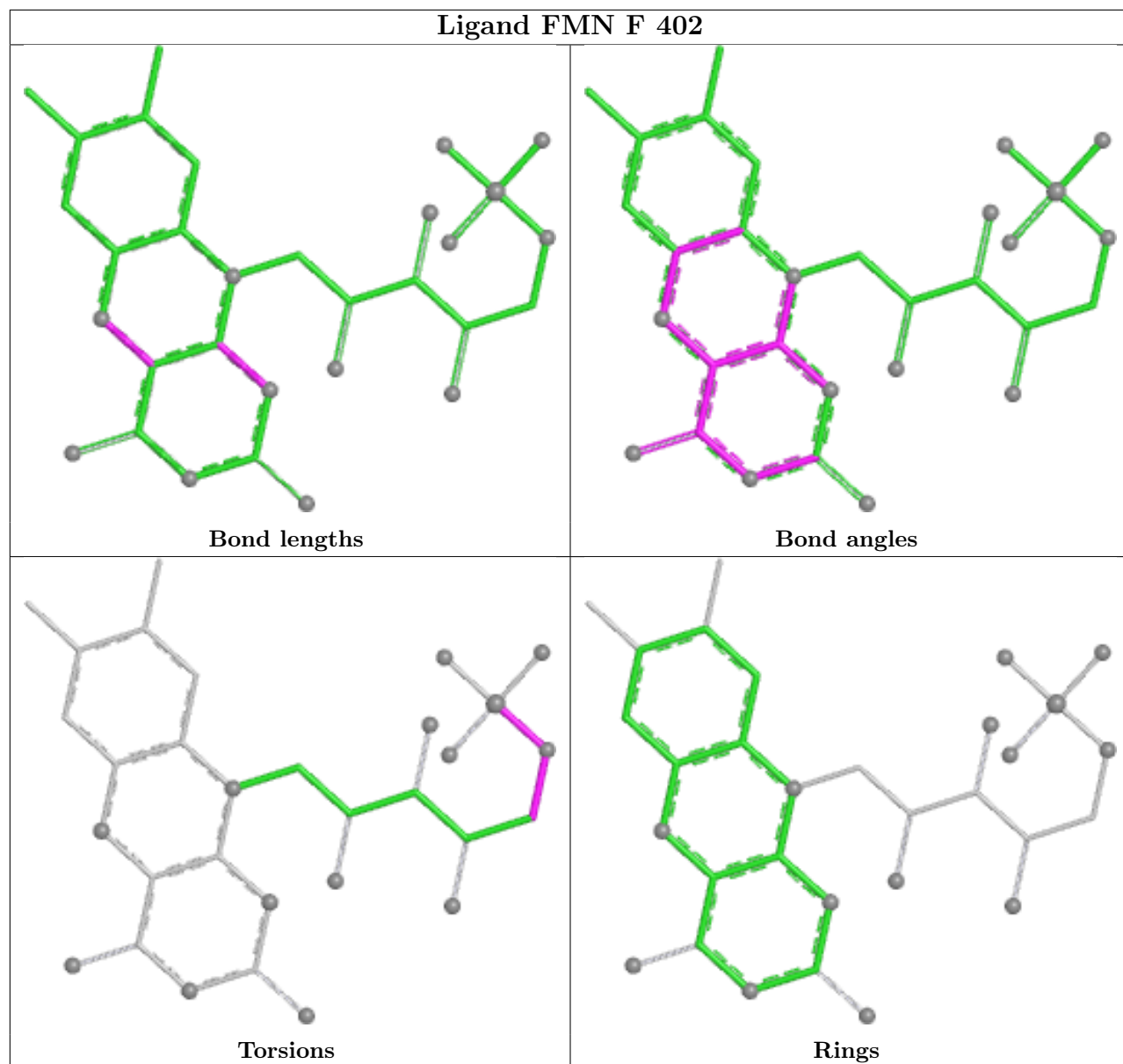


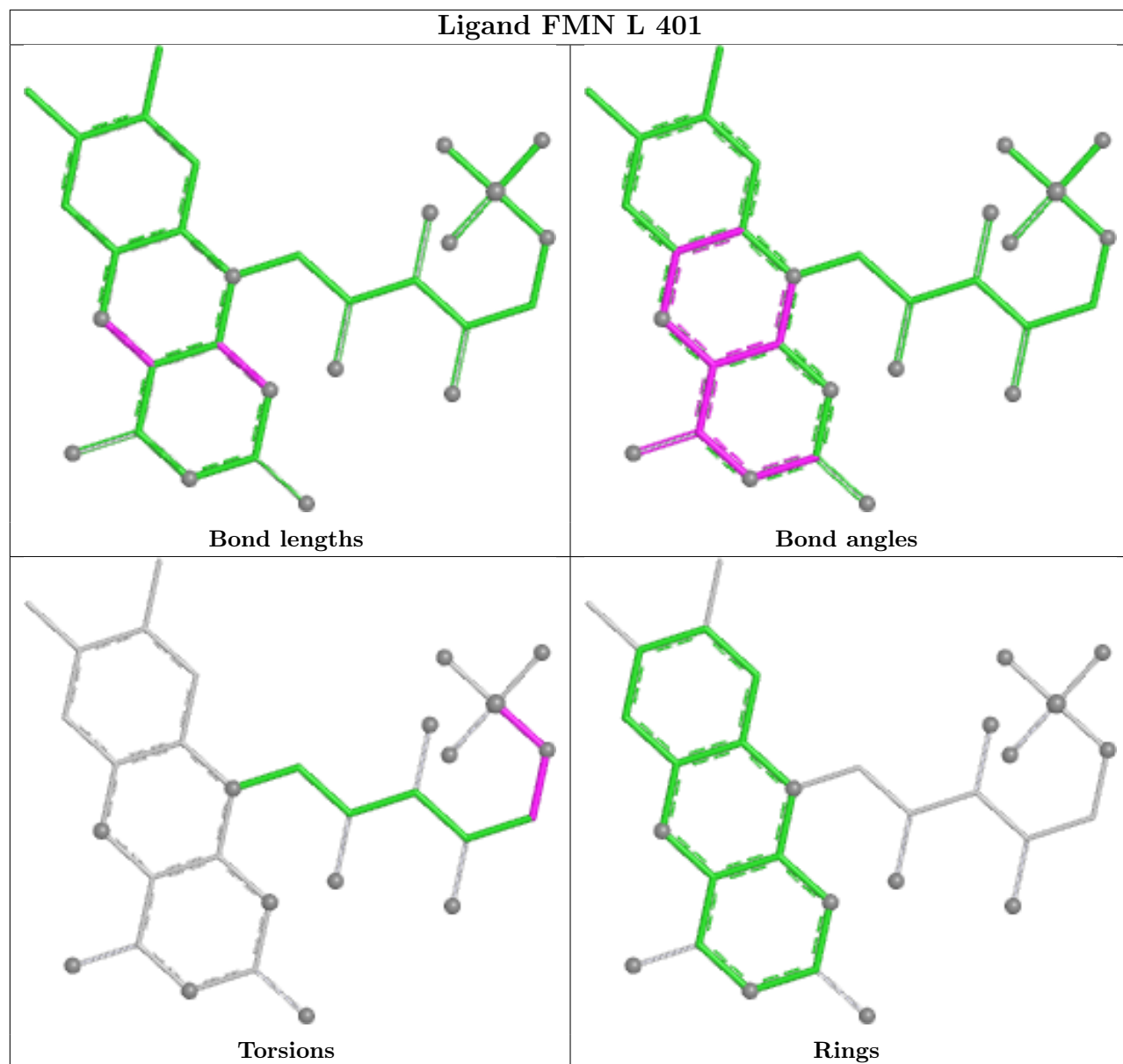
Ligand JEF B 405

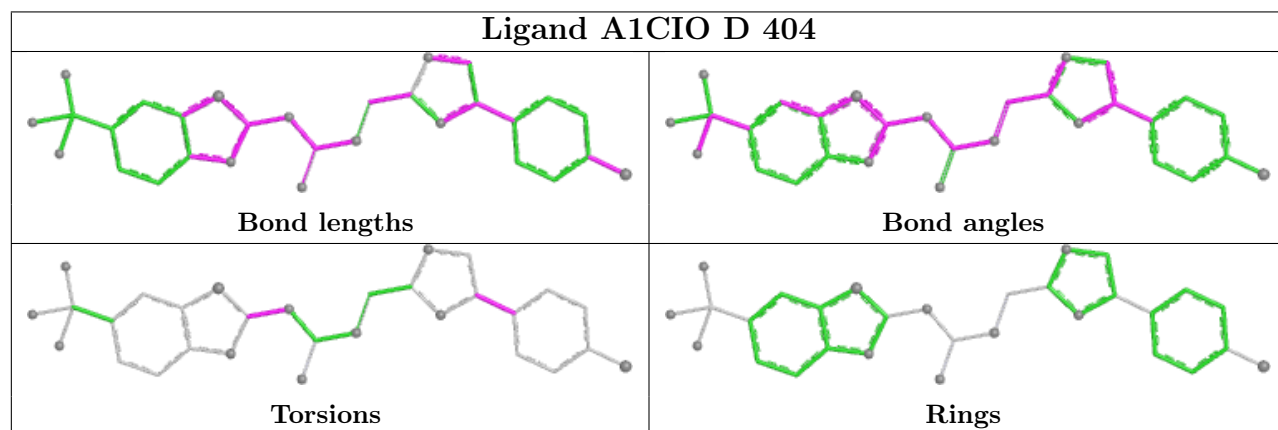
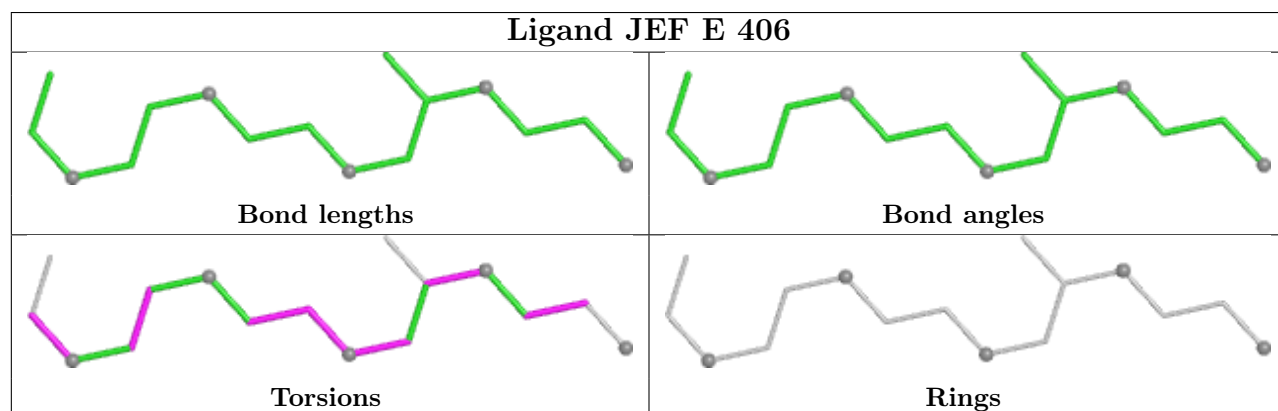
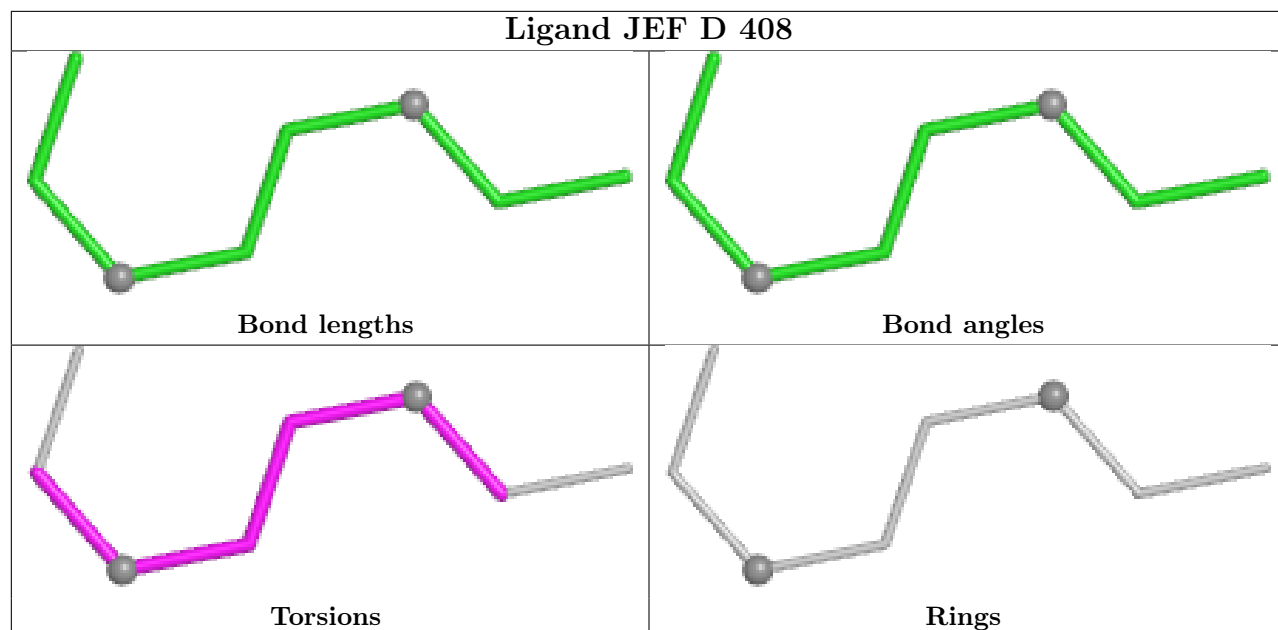




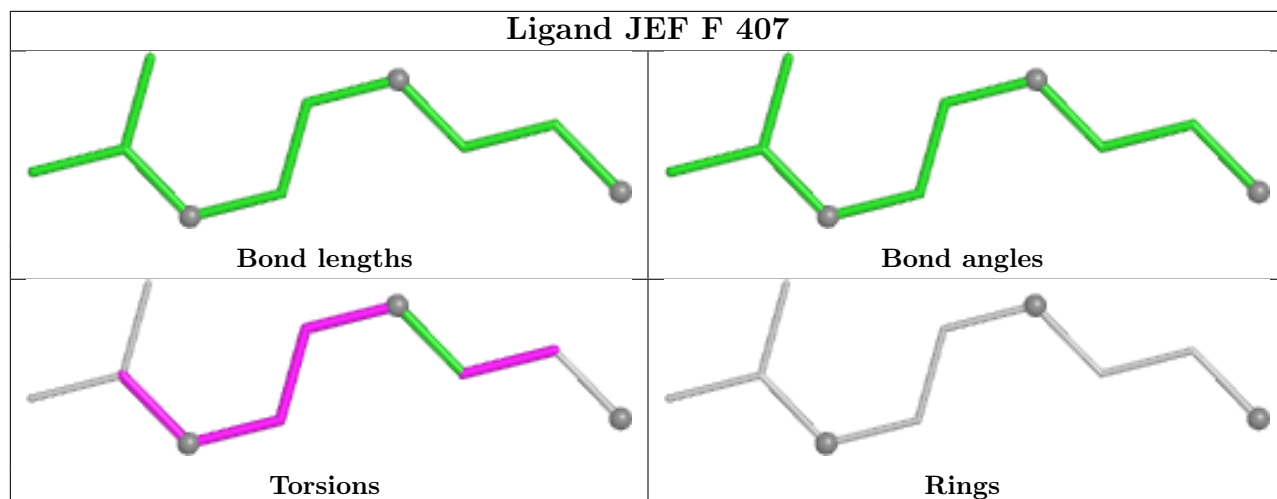




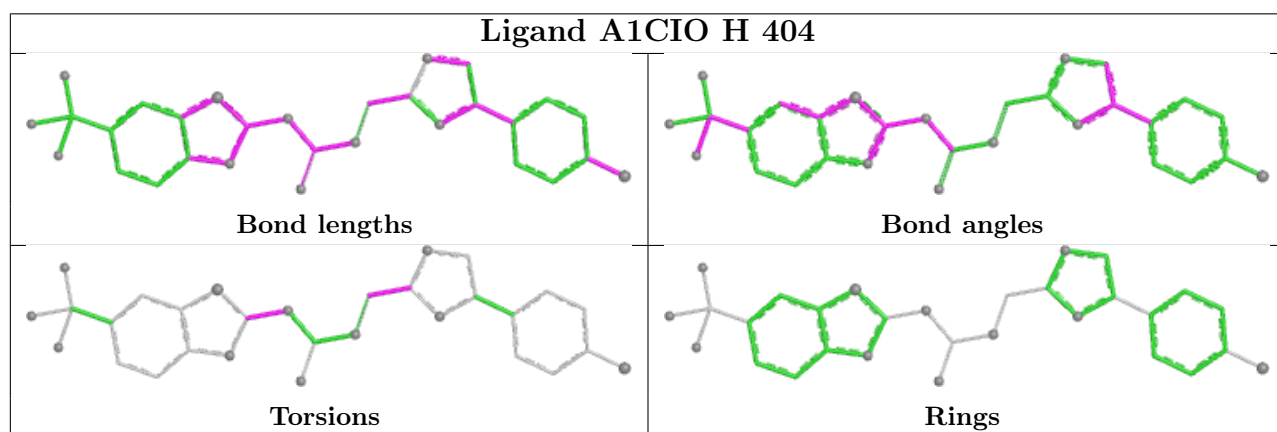




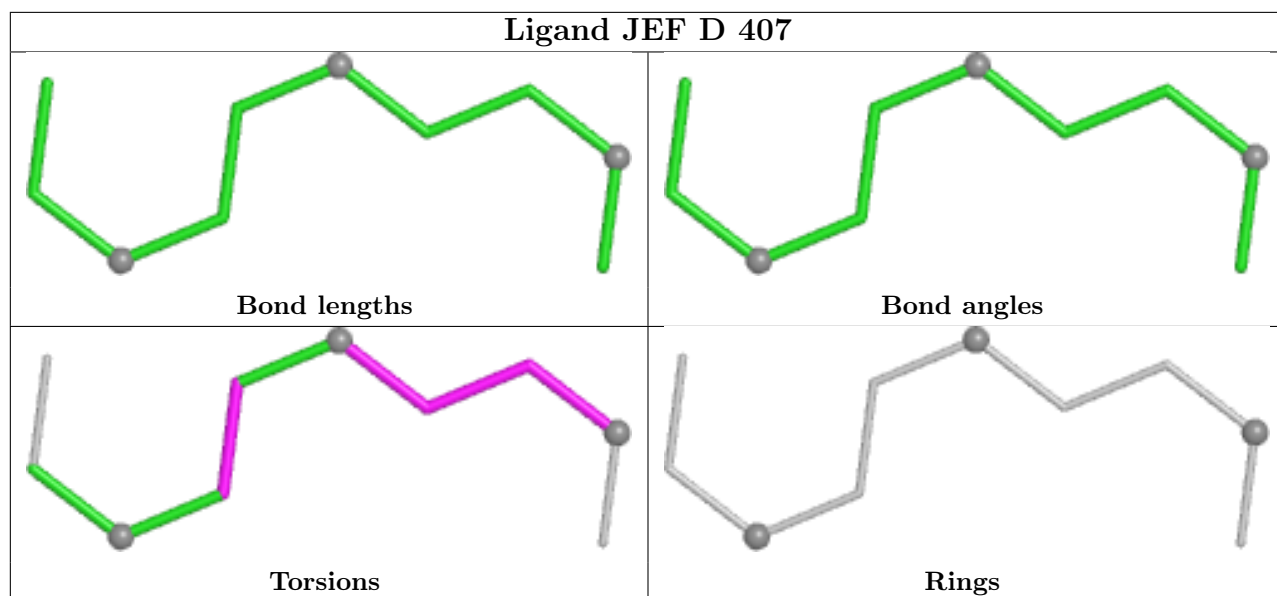
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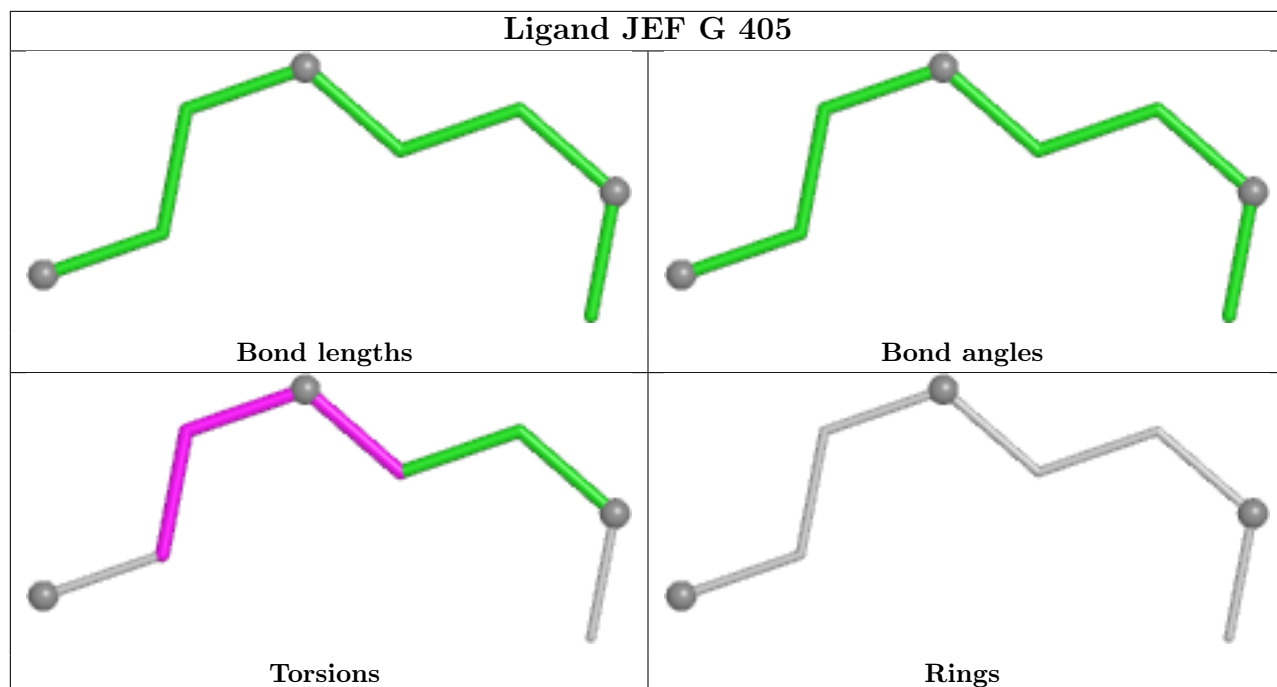
Ligand A1CIO H 404



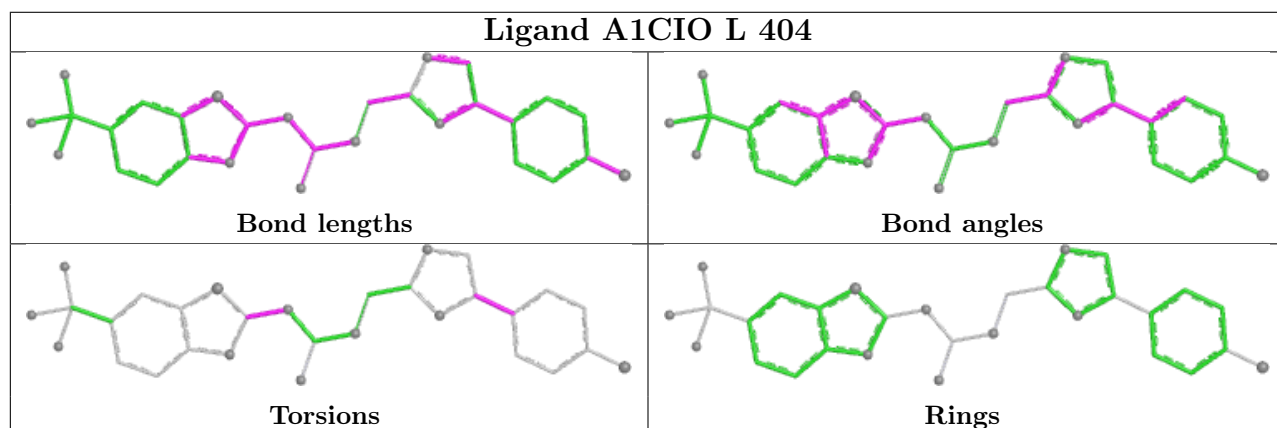
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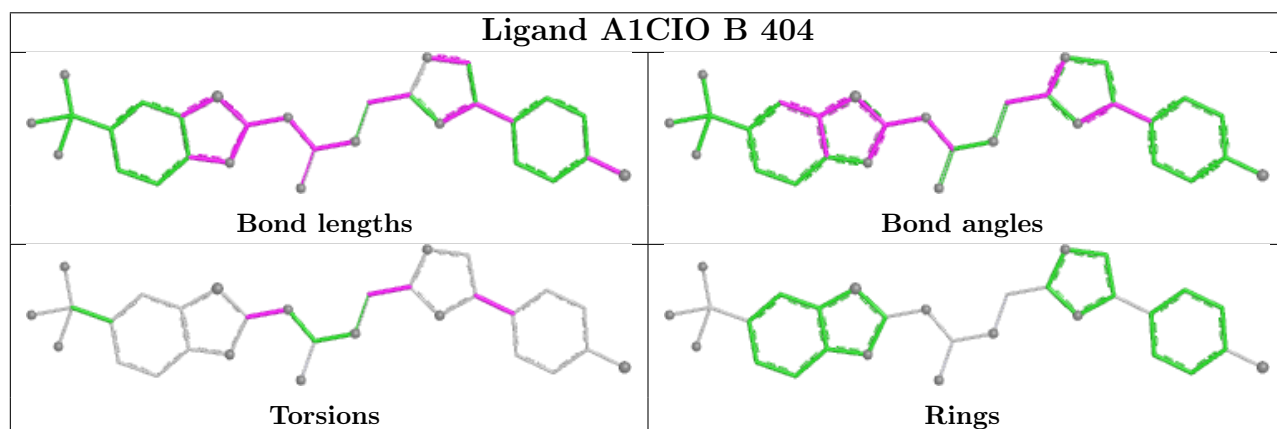
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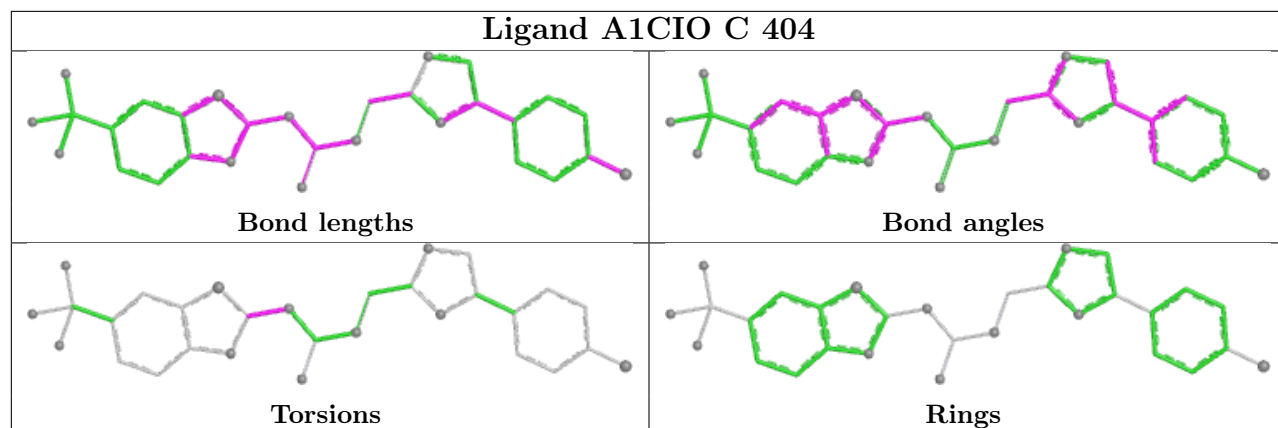
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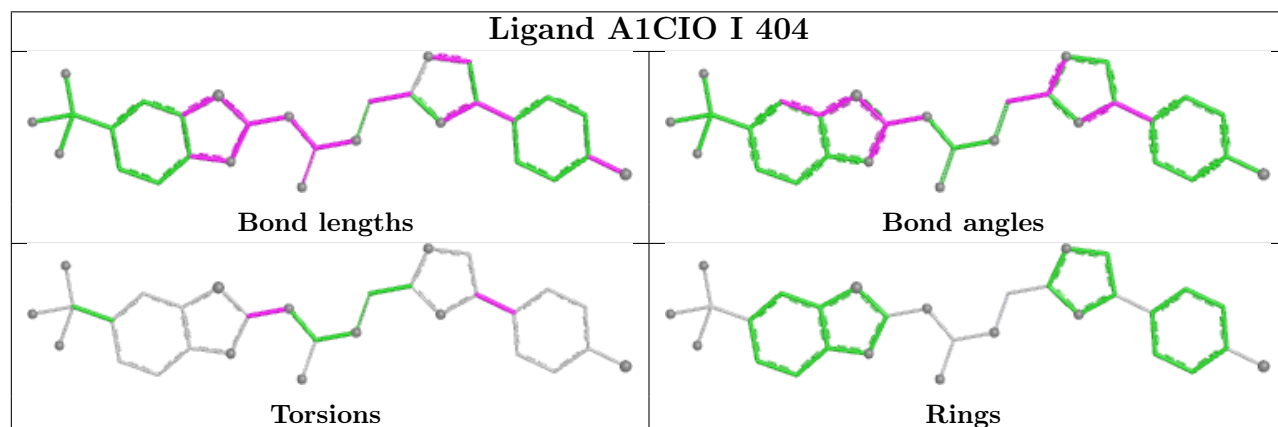
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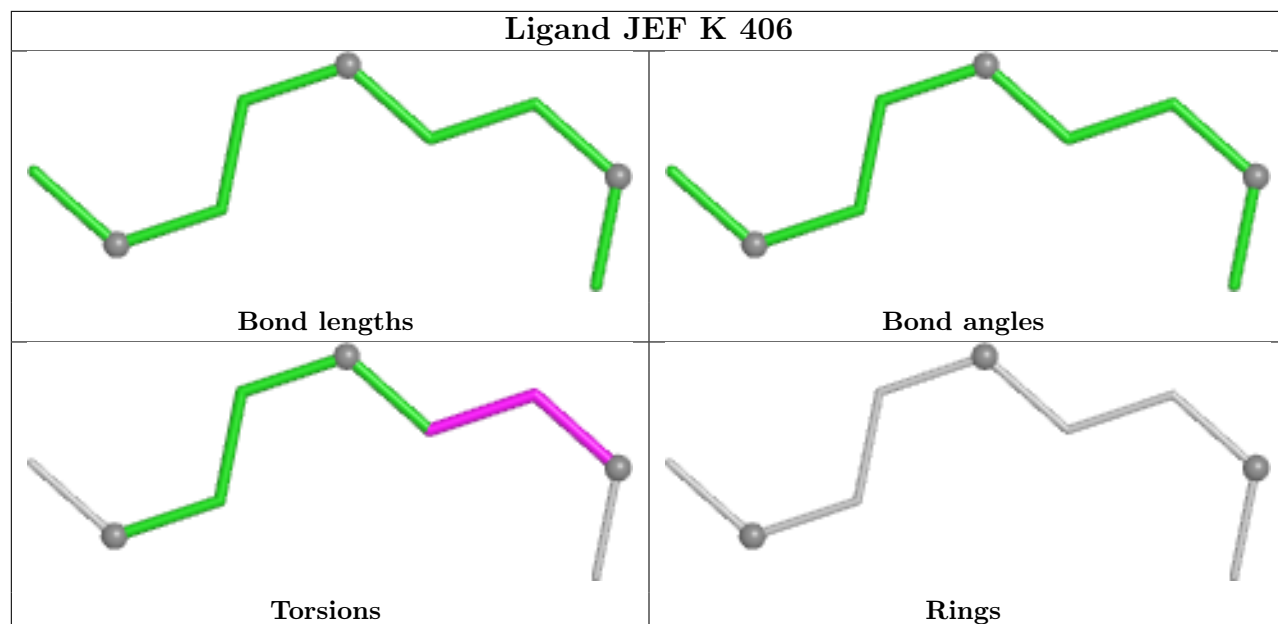
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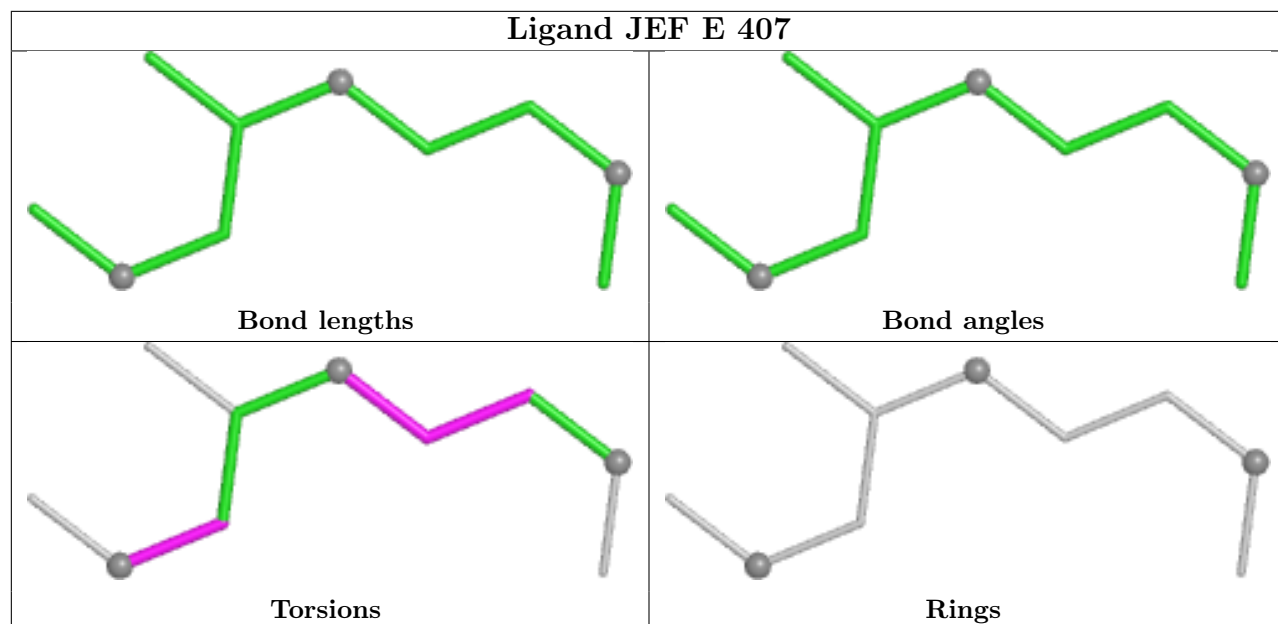
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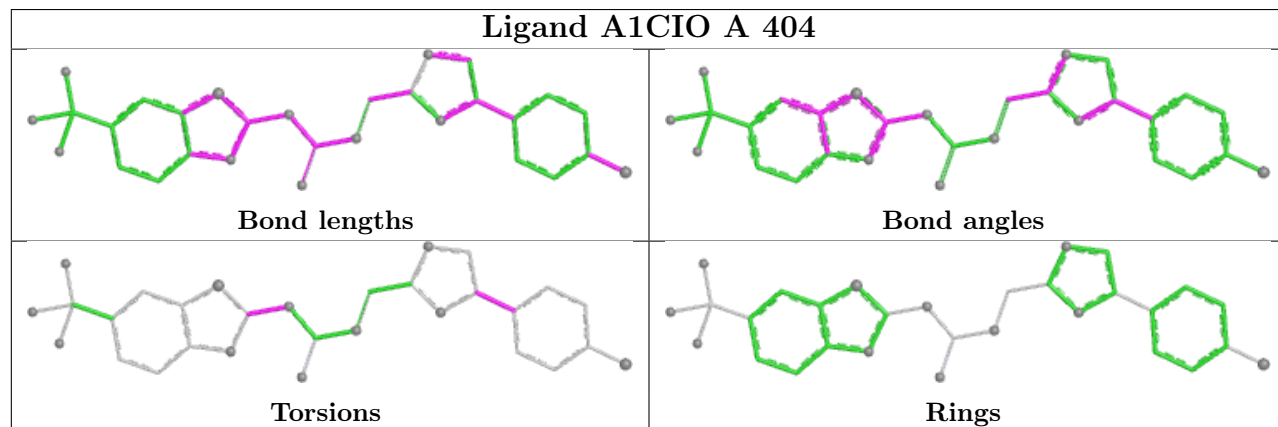
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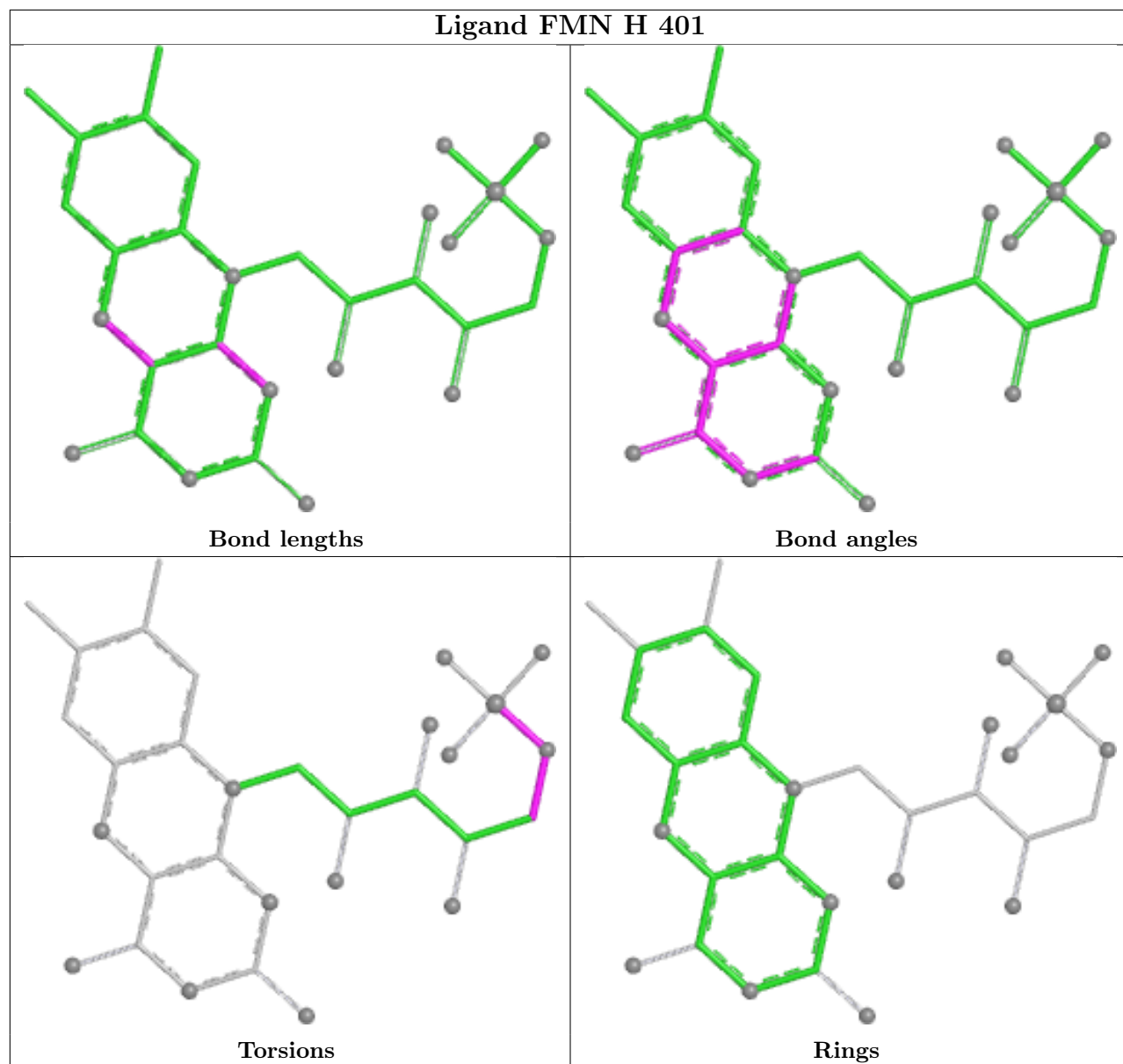


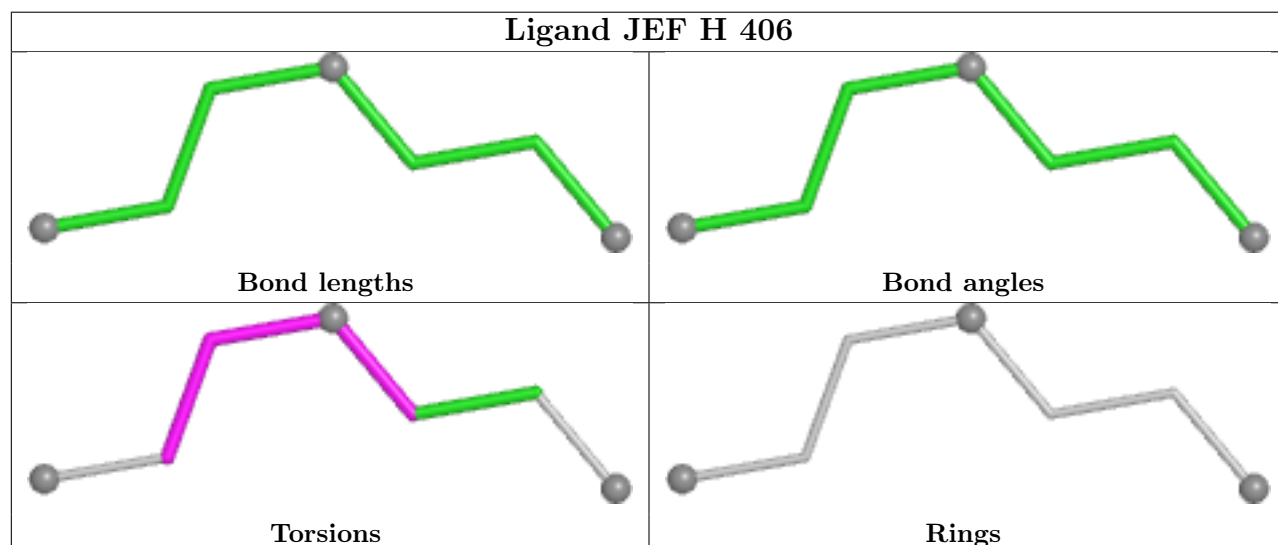
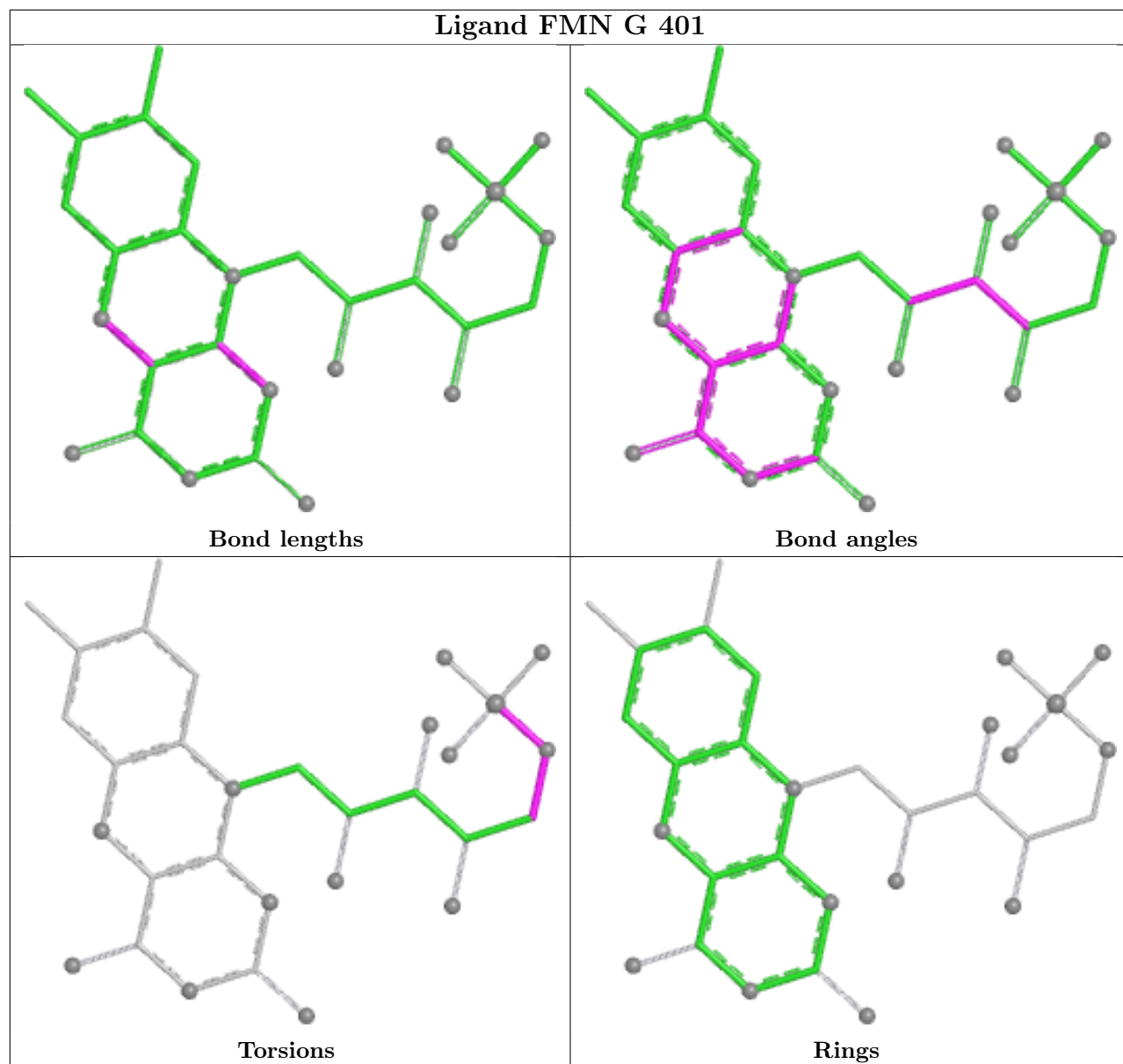
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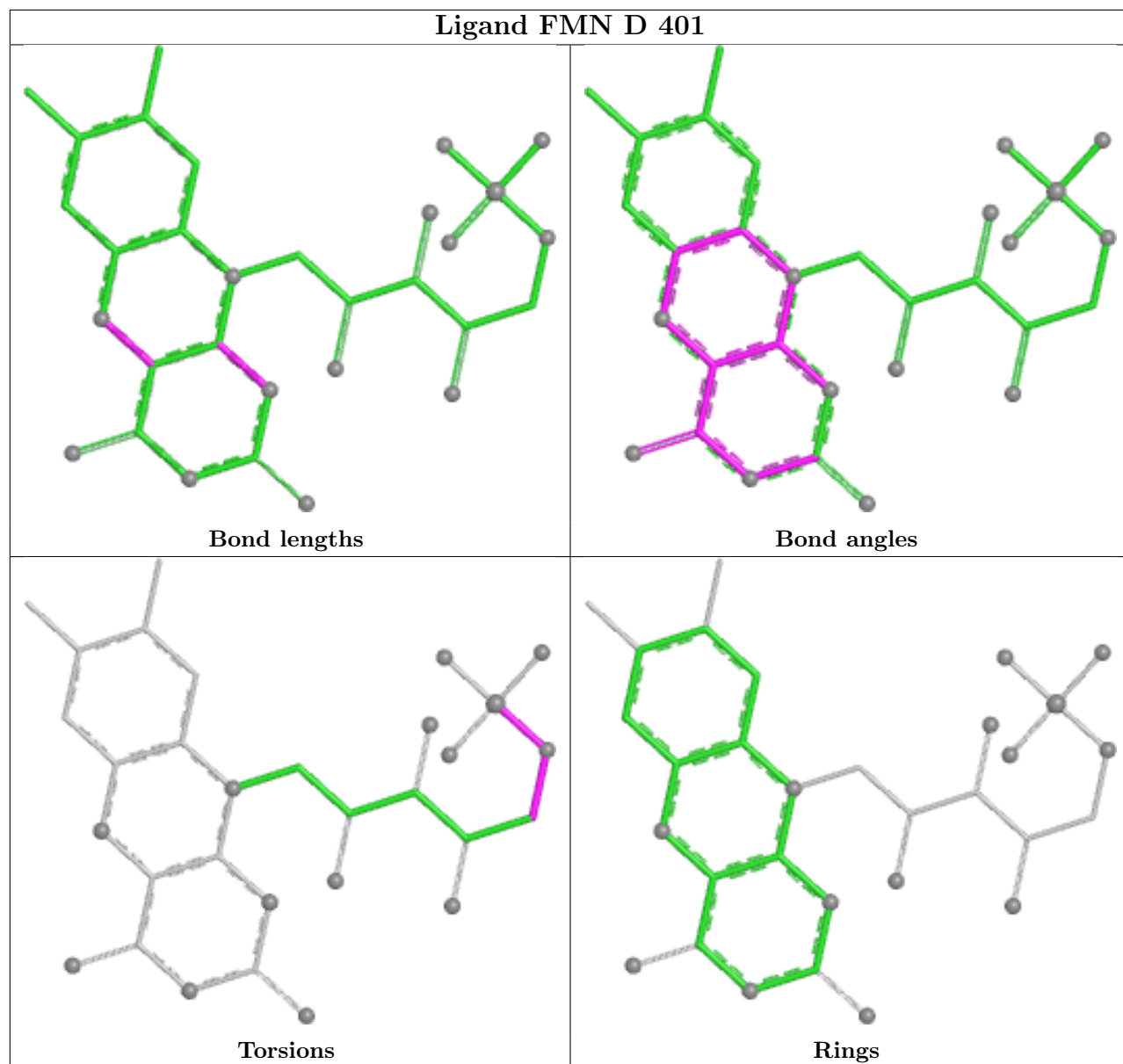


Ligand A1CIO A 404

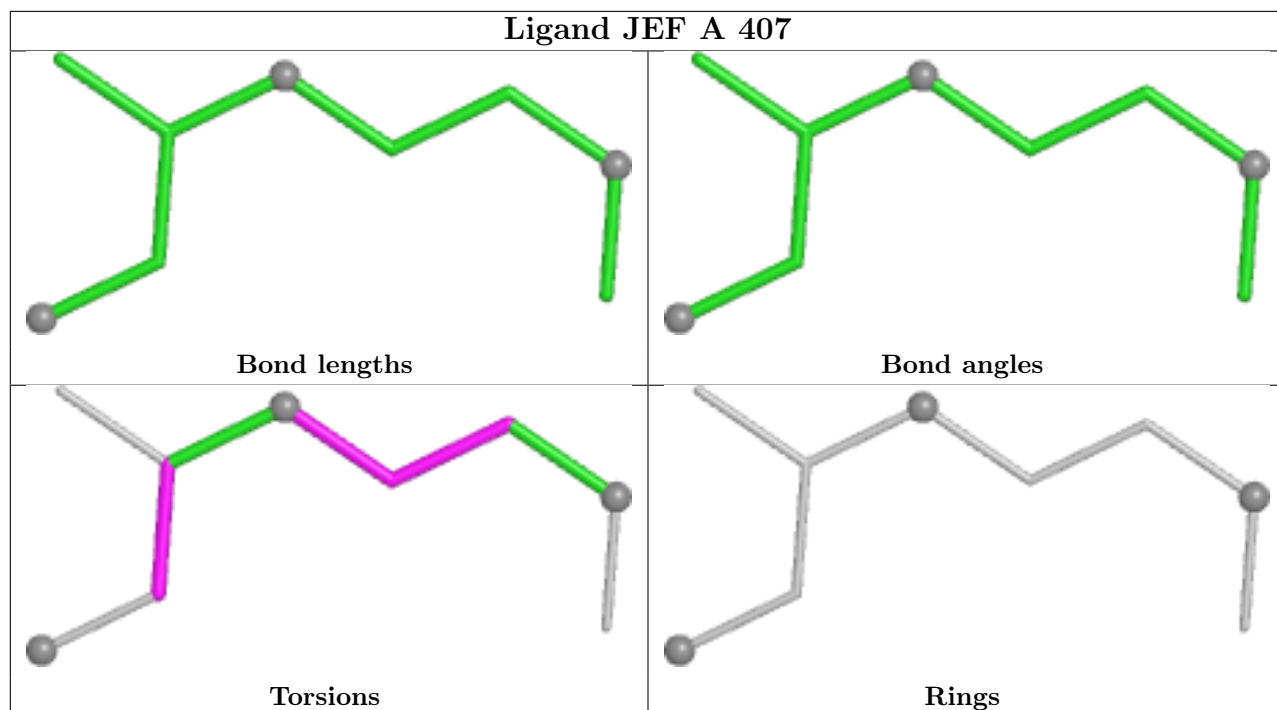




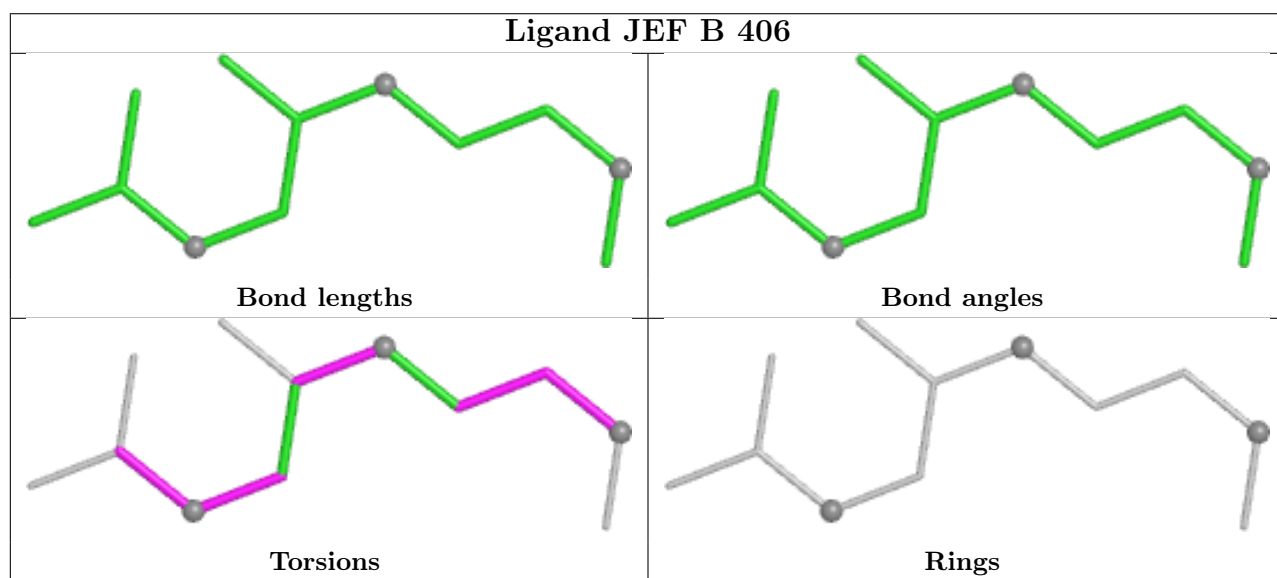


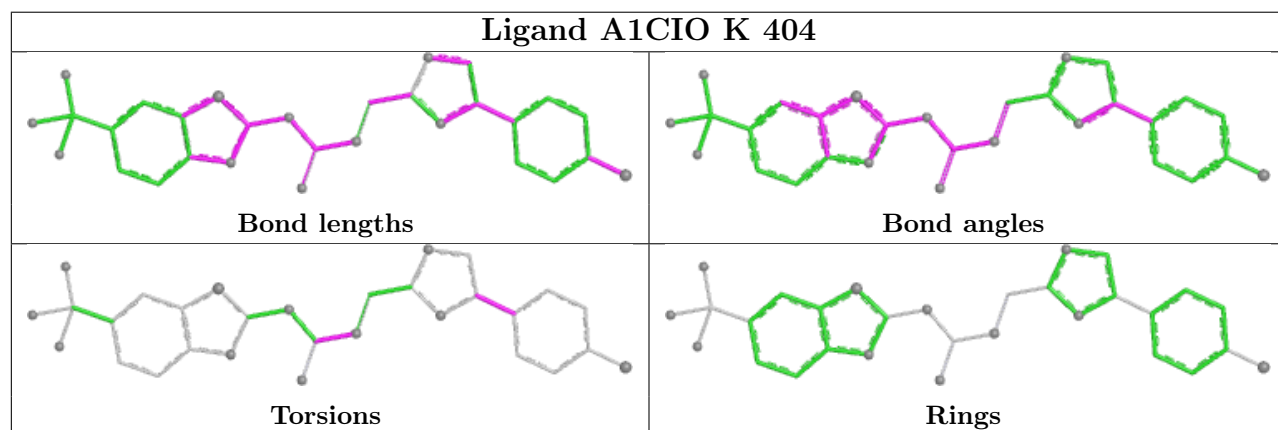
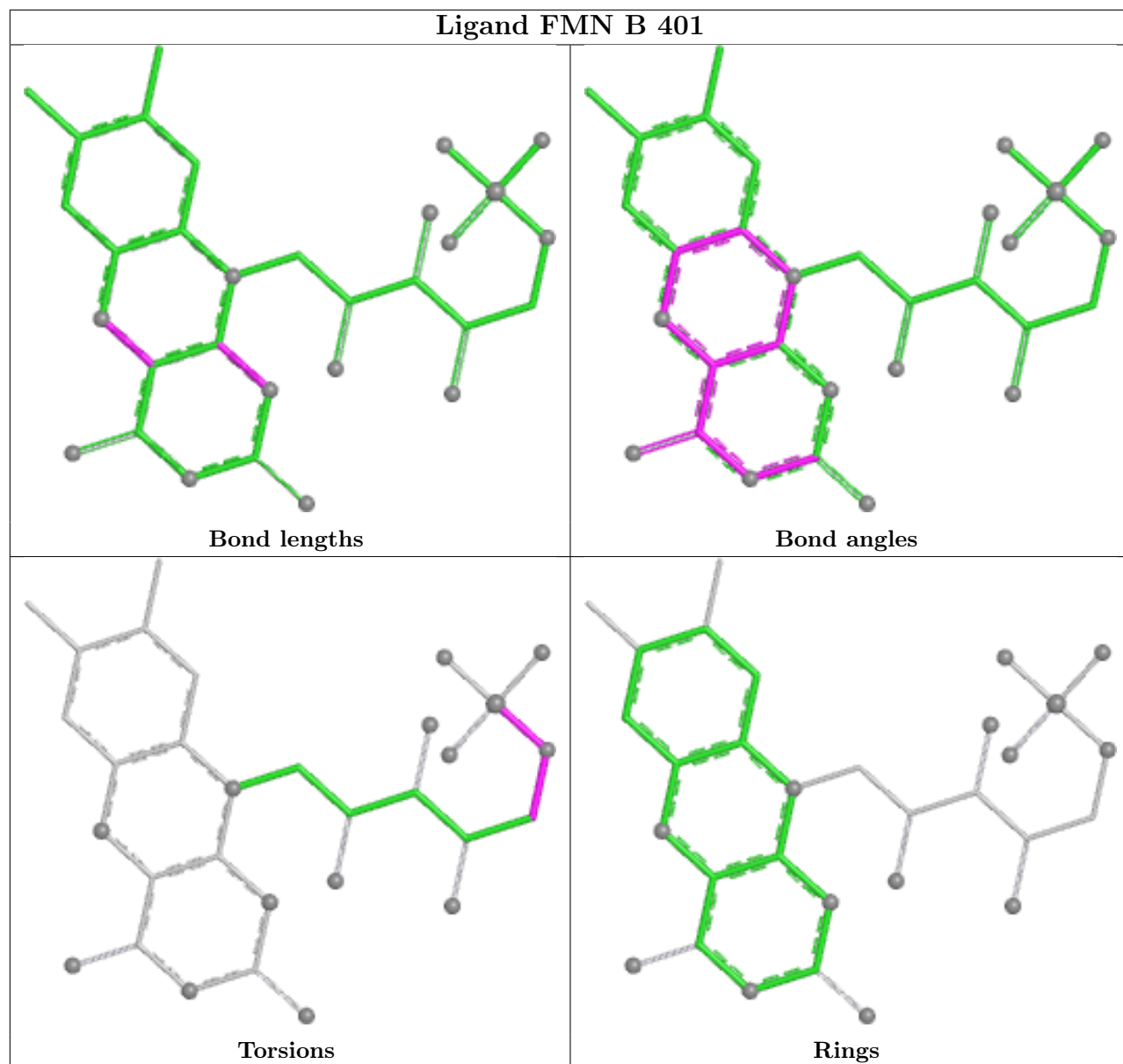


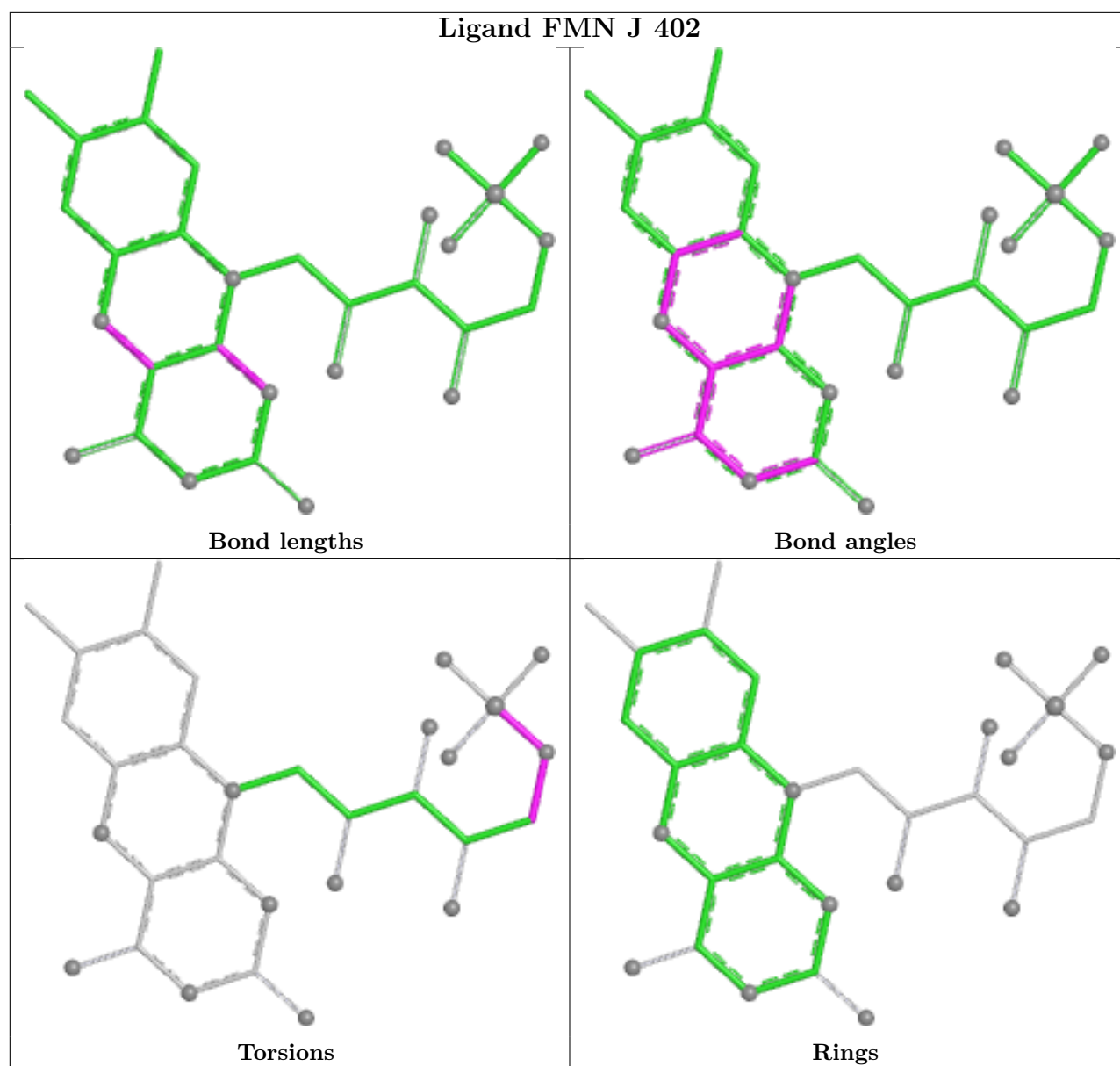
Ligand JEF A 407



Ligand JEF B 406







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/338 (93%)	0.40	11 (3%) 47 47	20, 32, 52, 80	2 (0%)
1	B	316/338 (93%)	0.30	12 (3%) 44 44	17, 30, 51, 72	1 (0%)
1	C	315/338 (93%)	0.67	16 (5%) 33 32	15, 38, 57, 82	2 (0%)
1	D	316/338 (93%)	0.50	12 (3%) 44 44	20, 34, 60, 85	2 (0%)
1	E	314/338 (92%)	0.49	13 (4%) 41 41	20, 35, 54, 70	1 (0%)
1	F	315/338 (93%)	0.51	17 (5%) 31 29	20, 32, 62, 81	0
1	G	315/338 (93%)	1.24	50 (15%) 5 4	29, 49, 68, 93	0
1	H	315/338 (93%)	0.66	18 (5%) 29 27	20, 37, 66, 108	0
1	I	314/338 (92%)	0.59	21 (6%) 24 22	18, 35, 58, 71	0
1	J	314/338 (92%)	0.47	11 (3%) 47 47	20, 34, 52, 70	0
1	K	314/338 (92%)	0.66	20 (6%) 25 24	19, 37, 62, 87	1 (0%)
1	L	314/338 (92%)	1.27	67 (21%) 2 2	28, 51, 72, 91	1 (0%)
All	All	3777/4056 (93%)	0.65	268 (7%) 22 20	15, 36, 63, 108	10 (0%)

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	260	GLY	5.4
1	K	250	PRO	5.1
1	K	257	LEU	5.0
1	F	97	ALA	4.8
1	A	96	GLY	4.8
1	I	97	ALA	4.7
1	D	316	TRP	4.7
1	L	103	PHE	4.5
1	G	309	LEU	4.4
1	F	313	LEU	4.4
1	F	98	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	89	GLY	4.3
1	L	110	ALA	4.0
1	D	97	ALA	4.0
1	I	74	LEU	3.9
1	G	96	GLY	3.9
1	I	313	LEU	3.9
1	B	96	GLY	3.8
1	L	271	VAL	3.8
1	L	309	LEU	3.8
1	F	1	MET	3.8
1	C	309	LEU	3.8
1	F	96	GLY	3.8
1	D	312[A]	ARG	3.7
1	E	309	LEU	3.7
1	E	313	LEU	3.7
1	L	89	GLY	3.7
1	F	310	LYS	3.5
1	G	59	ALA	3.5
1	G	312	ARG	3.5
1	L	102	ALA	3.5
1	L	228	HIS	3.5
1	D	309	LEU	3.5
1	K	247	SER	3.4
1	K	313	LEU	3.4
1	A	310	LYS	3.4
1	G	260	GLY	3.4
1	J	309	LEU	3.4
1	C	1	MET	3.4
1	K	256	LYS	3.4
1	L	77	ASP	3.3
1	B	313	LEU	3.3
1	C	313	LEU	3.3
1	G	48	GLU	3.3
1	G	97	ALA	3.3
1	J	248	GLY	3.3
1	L	96	GLY	3.3
1	F	102	ALA	3.3
1	L	315	ASN	3.3
1	G	62	ILE	3.3
1	L	76	PRO	3.3
1	K	2	LYS	3.3
1	L	109	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	9	ILE	3.2
1	L	226	THR	3.2
1	J	312	ARG	3.2
1	B	316	TRP	3.2
1	G	257	LEU	3.2
1	H	306	THR	3.2
1	G	130	ILE	3.1
1	D	1	MET	3.1
1	I	103	PHE	3.1
1	G	6	ILE	3.1
1	H	313	LEU	3.1
1	I	312	ARG	3.1
1	K	244	LEU	3.1
1	G	1	MET	3.1
1	G	100	PRO	3.0
1	B	312	ARG	3.0
1	A	260	GLY	3.0
1	C	3	ASN	3.0
1	F	315	ASN	3.0
1	G	310	LYS	2.9
1	L	307	GLU	2.9
1	B	102	ALA	2.9
1	I	73	LEU	2.9
1	G	3	ASN	2.9
1	L	3	ASN	2.9
1	C	310	LYS	2.8
1	H	311	ARG	2.8
1	A	1	MET	2.8
1	K	26	GLY	2.8
1	E	96	GLY	2.8
1	I	257	LEU	2.8
1	G	103	PHE	2.8
1	I	46	GLY	2.8
1	A	312	ARG	2.8
1	G	203	ILE	2.7
1	E	98	GLY	2.7
1	L	161	ALA	2.7
1	L	313	LEU	2.7
1	E	97	ALA	2.7
1	G	24	VAL	2.7
1	L	80	ASP	2.7
1	E	254	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	251	LYS	2.7
1	G	248	GLY	2.7
1	L	130	ILE	2.7
1	F	23	TRP	2.7
1	A	97	ALA	2.6
1	G	14	TYR	2.6
1	L	308	VAL	2.6
1	H	217	ARG	2.6
1	E	225	SER	2.6
1	H	250	PRO	2.6
1	L	91[A]	LYS	2.6
1	C	97	ALA	2.6
1	J	109	ALA	2.6
1	K	97	ALA	2.6
1	L	67	PHE	2.6
1	B	257	LEU	2.6
1	G	256	LYS	2.6
1	K	252	GLU	2.6
1	G	109	ALA	2.6
1	G	4	ASN	2.6
1	I	315	ASN	2.6
1	F	103	PHE	2.6
1	H	257	LEU	2.6
1	L	257	LEU	2.6
1	A	98	GLY	2.6
1	A	101	GLY	2.6
1	G	101	GLY	2.6
1	I	96	GLY	2.6
1	L	86	ILE	2.6
1	G	313	LEU	2.5
1	I	102	ALA	2.5
1	L	124	ALA	2.5
1	G	315	ASN	2.5
1	L	23	TRP	2.5
1	E	310	LYS	2.5
1	G	86	ILE	2.5
1	L	267	ILE	2.5
1	B	1	MET	2.5
1	J	310	LYS	2.5
1	I	100	PRO	2.5
1	H	254	ILE	2.5
1	H	54	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	47	MET	2.5
1	H	249	ALA	2.5
1	H	315	ASN	2.5
1	I	99	ASN	2.5
1	K	249	ALA	2.5
1	L	132	ALA	2.5
1	L	100	PRO	2.5
1	C	151	THR	2.5
1	L	88	GLU	2.4
1	G	67	PHE	2.4
1	I	254	ILE	2.4
1	F	2	LYS	2.4
1	D	315	ASN	2.4
1	L	265	ALA	2.4
1	C	89	GLY	2.4
1	I	272	GLU	2.4
1	L	101	GLY	2.4
1	L	258	GLY	2.4
1	C	254	ILE	2.4
1	J	9	ILE	2.4
1	G	93	ILE	2.4
1	L	9	ILE	2.4
1	G	47	MET	2.4
1	D	313	LEU	2.4
1	H	212	LEU	2.4
1	J	315	ASN	2.4
1	B	243	GLU	2.4
1	H	310	LYS	2.4
1	F	73	LEU	2.4
1	L	266	VAL	2.4
1	F	257	LEU	2.4
1	L	49	PRO	2.3
1	L	47	MET	2.3
1	C	308	VAL	2.3
1	L	90	VAL	2.3
1	K	309	LEU	2.3
1	L	74	LEU	2.3
1	A	3	ASN	2.3
1	D	99	ASN	2.3
1	G	127	MET	2.3
1	L	225	SER	2.3
1	B	103	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	85	CYS	2.3
1	G	98	GLY	2.3
1	K	258	GLY	2.3
1	L	31	GLY	2.3
1	B	97	ALA	2.3
1	A	2	LYS	2.3
1	L	115	ILE	2.3
1	D	257	LEU	2.2
1	G	107	LEU	2.2
1	G	133	ASP	2.2
1	C	246[A]	ARG	2.2
1	I	226	THR	2.2
1	J	313	LEU	2.2
1	G	117	VAL	2.2
1	L	78	VAL	2.2
1	G	55	ASN	2.2
1	H	312	ARG	2.2
1	K	109	ALA	2.2
1	K	310	LYS	2.2
1	G	63	THR	2.2
1	E	74	LEU	2.2
1	L	244	LEU	2.2
1	G	90	VAL	2.2
1	G	27	GLY	2.2
1	K	255	GLU	2.2
1	G	112	ILE	2.2
1	L	92	VAL	2.2
1	B	310	LYS	2.2
1	E	217	ARG	2.1
1	G	254	ILE	2.1
1	H	1	MET	2.1
1	G	84	VAL	2.1
1	G	285	VAL	2.1
1	D	2	LYS	2.1
1	D	310	LYS	2.1
1	H	252	GLU	2.1
1	H	253	GLU	2.1
1	I	253	GLU	2.1
1	L	97	ALA	2.1
1	C	257	LEU	2.1
1	I	309	LEU	2.1
1	K	254	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	6	ILE	2.1
1	L	73	LEU	2.1
1	L	93	ILE	2.1
1	B	315	ASN	2.1
1	I	54	GLU	2.1
1	I	245	GLU	2.1
1	L	133	ASP	2.1
1	G	121	VAL	2.1
1	A	263	ARG	2.1
1	C	226	THR	2.1
1	F	312	ARG	2.1
1	L	256	LYS	2.1
1	C	9	ILE	2.1
1	C	264	LEU	2.1
1	F	309	LEU	2.1
1	L	48	GLU	2.1
1	L	79	GLU	2.1
1	L	105	GLU	2.1
1	K	297	PHE	2.1
1	L	263	ARG	2.1
1	L	95	THR	2.1
1	E	255	GLU	2.1
1	G	314	GLU	2.1
1	L	187	GLU	2.1
1	F	250	PRO	2.1
1	J	98	GLY	2.1
1	L	223	GLY	2.1
1	C	218	SER	2.0
1	J	48	GLU	2.0
1	G	125	GLU	2.0
1	J	3	ASN	2.0
1	H	309	LEU	2.0
1	G	66	PRO	2.0
1	L	207	TYR	2.0
1	E	271	VAL	2.0
1	E	2	LYS	2.0
1	H	2	LYS	2.0
1	L	236	LYS	2.0
1	F	104	MET	2.0
1	L	94	THR	2.0
1	L	224	THR	2.0
1	L	259	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	270	ASP	2.0
1	K	202	LEU	2.0
1	L	51	LEU	2.0
1	L	56	ILE	2.0
1	G	2	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	J	401	4/4	0.33	0.22	48,56,59,95	0
5	DMS	D	406	4/4	0.46	0.22	44,50,61,77	0
4	A1CIO	L	404	30/30	0.50	0.26	56,75,97,164	30
6	JEF	J	407	12/41	0.52	0.23	54,67,70,75	0
5	DMS	F	401	4/4	0.53	0.22	37,53,67,82	0
6	JEF	B	406	12/41	0.55	0.20	68,71,77,79	0
4	A1CIO	G	404	30/30	0.57	0.24	49,71,95,151	30
6	JEF	E	408	7/41	0.57	0.25	55,60,65,66	0
4	A1CIO	K	404	30/30	0.57	0.25	34,65,90,188	30
6	JEF	A	407	9/41	0.58	0.22	38,43,53,60	0
6	JEF	E	406	16/41	0.58	0.20	62,77,87,90	0
6	JEF	I	406	8/41	0.58	0.20	44,52,58,65	0
5	DMS	C	407	4/4	0.61	0.18	54,67,68,89	0
5	DMS	A	406	4/4	0.62	0.19	66,68,71,88	0
4	A1CIO	C	404	30/30	0.63	0.25	40,62,86,154	30
4	A1CIO	J	405	30/30	0.63	0.24	32,56,91,146	30
6	JEF	E	407	10/41	0.65	0.20	49,57,62,66	0
4	A1CIO	E	404	30/30	0.65	0.27	36,58,86,162	30

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	JEF	K	406	9/41	0.65	0.19	51,64,75,75	0
7	CIT	D	405	13/13	0.65	0.18	54,65,72,74	0
4	A1CIO	B	404	30/30	0.66	0.22	28,50,80,151	30
4	A1CIO	A	404	30/30	0.67	0.23	34,53,87,158	30
6	JEF	F	407	10/41	0.67	0.19	45,61,66,68	0
4	A1CIO	D	404	30/30	0.67	0.23	39,57,83,142	30
5	DMS	C	406	4/4	0.68	0.19	60,76,83,87	0
5	DMS	E	405	4/4	0.68	0.18	52,54,57,82	0
4	A1CIO	H	404	30/30	0.68	0.23	34,55,82,136	30
6	JEF	D	408	8/41	0.68	0.19	54,65,70,73	0
6	JEF	A	408	6/41	0.69	0.17	41,46,56,57	0
4	A1CIO	F	405	30/30	0.69	0.21	35,47,86,156	30
6	JEF	D	407	10/41	0.69	0.17	51,56,61,66	0
6	JEF	B	405	16/41	0.70	0.18	40,51,59,64	0
6	JEF	H	406	7/41	0.71	0.16	42,47,50,59	0
4	A1CIO	I	404	30/30	0.72	0.22	30,52,83,184	30
6	JEF	C	405	6/41	0.73	0.19	49,52,56,61	0
5	DMS	A	405	4/4	0.73	0.27	49,58,58,81	0
5	DMS	F	406	4/4	0.75	0.15	42,52,58,82	0
3	NA	K	403	1/1	0.76	0.20	46,46,46,46	0
6	JEF	G	405	8/41	0.76	0.17	47,58,62,64	0
5	DMS	K	405	4/4	0.78	0.18	46,49,64,81	0
5	DMS	H	405	4/4	0.80	0.17	46,60,66,78	0
3	NA	E	402	1/1	0.82	0.08	28,28,28,28	0
3	NA	G	402	1/1	0.83	0.08	45,45,45,45	0
5	DMS	J	406	4/4	0.86	0.17	57,57,60,77	0
3	NA	C	403	1/1	0.86	0.07	31,31,31,31	0
3	NA	F	403	1/1	0.87	0.14	36,36,36,36	0
3	NA	L	402	1/1	0.88	0.08	44,44,44,44	0
3	NA	I	403	1/1	0.88	0.09	28,28,28,28	0
3	NA	D	403	1/1	0.88	0.07	31,31,31,31	0
3	NA	D	402	1/1	0.90	0.08	43,43,43,43	0
3	NA	E	403	1/1	0.90	0.06	29,29,29,29	0
3	NA	B	402	1/1	0.91	0.08	32,32,32,32	0
2	FMN	L	401	31/31	0.91	0.10	27,42,51,52	0
3	NA	H	402	1/1	0.91	0.07	41,41,41,41	0
3	NA	H	403	1/1	0.91	0.05	30,30,30,30	0
3	NA	B	403	1/1	0.92	0.07	24,24,24,24	0
3	NA	J	403	1/1	0.92	0.09	32,32,32,32	0
2	FMN	H	401	31/31	0.92	0.10	23,29,33,37	0
2	FMN	K	401	31/31	0.92	0.10	21,34,41,44	0
2	FMN	C	401	31/31	0.92	0.09	19,28,35,39	0

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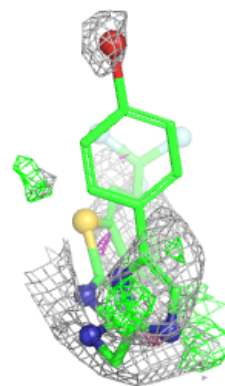
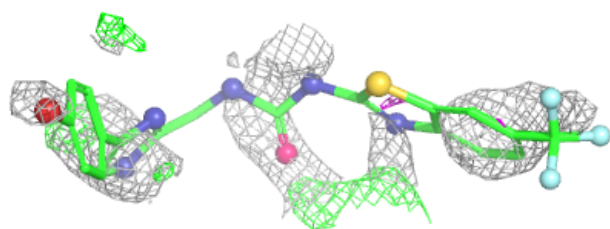
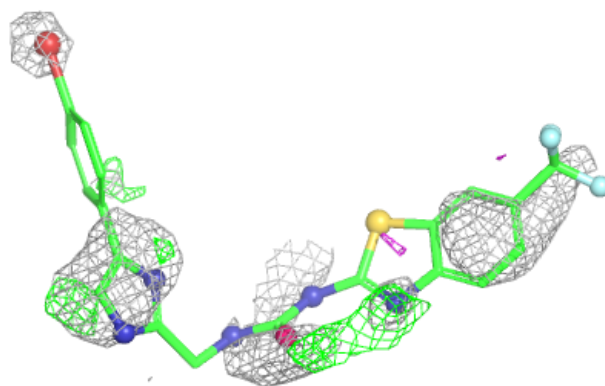
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	403	1/1	0.92	0.11	30,30,30,30	0
2	FMN	G	401	31/31	0.92	0.09	20,35,43,47	0
2	FMN	I	401	31/31	0.93	0.08	18,26,33,35	0
2	FMN	E	401	31/31	0.93	0.09	17,28,33,35	0
5	DMS	I	405	4/4	0.93	0.13	39,46,51,77	0
2	FMN	D	401	31/31	0.94	0.08	19,24,35,40	0
3	NA	I	402	1/1	0.94	0.07	40,40,40,40	0
3	NA	F	404	1/1	0.94	0.04	28,28,28,28	0
3	NA	K	402	1/1	0.94	0.05	43,43,43,43	0
2	FMN	B	401	31/31	0.94	0.08	15,22,30,30	0
2	FMN	J	402	31/31	0.94	0.08	15,23,32,33	0
3	NA	G	403	1/1	0.94	0.10	38,38,38,38	0
2	FMN	A	401	31/31	0.94	0.08	14,26,33,35	0
2	FMN	F	402	31/31	0.95	0.07	16,24,33,37	0
3	NA	L	403	1/1	0.95	0.06	34,34,34,34	0
3	NA	C	402	1/1	0.96	0.08	34,34,34,34	0
3	NA	J	404	1/1	0.96	0.04	29,29,29,29	0
3	NA	A	402	1/1	0.96	0.04	36,36,36,36	0

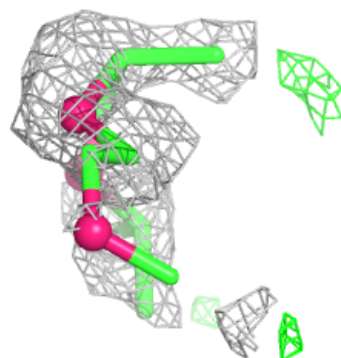
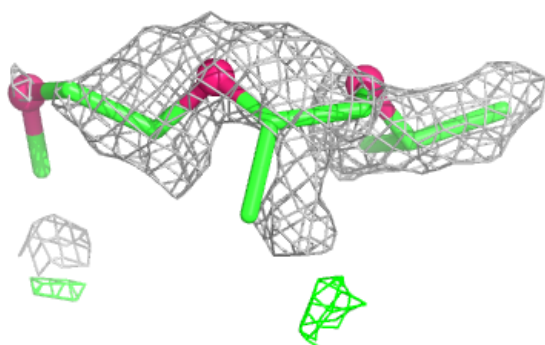
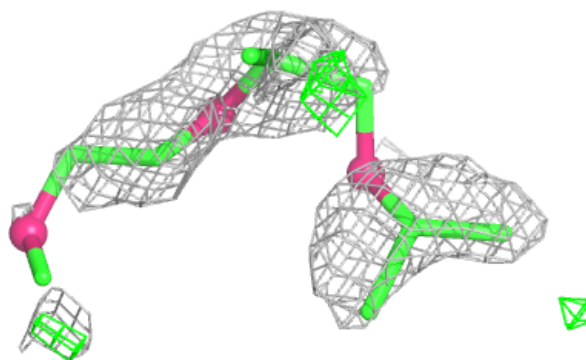
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CIO L 404:

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

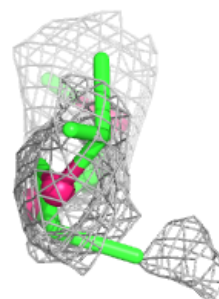
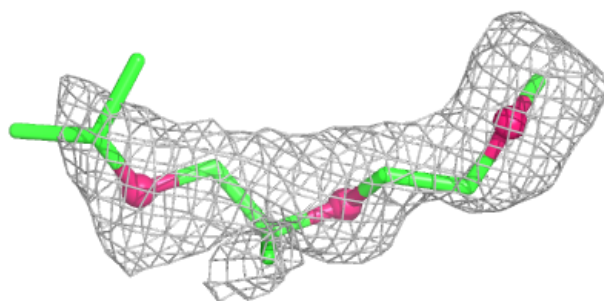
**Electron density around JEF J 407:**

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



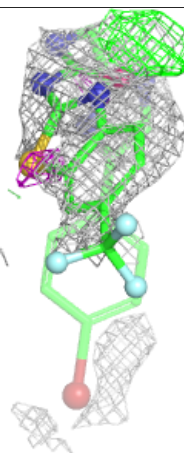
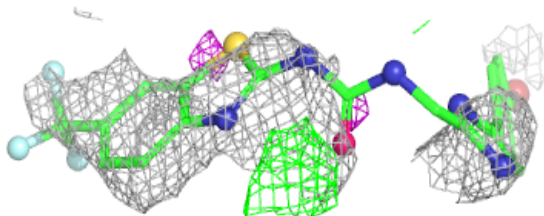
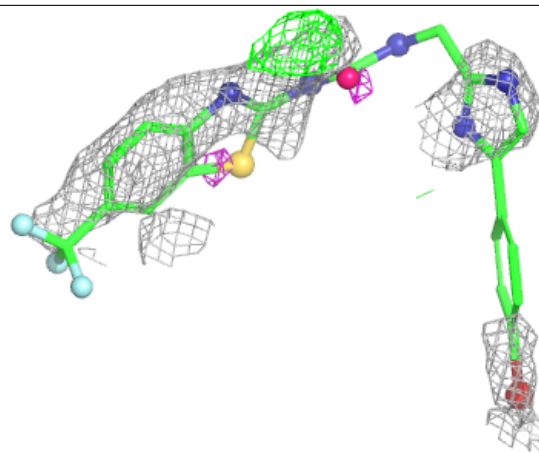
Electron density around JEF B 406:

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

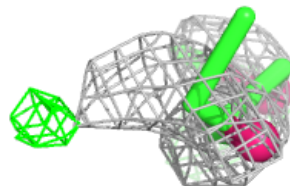
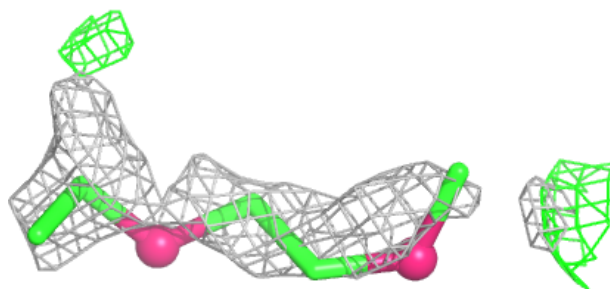
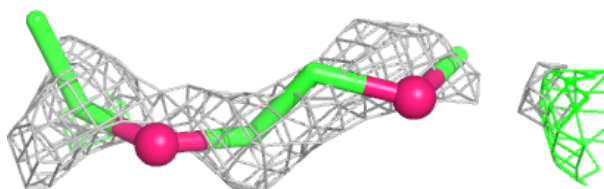


Electron density around A1CIO G 404:

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

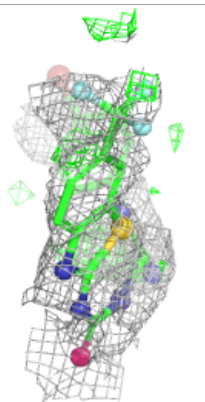
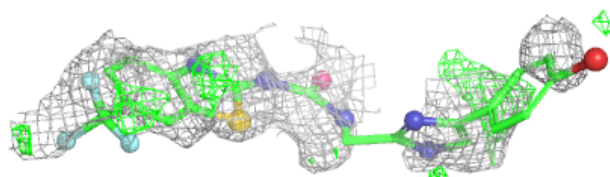
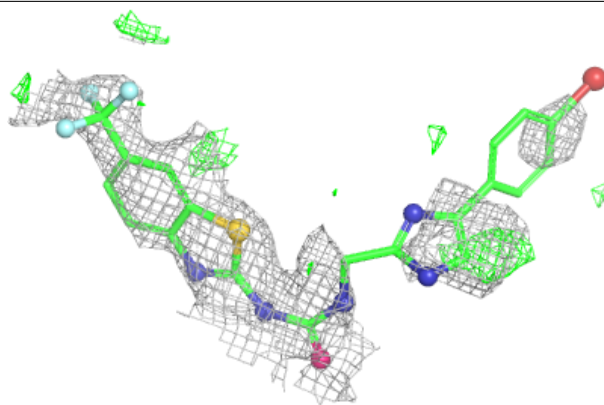
**Electron density around JEF E 408:**

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

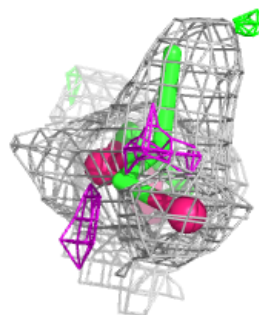
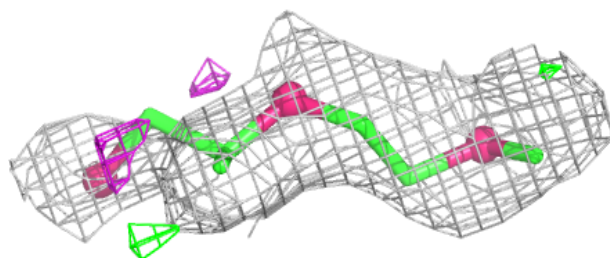
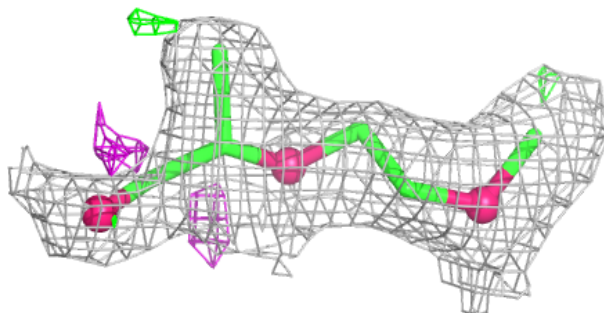


Electron density around A1CIO K 404:

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

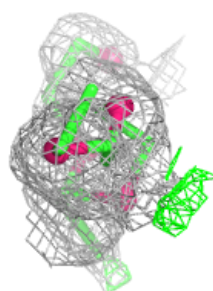
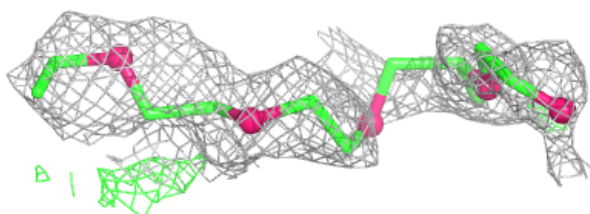
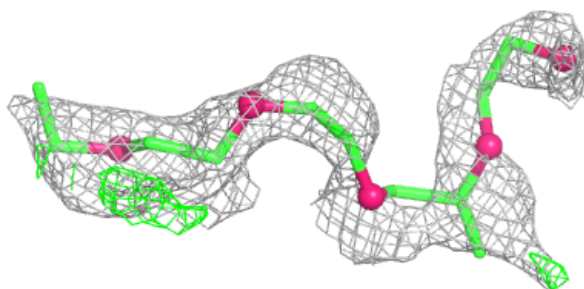
**Electron density around JEF A 407:**

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

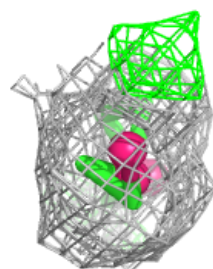
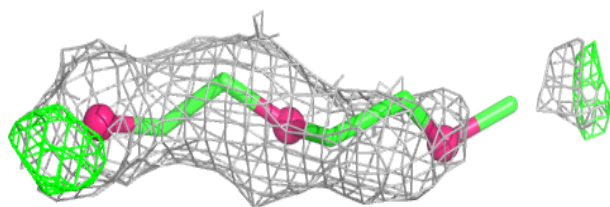
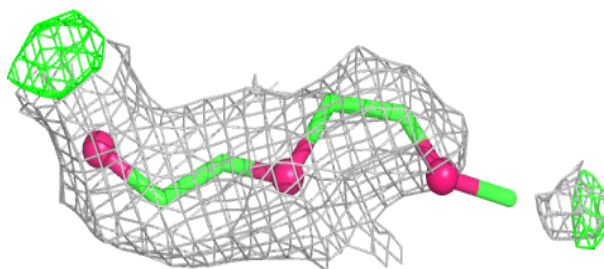


Electron density around JEF E 406:

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

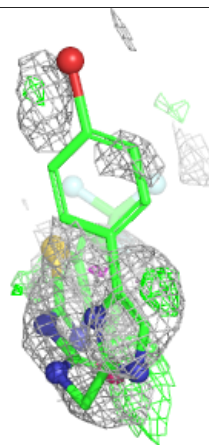
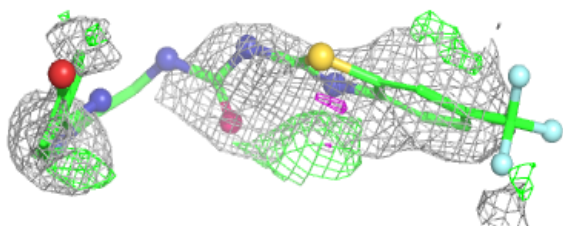
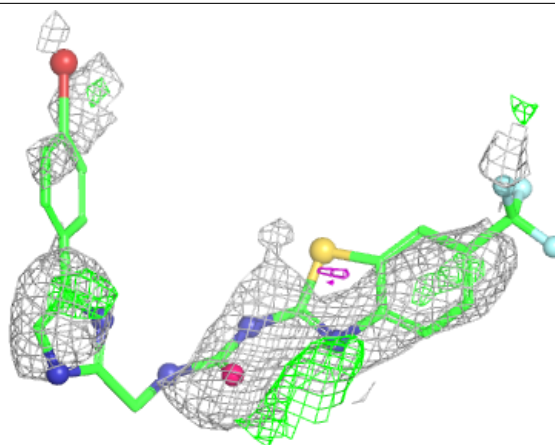
**Electron density around JEF I 406:**

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

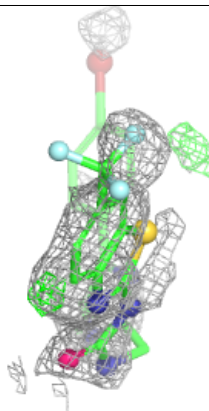
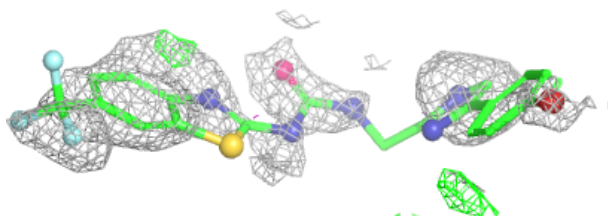
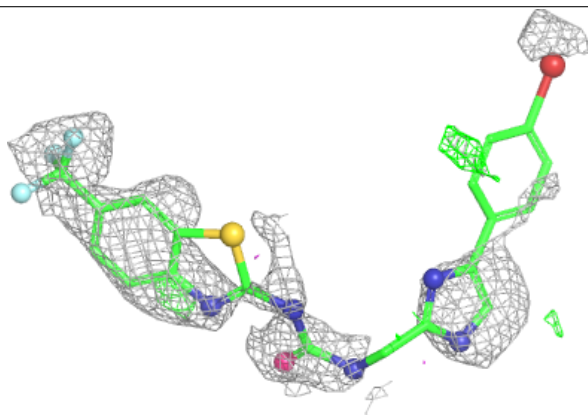


Electron density around A1CIO C 404:

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

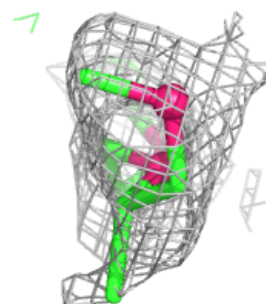
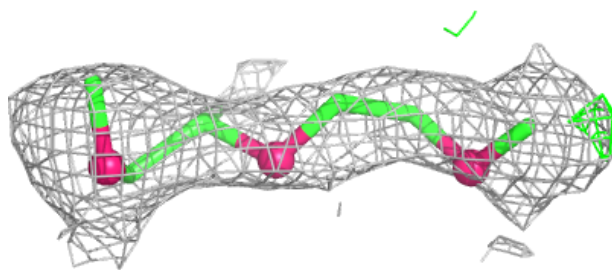
**Electron density around A1CIO J 405:**

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

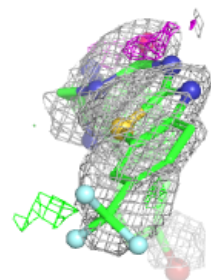
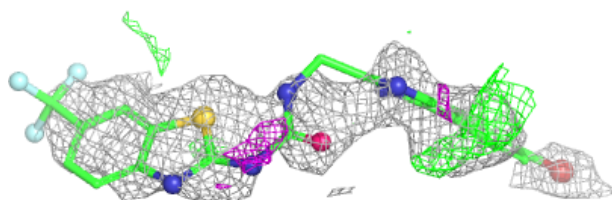
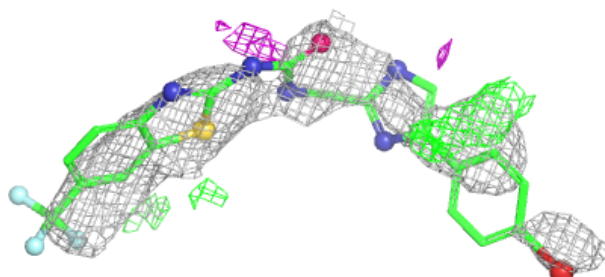


Electron density around JEF E 407:

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

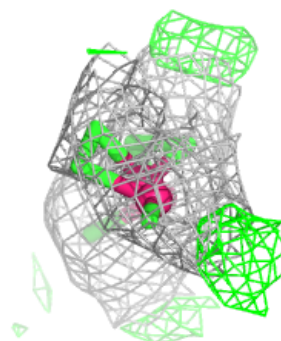
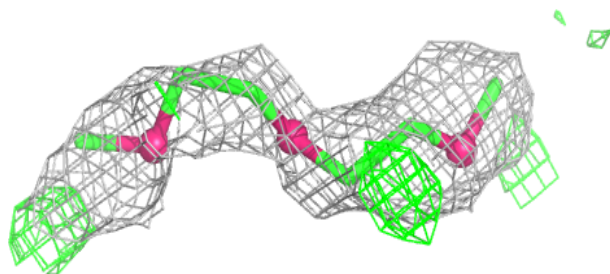
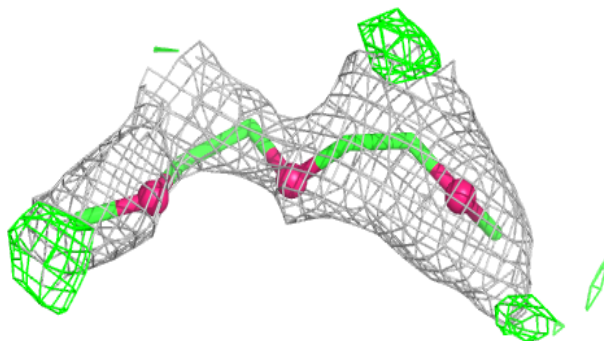
**Electron density around A1CIO E 404:**

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

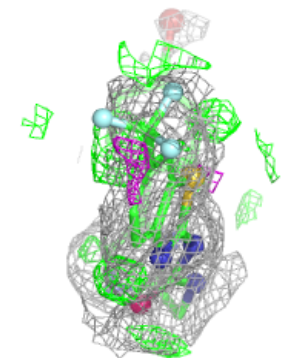
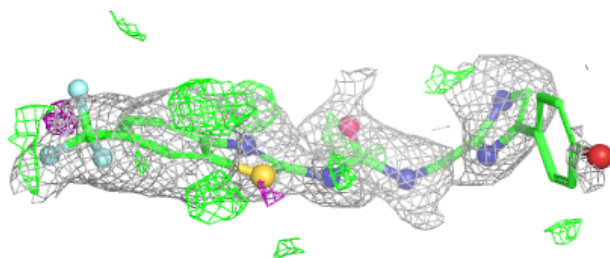
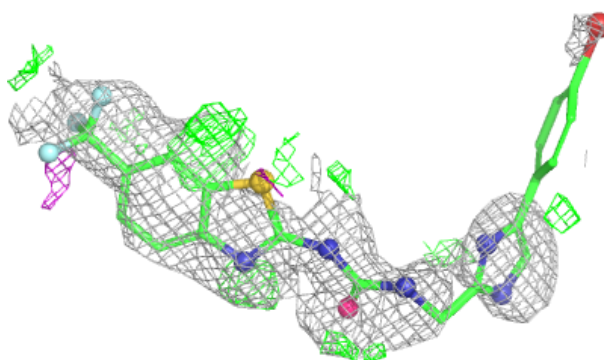


Electron density around JEF K 406:

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

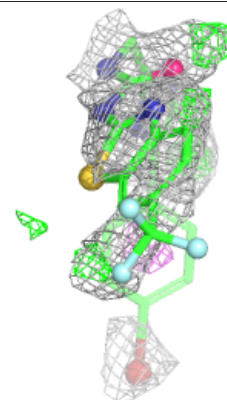
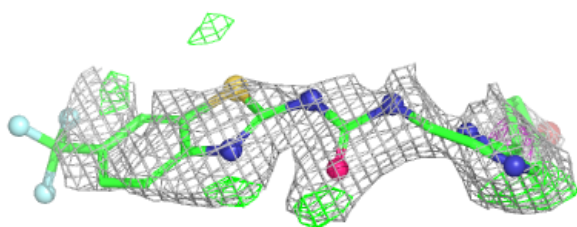
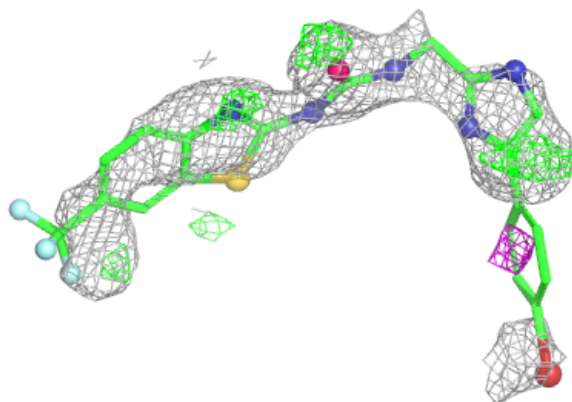
**Electron density around A1CIO B 404:**

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

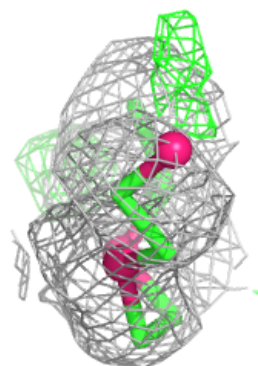
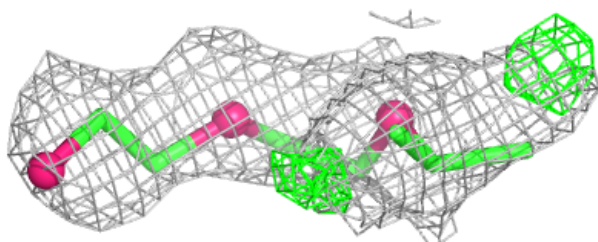
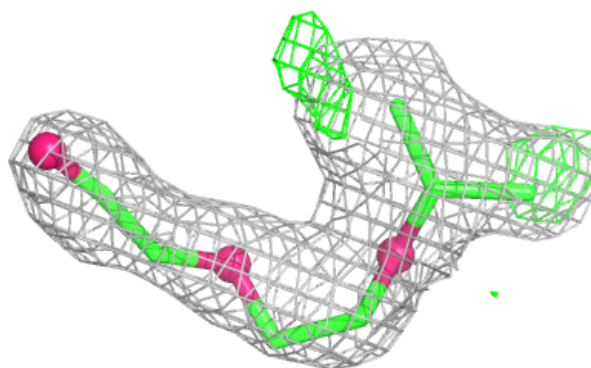


Electron density around A1CIO A 404:

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

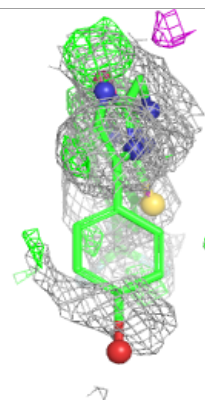
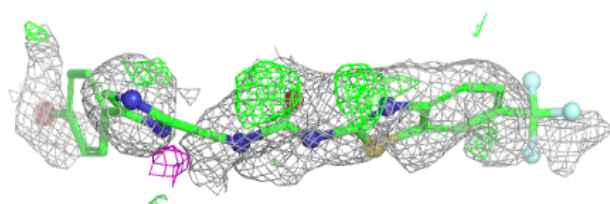
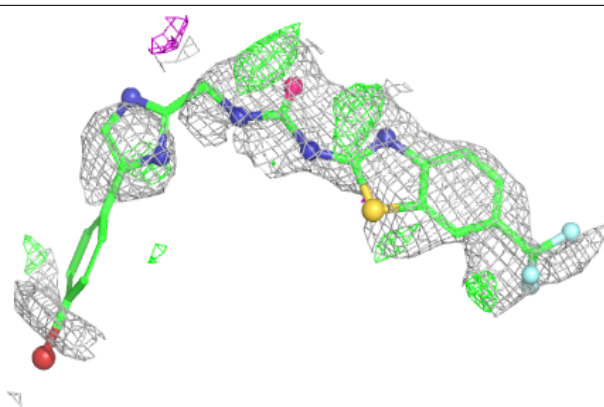
**Electron density around JEF F 407:**

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

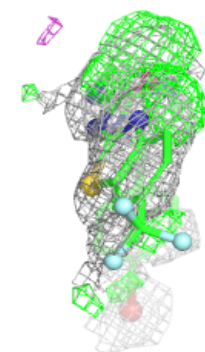
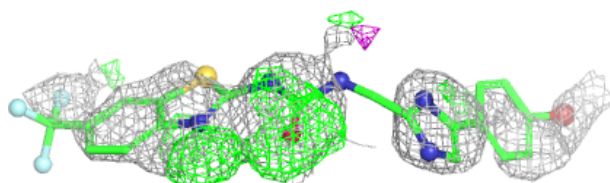
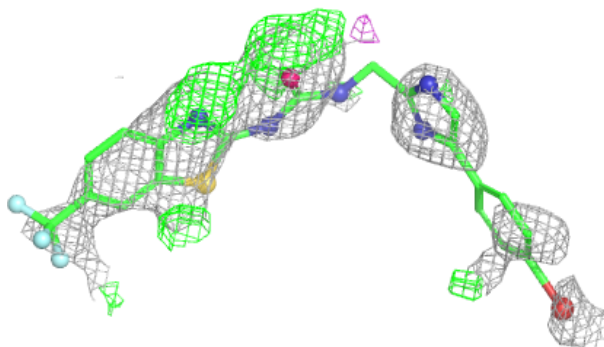


Electron density around A1CIO D 404:

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

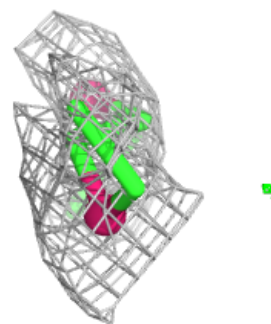
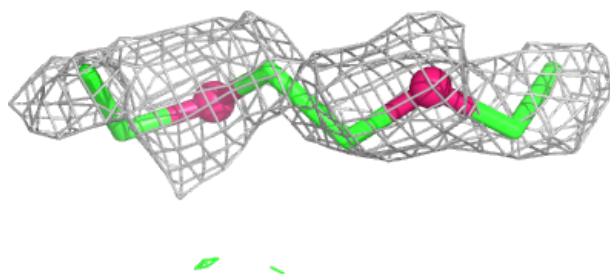
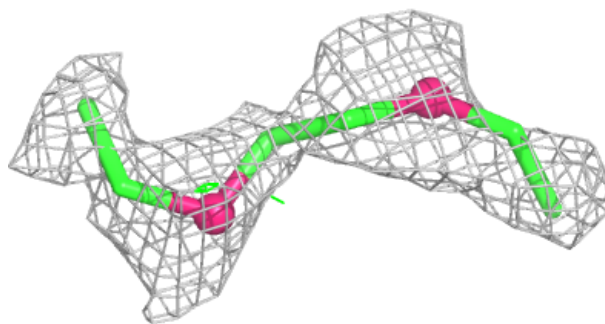
**Electron density around A1CIO H 404:**

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



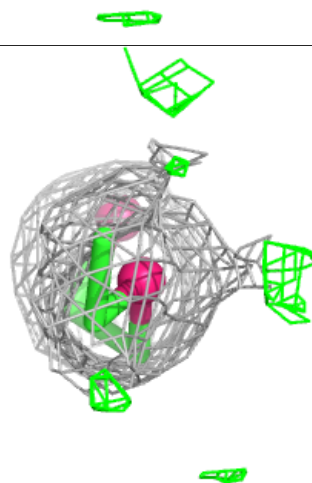
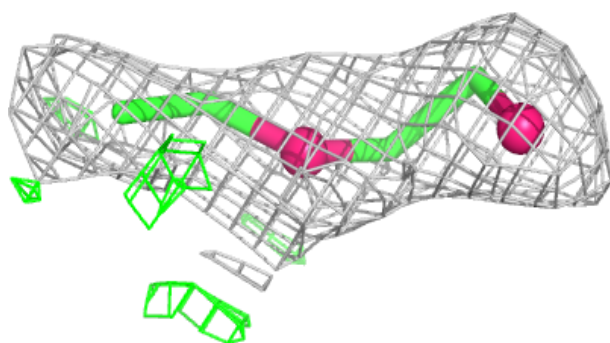
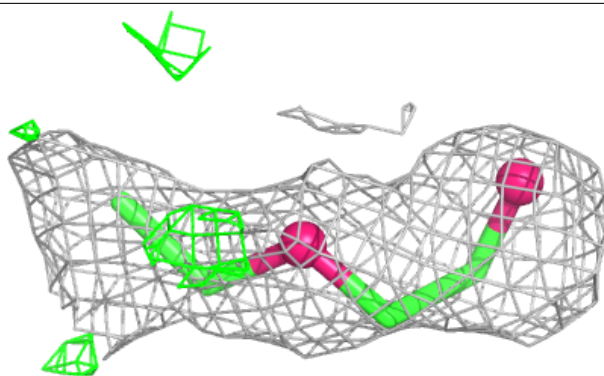
Electron density around JEF D 408:

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

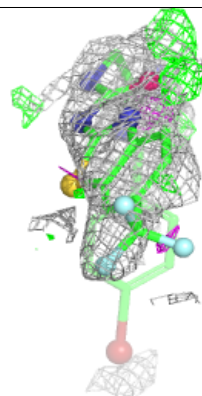
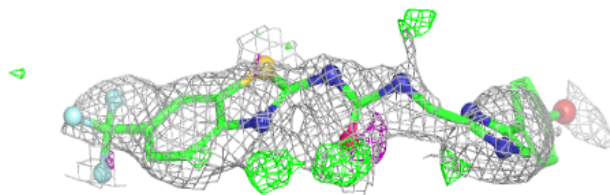
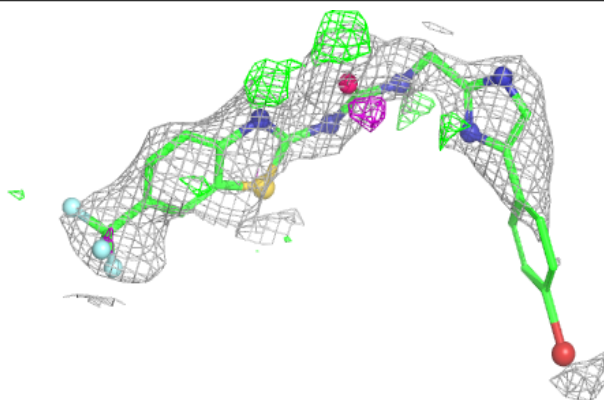


Electron density around JEF A 408:

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

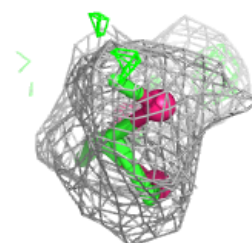
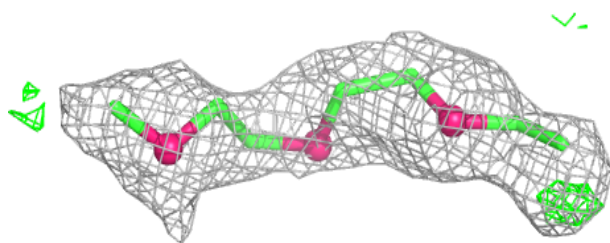
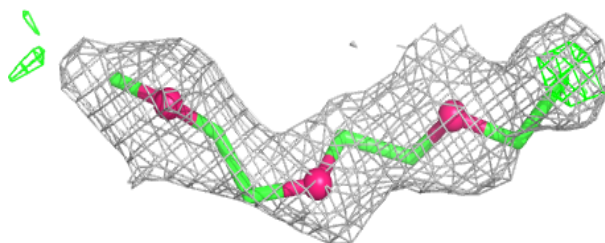
**Electron density around A1CIO F 405:**

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

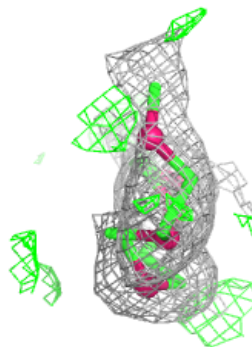
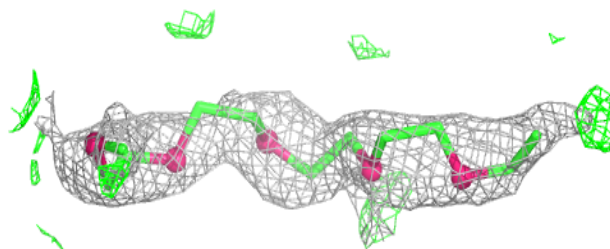
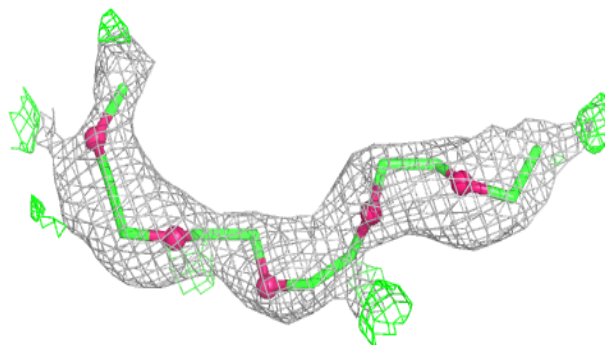


Electron density around JEF D 407:

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

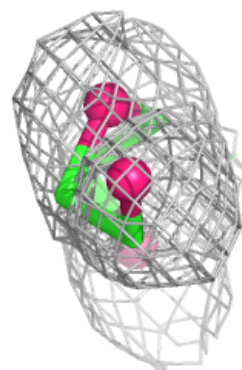
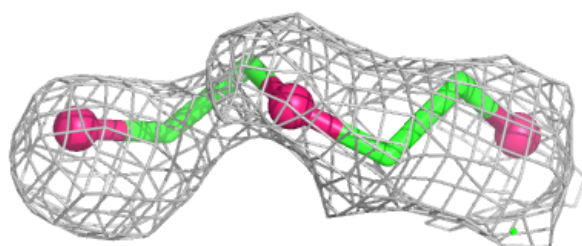
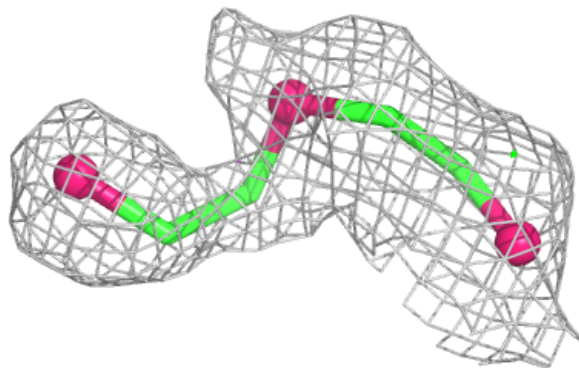
**Electron density around JEF B 405:**

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

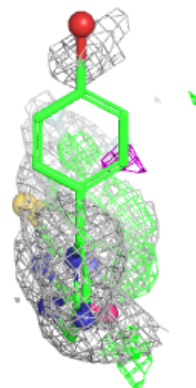
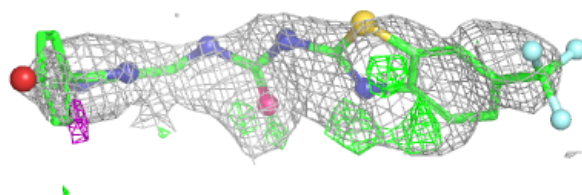
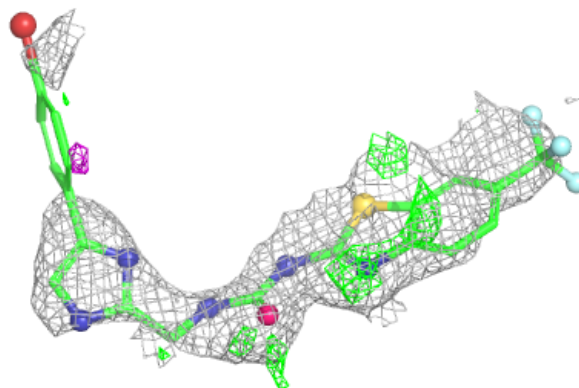


Electron density around JEF H 406:

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

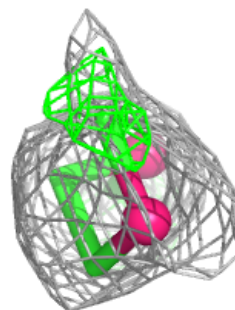
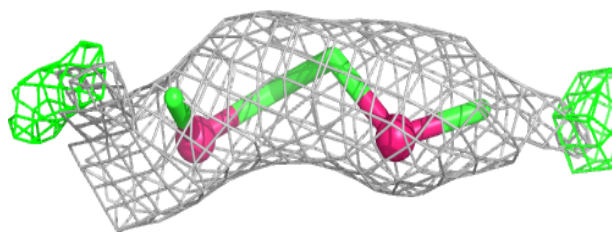
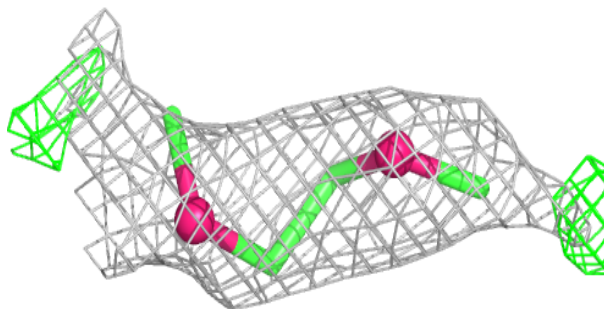
**Electron density around A1CIO I 404:**

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

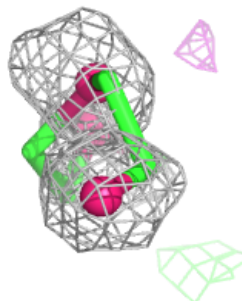
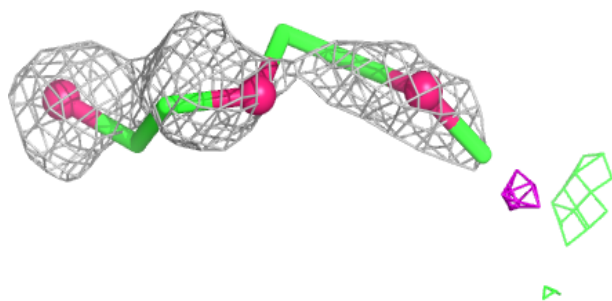
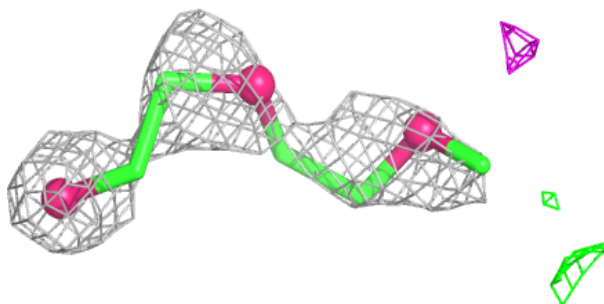


Electron density around JEF C 405:

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

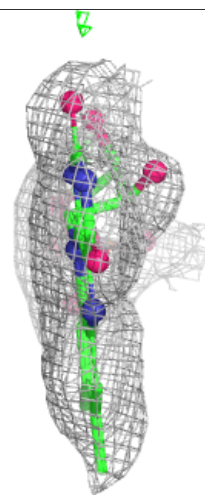
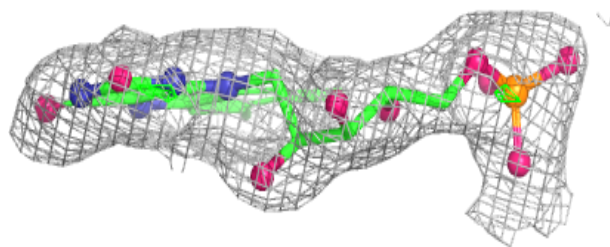
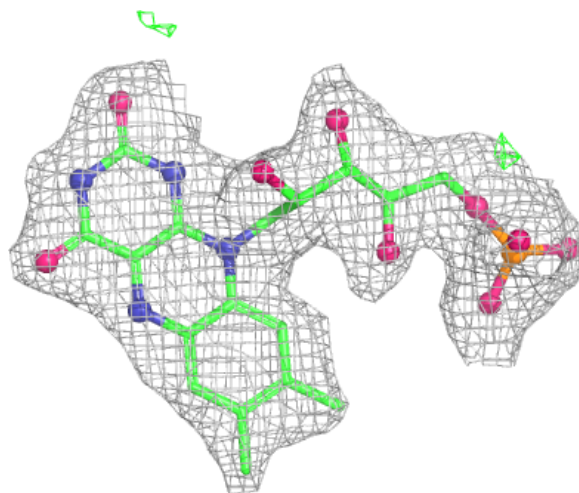
**Electron density around JEF G 405:**

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



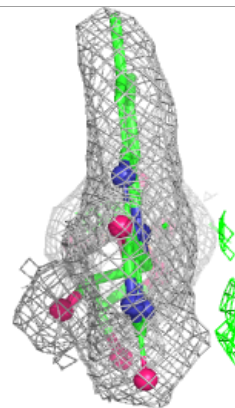
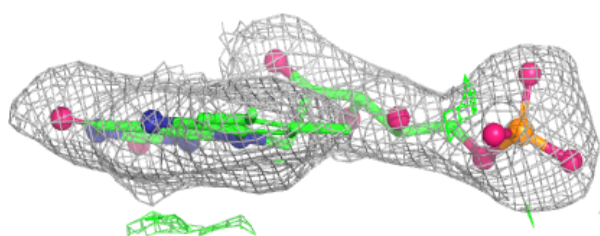
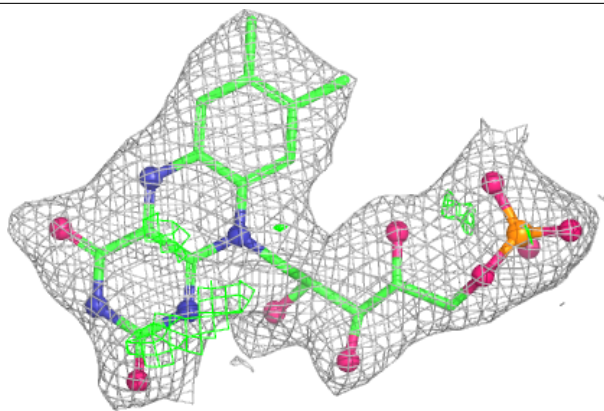
Electron density around FMN L 401:

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



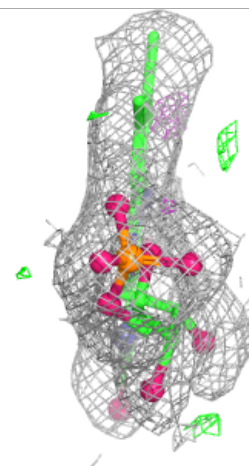
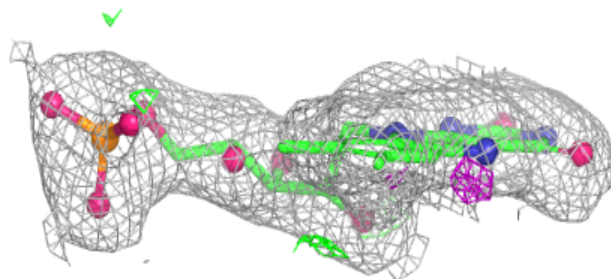
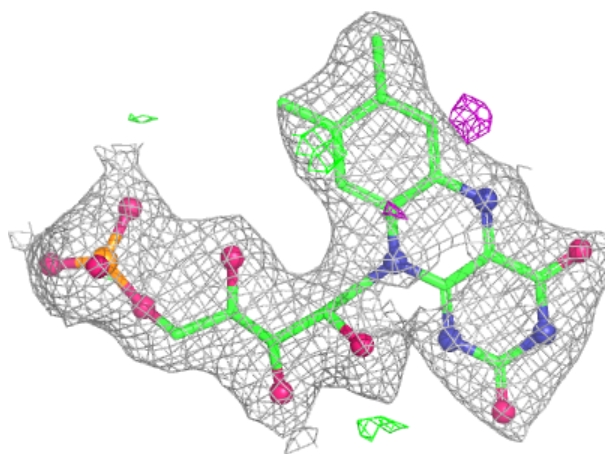
Electron density around FMN H 401:

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



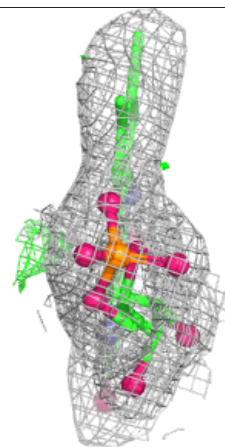
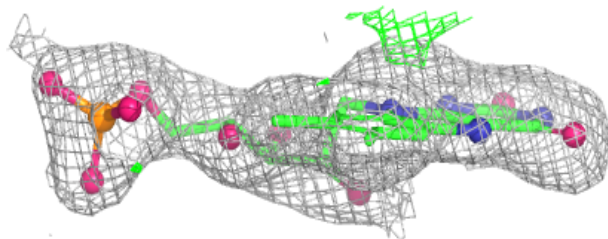
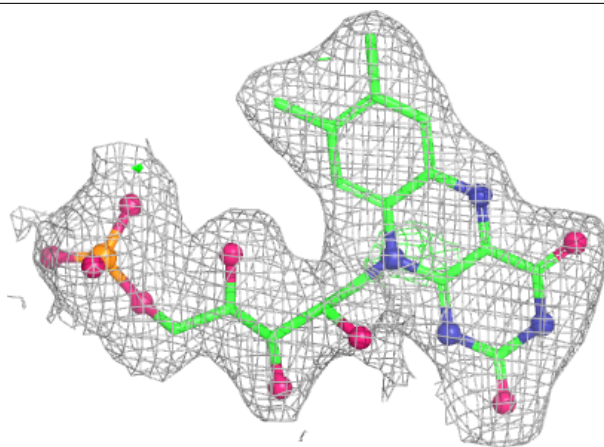
Electron density around FMN K 401:

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



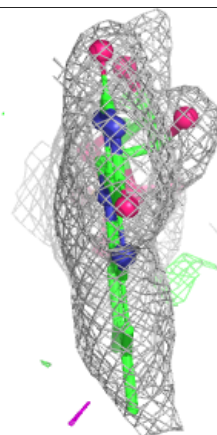
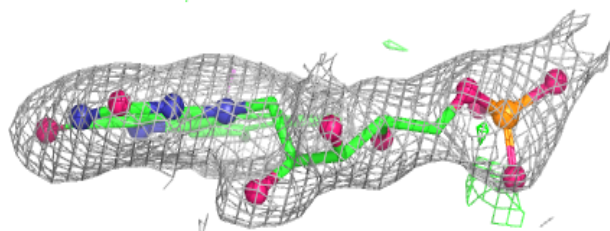
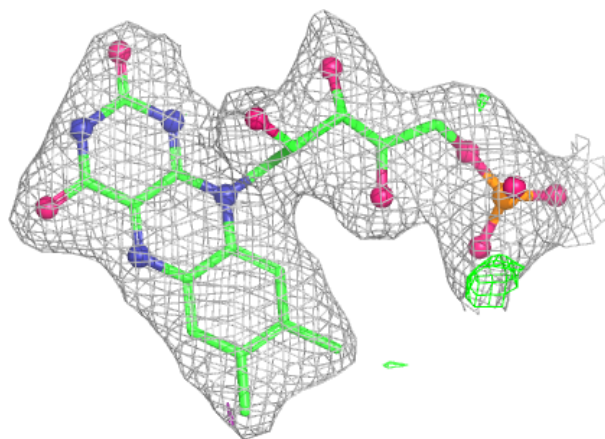
Electron density around FMN C 401:

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



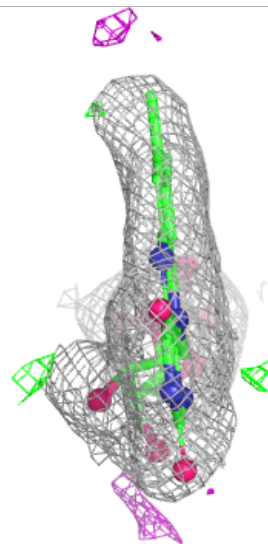
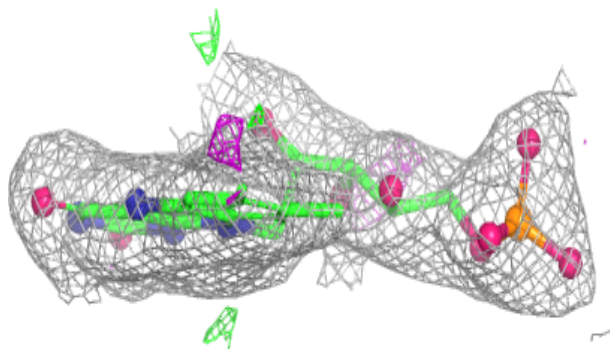
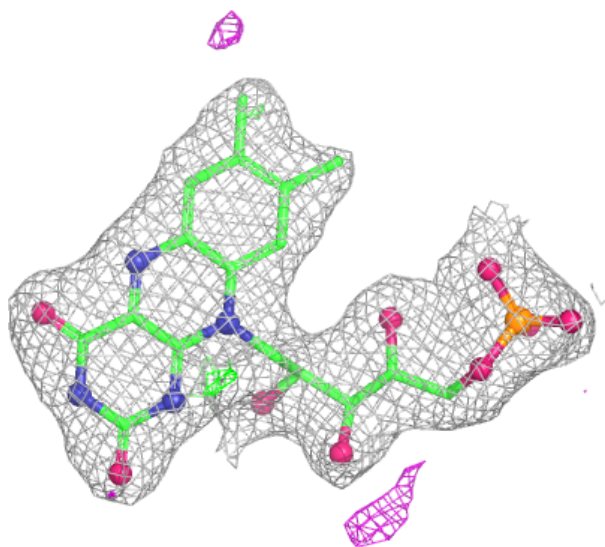
Electron density around FMN G 401:

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



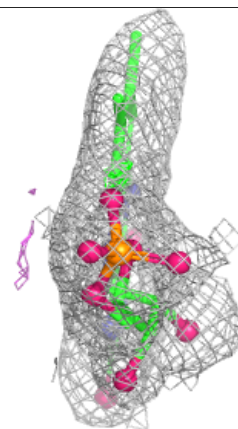
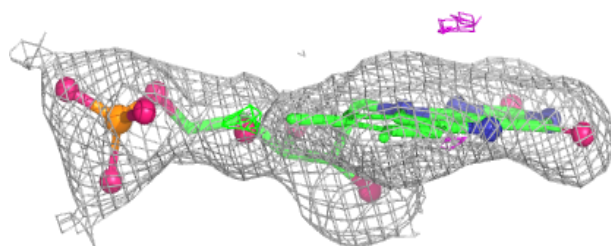
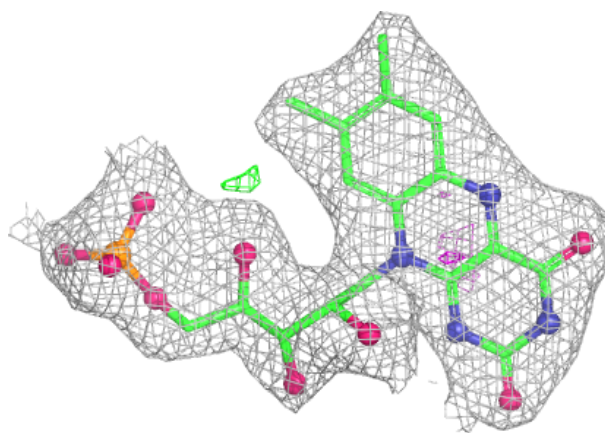
Electron density around FMN I 401:

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



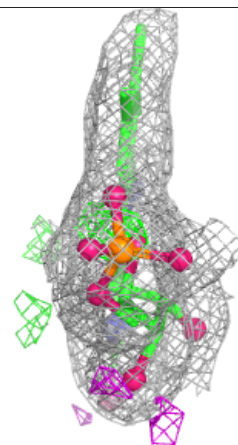
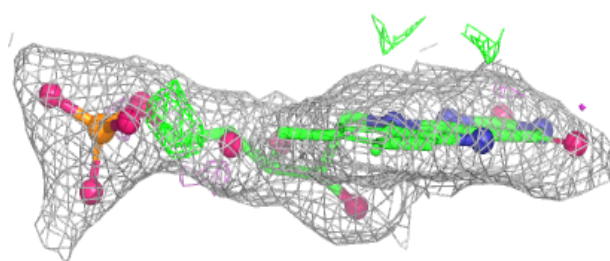
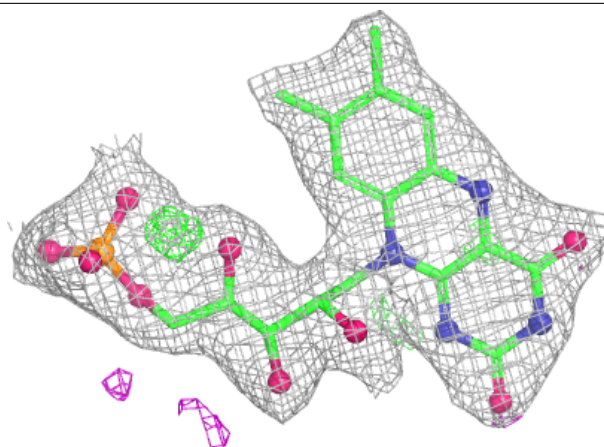
Electron density around FMN E 401:

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

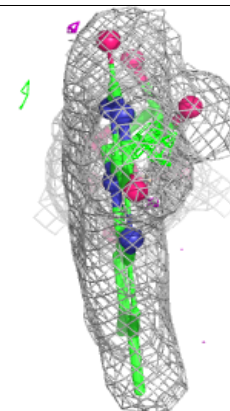
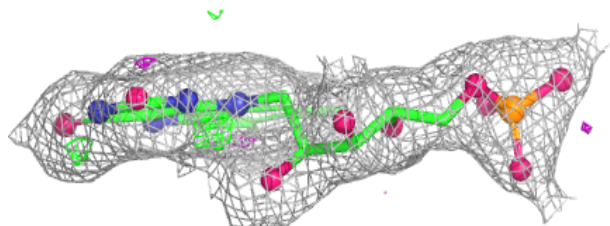
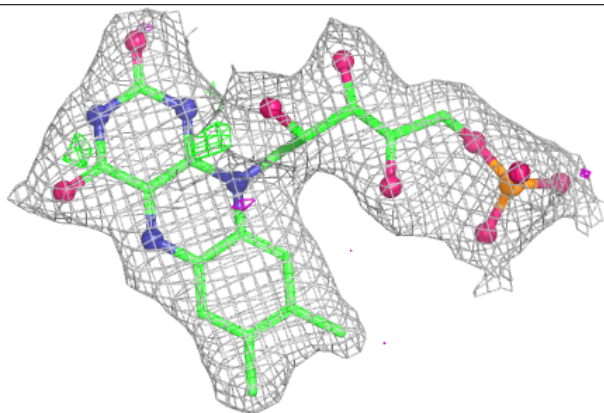


Electron density around FMN D 401:

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

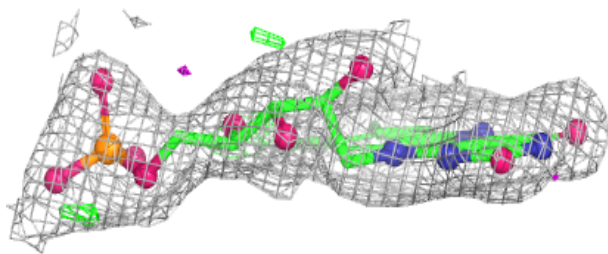
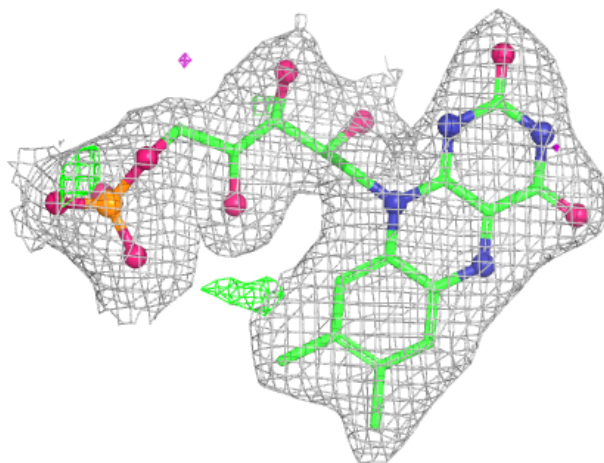
**Electron density around FMN B 401:**

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



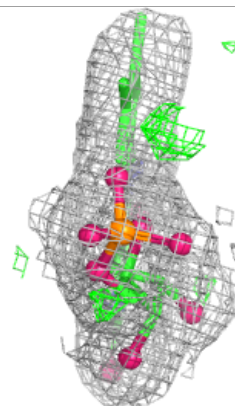
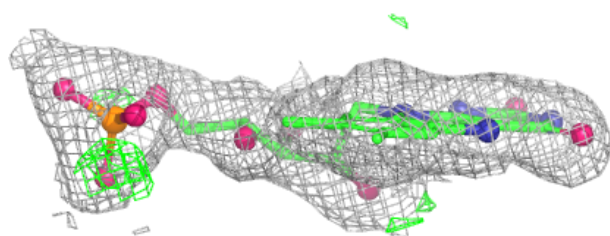
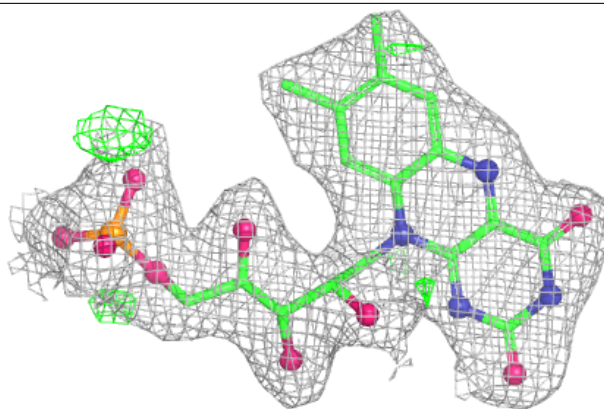
Electron density around FMN J 402:

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

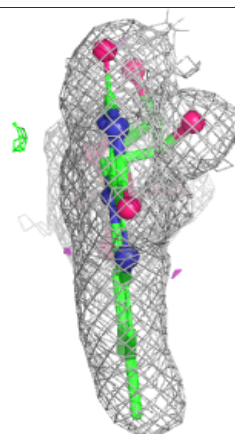
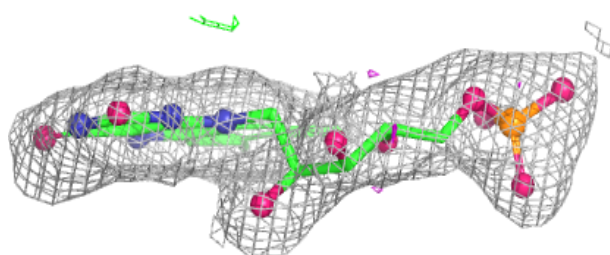
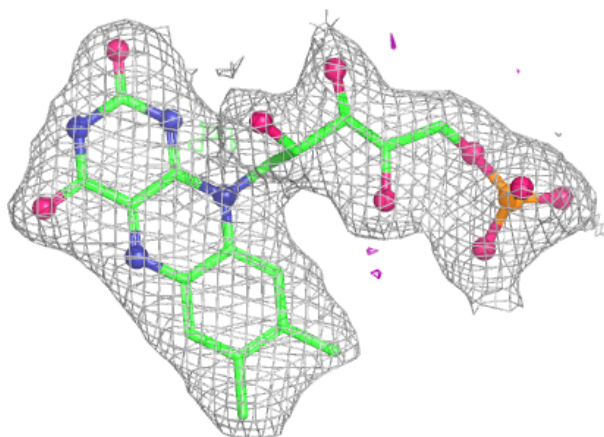


Electron density around FMN A 401:

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

**Electron density around FMN F 402:**

$2mF_o-DF_c$ (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.