WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 08:24 AM EDT

PDB ID	:	7K64
Title	:	Binary titrated soak structure of alkanesulfonate monooxygenase MsuD from Pseudomonas fluorescens with FMN
Authors	:	Liew, J.J.M.; Dowling, D.P.
Deposited on	:	2020-09-18
Resolution	:	2.80 Å(reported)

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

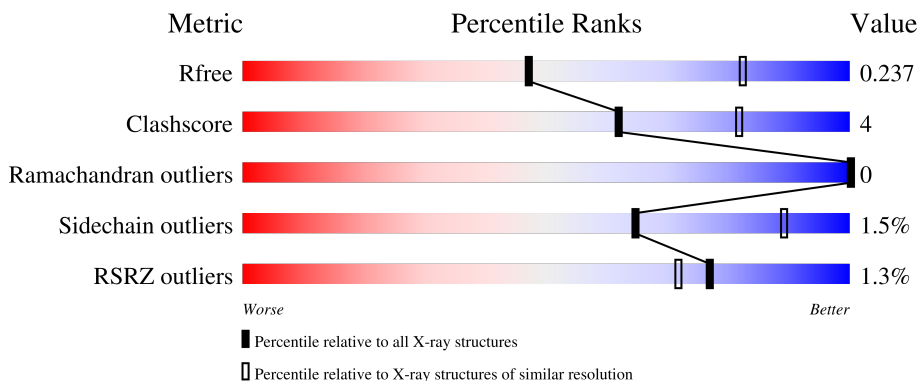|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.237
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.5%
RSRZ outliers		1.3%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	404	76% 12% 12%
1	B	404	2% 72% 12% 16%
1	C	404	78% 9% 12%
1	D	404	2% 73% 11% 15%
1	E	404	76% 11% 12%

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Mol	Chain	Length	Quality of chain
1	F	404	% 70% 10% 21%
1	G	404	% 70% 11% 19%
1	H	404	3% 75% 11% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	G	401	-	-	-	X
2	FMN	H	401	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 21571 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 Alkanesulfonate monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	2	0
			2792	1774	497	517	4			
1	B	338	Total	C	N	O	S	0	1	0
			2619	1677	455	483	4			
1	C	356	Total	C	N	O	S	0	0	0
			2764	1757	488	515	4			
1	D	342	Total	C	N	O	S	0	1	0
			2637	1687	459	487	4			
1	E	356	Total	C	N	O	S	0	1	0
			2779	1766	493	516	4			
1	F	321	Total	C	N	O	S	0	0	0
			2491	1597	432	459	3			
1	G	326	Total	C	N	O	S	0	0	0
			2522	1614	438	467	3			
1	H	348	Total	C	N	O	S	0	1	0
			2692	1720	470	498	4			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q3K9A1
A	-21	GLY	-	expression tag	UNP Q3K9A1
A	-20	SER	-	expression tag	UNP Q3K9A1
A	-19	SER	-	expression tag	UNP Q3K9A1
A	-18	HIS	-	expression tag	UNP Q3K9A1
A	-17	HIS	-	expression tag	UNP Q3K9A1
A	-16	HIS	-	expression tag	UNP Q3K9A1
A	-15	HIS	-	expression tag	UNP Q3K9A1
A	-14	HIS	-	expression tag	UNP Q3K9A1
A	-13	HIS	-	expression tag	UNP Q3K9A1
A	-12	SER	-	expression tag	UNP Q3K9A1
A	-11	SER	-	expression tag	UNP Q3K9A1
A	-10	GLY	-	expression tag	UNP Q3K9A1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	LEU	-	expression tag	UNP Q3K9A1
A	-8	VAL	-	expression tag	UNP Q3K9A1
A	-7	PRO	-	expression tag	UNP Q3K9A1
A	-6	ARG	-	expression tag	UNP Q3K9A1
A	-5	GLY	-	expression tag	UNP Q3K9A1
A	-4	SER	-	expression tag	UNP Q3K9A1
A	-3	HIS	-	expression tag	UNP Q3K9A1
A	-2	MET	-	expression tag	UNP Q3K9A1
A	-1	ALA	-	expression tag	UNP Q3K9A1
A	0	SER	-	expression tag	UNP Q3K9A1
B	-22	MET	-	initiating methionine	UNP Q3K9A1
B	-21	GLY	-	expression tag	UNP Q3K9A1
B	-20	SER	-	expression tag	UNP Q3K9A1
B	-19	SER	-	expression tag	UNP Q3K9A1
B	-18	HIS	-	expression tag	UNP Q3K9A1
B	-17	HIS	-	expression tag	UNP Q3K9A1
B	-16	HIS	-	expression tag	UNP Q3K9A1
B	-15	HIS	-	expression tag	UNP Q3K9A1
B	-14	HIS	-	expression tag	UNP Q3K9A1
B	-13	HIS	-	expression tag	UNP Q3K9A1
B	-12	SER	-	expression tag	UNP Q3K9A1
B	-11	SER	-	expression tag	UNP Q3K9A1
B	-10	GLY	-	expression tag	UNP Q3K9A1
B	-9	LEU	-	expression tag	UNP Q3K9A1
B	-8	VAL	-	expression tag	UNP Q3K9A1
B	-7	PRO	-	expression tag	UNP Q3K9A1
B	-6	ARG	-	expression tag	UNP Q3K9A1
B	-5	GLY	-	expression tag	UNP Q3K9A1
B	-4	SER	-	expression tag	UNP Q3K9A1
B	-3	HIS	-	expression tag	UNP Q3K9A1
B	-2	MET	-	expression tag	UNP Q3K9A1
B	-1	ALA	-	expression tag	UNP Q3K9A1
B	0	SER	-	expression tag	UNP Q3K9A1
C	-22	MET	-	initiating methionine	UNP Q3K9A1
C	-21	GLY	-	expression tag	UNP Q3K9A1
C	-20	SER	-	expression tag	UNP Q3K9A1
C	-19	SER	-	expression tag	UNP Q3K9A1
C	-18	HIS	-	expression tag	UNP Q3K9A1
C	-17	HIS	-	expression tag	UNP Q3K9A1
C	-16	HIS	-	expression tag	UNP Q3K9A1
C	-15	HIS	-	expression tag	UNP Q3K9A1
C	-14	HIS	-	expression tag	UNP Q3K9A1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP Q3K9A1
C	-12	SER	-	expression tag	UNP Q3K9A1
C	-11	SER	-	expression tag	UNP Q3K9A1
C	-10	GLY	-	expression tag	UNP Q3K9A1
C	-9	LEU	-	expression tag	UNP Q3K9A1
C	-8	VAL	-	expression tag	UNP Q3K9A1
C	-7	PRO	-	expression tag	UNP Q3K9A1
C	-6	ARG	-	expression tag	UNP Q3K9A1
C	-5	GLY	-	expression tag	UNP Q3K9A1
C	-4	SER	-	expression tag	UNP Q3K9A1
C	-3	HIS	-	expression tag	UNP Q3K9A1
C	-2	MET	-	expression tag	UNP Q3K9A1
C	-1	ALA	-	expression tag	UNP Q3K9A1
C	0	SER	-	expression tag	UNP Q3K9A1
D	-22	MET	-	initiating methionine	UNP Q3K9A1
D	-21	GLY	-	expression tag	UNP Q3K9A1
D	-20	SER	-	expression tag	UNP Q3K9A1
D	-19	SER	-	expression tag	UNP Q3K9A1
D	-18	HIS	-	expression tag	UNP Q3K9A1
D	-17	HIS	-	expression tag	UNP Q3K9A1
D	-16	HIS	-	expression tag	UNP Q3K9A1
D	-15	HIS	-	expression tag	UNP Q3K9A1
D	-14	HIS	-	expression tag	UNP Q3K9A1
D	-13	HIS	-	expression tag	UNP Q3K9A1
D	-12	SER	-	expression tag	UNP Q3K9A1
D	-11	SER	-	expression tag	UNP Q3K9A1
D	-10	GLY	-	expression tag	UNP Q3K9A1
D	-9	LEU	-	expression tag	UNP Q3K9A1
D	-8	VAL	-	expression tag	UNP Q3K9A1
D	-7	PRO	-	expression tag	UNP Q3K9A1
D	-6	ARG	-	expression tag	UNP Q3K9A1
D	-5	GLY	-	expression tag	UNP Q3K9A1
D	-4	SER	-	expression tag	UNP Q3K9A1
D	-3	HIS	-	expression tag	UNP Q3K9A1
D	-2	MET	-	expression tag	UNP Q3K9A1
D	-1	ALA	-	expression tag	UNP Q3K9A1
D	0	SER	-	expression tag	UNP Q3K9A1
E	-22	MET	-	initiating methionine	UNP Q3K9A1
E	-21	GLY	-	expression tag	UNP Q3K9A1
E	-20	SER	-	expression tag	UNP Q3K9A1
E	-19	SER	-	expression tag	UNP Q3K9A1
E	-18	HIS	-	expression tag	UNP Q3K9A1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	expression tag	UNP Q3K9A1
E	-16	HIS	-	expression tag	UNP Q3K9A1
E	-15	HIS	-	expression tag	UNP Q3K9A1
E	-14	HIS	-	expression tag	UNP Q3K9A1
E	-13	HIS	-	expression tag	UNP Q3K9A1
E	-12	SER	-	expression tag	UNP Q3K9A1
E	-11	SER	-	expression tag	UNP Q3K9A1
E	-10	GLY	-	expression tag	UNP Q3K9A1
E	-9	LEU	-	expression tag	UNP Q3K9A1
E	-8	VAL	-	expression tag	UNP Q3K9A1
E	-7	PRO	-	expression tag	UNP Q3K9A1
E	-6	ARG	-	expression tag	UNP Q3K9A1
E	-5	GLY	-	expression tag	UNP Q3K9A1
E	-4	SER	-	expression tag	UNP Q3K9A1
E	-3	HIS	-	expression tag	UNP Q3K9A1
E	-2	MET	-	expression tag	UNP Q3K9A1
E	-1	ALA	-	expression tag	UNP Q3K9A1
E	0	SER	-	expression tag	UNP Q3K9A1
F	-22	MET	-	initiating methionine	UNP Q3K9A1
F	-21	GLY	-	expression tag	UNP Q3K9A1
F	-20	SER	-	expression tag	UNP Q3K9A1
F	-19	SER	-	expression tag	UNP Q3K9A1
F	-18	HIS	-	expression tag	UNP Q3K9A1
F	-17	HIS	-	expression tag	UNP Q3K9A1
F	-16	HIS	-	expression tag	UNP Q3K9A1
F	-15	HIS	-	expression tag	UNP Q3K9A1
F	-14	HIS	-	expression tag	UNP Q3K9A1
F	-13	HIS	-	expression tag	UNP Q3K9A1
F	-12	SER	-	expression tag	UNP Q3K9A1
F	-11	SER	-	expression tag	UNP Q3K9A1
F	-10	GLY	-	expression tag	UNP Q3K9A1
F	-9	LEU	-	expression tag	UNP Q3K9A1
F	-8	VAL	-	expression tag	UNP Q3K9A1
F	-7	PRO	-	expression tag	UNP Q3K9A1
F	-6	ARG	-	expression tag	UNP Q3K9A1
F	-5	GLY	-	expression tag	UNP Q3K9A1
F	-4	SER	-	expression tag	UNP Q3K9A1
F	-3	HIS	-	expression tag	UNP Q3K9A1
F	-2	MET	-	expression tag	UNP Q3K9A1
F	-1	ALA	-	expression tag	UNP Q3K9A1
F	0	SER	-	expression tag	UNP Q3K9A1
G	-22	MET	-	initiating methionine	UNP Q3K9A1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	GLY	-	expression tag	UNP Q3K9A1
G	-20	SER	-	expression tag	UNP Q3K9A1
G	-19	SER	-	expression tag	UNP Q3K9A1
G	-18	HIS	-	expression tag	UNP Q3K9A1
G	-17	HIS	-	expression tag	UNP Q3K9A1
G	-16	HIS	-	expression tag	UNP Q3K9A1
G	-15	HIS	-	expression tag	UNP Q3K9A1
G	-14	HIS	-	expression tag	UNP Q3K9A1
G	-13	HIS	-	expression tag	UNP Q3K9A1
G	-12	SER	-	expression tag	UNP Q3K9A1
G	-11	SER	-	expression tag	UNP Q3K9A1
G	-10	GLY	-	expression tag	UNP Q3K9A1
G	-9	LEU	-	expression tag	UNP Q3K9A1
G	-8	VAL	-	expression tag	UNP Q3K9A1
G	-7	PRO	-	expression tag	UNP Q3K9A1
G	-6	ARG	-	expression tag	UNP Q3K9A1
G	-5	GLY	-	expression tag	UNP Q3K9A1
G	-4	SER	-	expression tag	UNP Q3K9A1
G	-3	HIS	-	expression tag	UNP Q3K9A1
G	-2	MET	-	expression tag	UNP Q3K9A1
G	-1	ALA	-	expression tag	UNP Q3K9A1
G	0	SER	-	expression tag	UNP Q3K9A1
H	-22	MET	-	initiating methionine	UNP Q3K9A1
H	-21	GLY	-	expression tag	UNP Q3K9A1
H	-20	SER	-	expression tag	UNP Q3K9A1
H	-19	SER	-	expression tag	UNP Q3K9A1
H	-18	HIS	-	expression tag	UNP Q3K9A1
H	-17	HIS	-	expression tag	UNP Q3K9A1
H	-16	HIS	-	expression tag	UNP Q3K9A1
H	-15	HIS	-	expression tag	UNP Q3K9A1
H	-14	HIS	-	expression tag	UNP Q3K9A1
H	-13	HIS	-	expression tag	UNP Q3K9A1
H	-12	SER	-	expression tag	UNP Q3K9A1
H	-11	SER	-	expression tag	UNP Q3K9A1
H	-10	GLY	-	expression tag	UNP Q3K9A1
H	-9	LEU	-	expression tag	UNP Q3K9A1
H	-8	VAL	-	expression tag	UNP Q3K9A1
H	-7	PRO	-	expression tag	UNP Q3K9A1
H	-6	ARG	-	expression tag	UNP Q3K9A1
H	-5	GLY	-	expression tag	UNP Q3K9A1
H	-4	SER	-	expression tag	UNP Q3K9A1
H	-3	HIS	-	expression tag	UNP Q3K9A1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	MET	-	expression tag	UNP Q3K9A1
H	-1	ALA	-	expression tag	UNP Q3K9A1
H	0	SER	-	expression tag	UNP Q3K9A1

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).


FMN
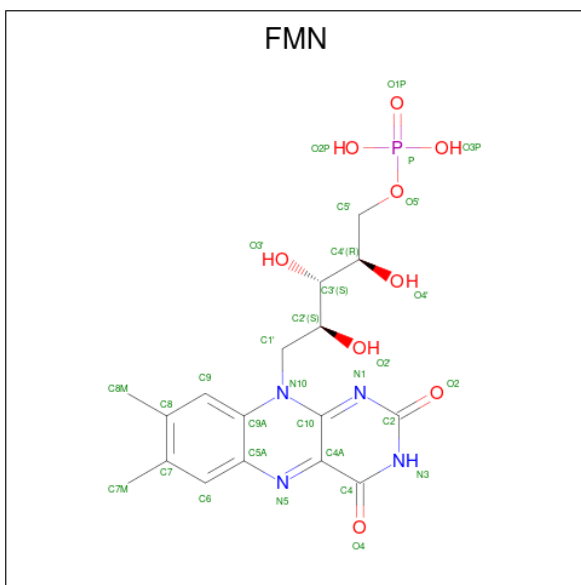
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: $C_4H_6O_4$).

SIN
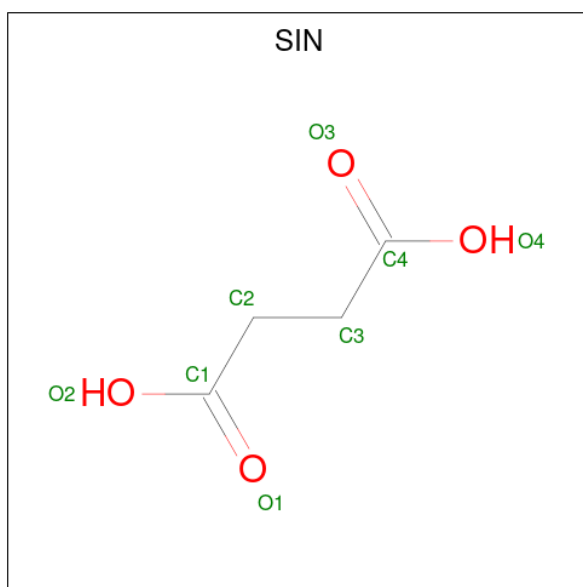
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	C 4	O 4	0	0
3	C	1	Total 8	C 4	O 4	0	0
3	E	1	Total 8	C 4	O 4	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4
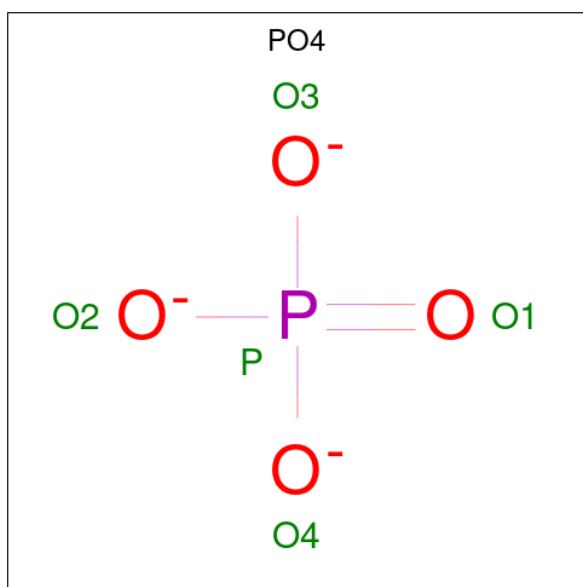
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total 5	O 4	P 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total 1	Na 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
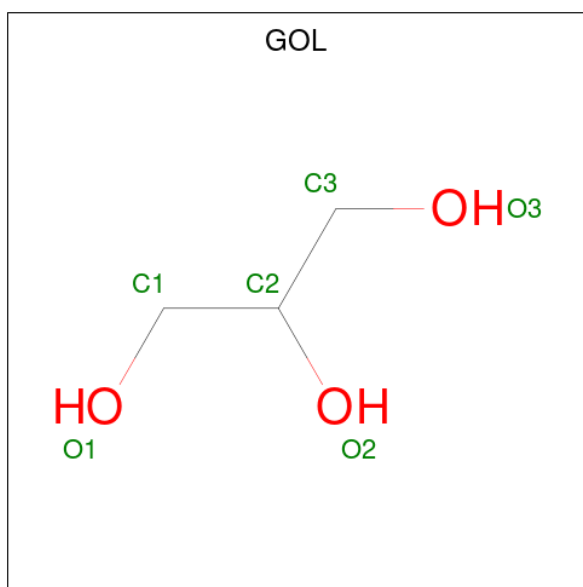
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 6	C 3	O 3	0	0
6	F	1	Total 6	C 3	O 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

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

3 Residue-property plots ⓘ

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.
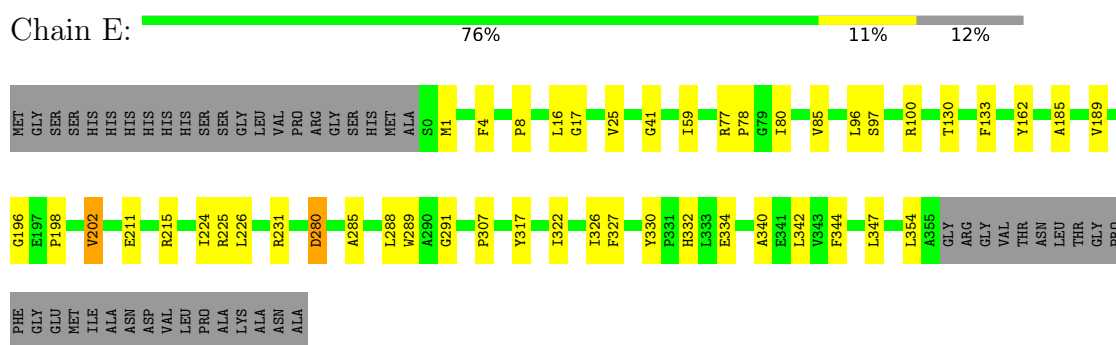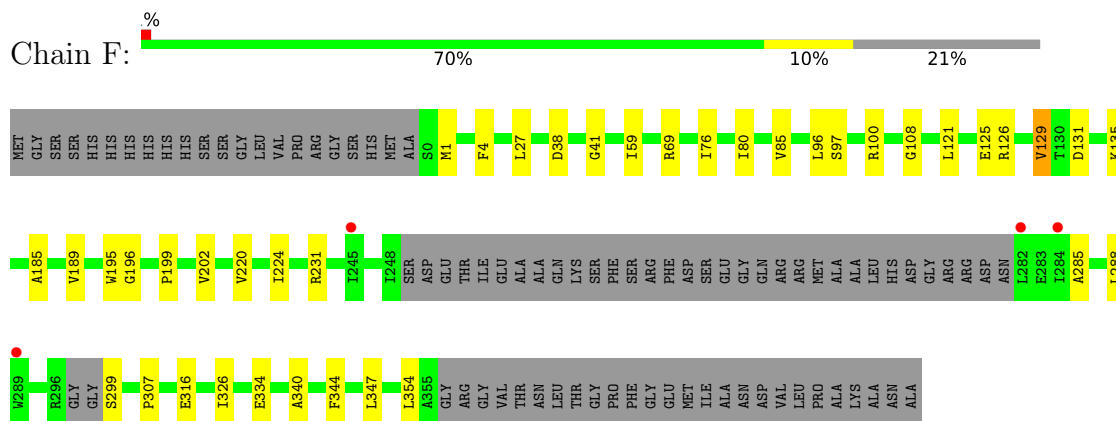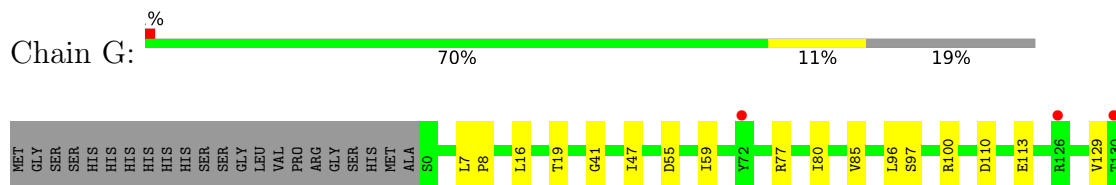
- Molecule 1: Alkanesulfonate monooxygenase

Chain A:
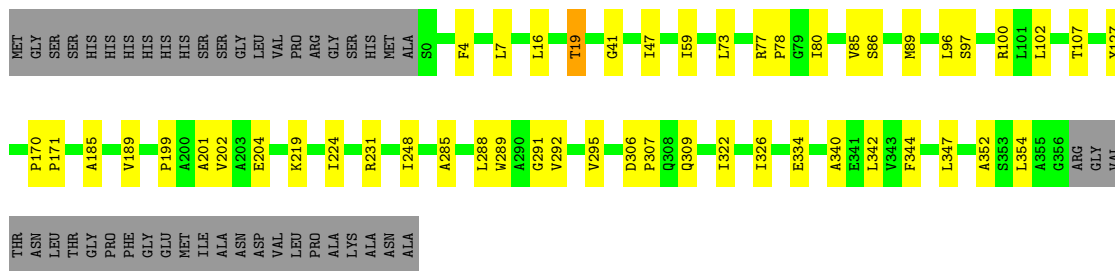
- Molecule 1: Alkanesulfonate monooxygenase

Chain B:
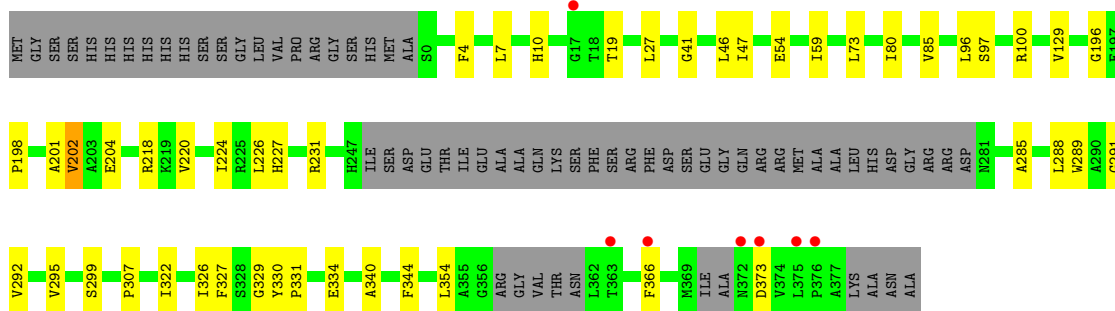
- Molecule 1: Alkanesulfonate monooxygenase

Chain C:

ALA

• Molecule 1: Alkanesulfonate monooxygenase

Chain D:

• Molecule 1: Alkanesulfonate monooxygenase

Chain E:

• Molecule 1: Alkanesulfonate monooxygenase

Chain F:

• Molecule 1: Alkanesulfonate monooxygenase

Chain G:

W137 H152 A185 V189 G196 E197 P198 V202 L206 V220 I224 R225 L226 R231 I248 S249 D250 GLU THR ILE GLU ALA ALA GLN LYS SER PHE SER ARG PHE ASP SER GLU GLY GLN ARG ARG MET ALA ALA LEU HIS ASP GLY ARG ARG ASP N281

I284 A285 L288 W289 A290 G291 V292 P307 I322 F327 Y330 P331 H332 L333 E334 A340 F344 L354 A355 GLY ARG GLY VAL THR ASN LEU THR GLY PRO PHE GLY GLU MET ILE ALA ASN ASP VAL LEU PRO ALA LYS ALA ASN ALA

• Molecule 1: Alkanesulfonate monooxygenase

Chain H:

3%

75%   11%   14%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA S0 M1 F4 L7 Y15 L16 G17 L27 K31 Q35 I47 I59 L66 I80 V85 S86 M89 L96 S97 R100 G109 V129

P170 P171 A185 V189 G196 R210 V220 I224 R225 L226 R231 K243 L244 I245 E246 H247 I248 S249 D250 GLU THR ILE GLU ALA ALA GLN LYS SER PHE SER ARG PHE ASP SER GLU GLY GLN ARG ARG MET ALA ALA LEU HIS ASP GLY ARG ARG ASP N281

A285 L288 W289 A290 G291 V292 G293 L294 V295 R296 G297 G298 T301 P307 Y317 I322 I326 F327 E334 L347 L354 G358 V359 I370 A377 LYS ALA ASN ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.01Å 212.01Å 94.46Å 90.00° 118.85° 90.00°	Depositor
Resolution (Å)	65.03 – 2.80 82.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (65.03-2.80) 91.4 (82.74-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.199 , 0.238 0.199 , 0.237	Depositor DCC
R_{free} test set	3902 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.023 for h,-k,-h-l 0.024 for -h-l,-k,l 0.020 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21571	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, FMN, NA, GOL, CL, SIN

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	0.24	0/2866	0.42	0/3894
1	B	0.24	0/2688	0.42	0/3658
1	C	0.24	0/2832	0.42	0/3851
1	D	0.24	0/2706	0.43	0/3688
1	E	0.25	0/2850	0.43	0/3874
1	F	0.24	0/2554	0.42	0/3480
1	G	0.24	0/2586	0.43	0/3523
1	H	0.24	0/2762	0.42	0/3761
All	All	0.24	0/21844	0.42	0/29729

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2792	0	2755	31	0
1	B	2619	0	2580	23	0
1	C	2764	0	2709	22	0
1	D	2637	0	2592	27	0
1	E	2779	0	2737	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2491	0	2451	25	0
1	G	2522	0	2480	27	0
1	H	2692	0	2662	28	0
2	A	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
3	A	8	0	4	0	0
3	C	8	0	4	1	0
3	E	8	0	4	1	0
4	B	5	0	0	0	0
4	F	5	0	0	0	0
5	E	1	0	0	0	0
6	E	6	0	8	0	0
6	F	6	0	8	1	0
7	G	1	0	0	0	0
8	A	6	0	0	0	0
8	B	8	0	0	0	0
8	C	6	0	0	0	0
8	D	6	0	0	0	0
8	E	8	0	0	0	0
8	F	3	0	0	0	0
8	G	1	0	0	0	0
8	H	3	0	0	0	0
All	All	21571	0	21108	189	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 4.

The worst 5 of 189 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HD12	1:B:85:VAL:HG21	1.52	0.91
1:E:80:ILE:HD12	1:F:85:VAL:HG21	1.53	0.89
1:C:85:VAL:HG21	1:D:80:ILE:HD12	1.64	0.80
1:G:80:ILE:HD12	1:H:85:VAL:HG21	1.65	0.79
1:A:85:VAL:HG21	1:B:80:ILE:HD12	1.68	0.76

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/404 (88%)	345 (97%)	12 (3%)	0	100	100
1	B	331/404 (82%)	322 (97%)	9 (3%)	0	100	100
1	C	354/404 (88%)	344 (97%)	10 (3%)	0	100	100
1	D	337/404 (83%)	327 (97%)	10 (3%)	0	100	100
1	E	355/404 (88%)	347 (98%)	8 (2%)	0	100	100
1	F	315/404 (78%)	308 (98%)	7 (2%)	0	100	100
1	G	322/404 (80%)	314 (98%)	8 (2%)	0	100	100
1	H	345/404 (85%)	332 (96%)	13 (4%)	0	100	100
All	All	2716/3232 (84%)	2639 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	286/321 (89%)	285 (100%)	1 (0%)	92	98
1	B	269/321 (84%)	259 (96%)	10 (4%)	34	68
1	C	282/321 (88%)	278 (99%)	4 (1%)	67	90
1	D	269/321 (84%)	264 (98%)	5 (2%)	57	85
1	E	285/321 (89%)	282 (99%)	3 (1%)	73	92
1	F	255/321 (79%)	252 (99%)	3 (1%)	71	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	258/321 (80%)	253 (98%)	5 (2%)	57	85
1	H	277/321 (86%)	275 (99%)	2 (1%)	84	95
All	All	2181/2568 (85%)	2148 (98%)	33 (2%)	65	89

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	220	VAL
1	G	248	ILE
1	H	220	VAL
1	C	129	VAL
1	C	19	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	10	HIS
1	H	35	GLN
1	E	35	GLN
1	H	361	ASN
1	G	10	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	#$|Z| > 2$
2	FMN	H	401	-	33,33,33	1.05	1 (3%)	48,50,50	1.28	8 (16%)
3	SIN	E	402	-	7,7,7	1.02	0	8,8,8	1.70	2 (25%)
6	GOL	E	404	-	5,5,5	0.92	0	5,5,5	0.96	0
4	PO4	F	501	-	4,4,4	0.89	0	6,6,6	0.44	0
2	FMN	A	401	-	33,33,33	1.05	2 (6%)	48,50,50	1.27	8 (16%)
2	FMN	G	401	-	33,33,33	1.06	2 (6%)	48,50,50	1.30	8 (16%)
2	FMN	D	401	-	33,33,33	1.06	2 (6%)	48,50,50	1.28	8 (16%)
2	FMN	E	401	-	33,33,33	1.07	2 (6%)	48,50,50	1.29	8 (16%)
3	SIN	C	402	-	7,7,7	1.01	0	8,8,8	1.71	2 (25%)
6	GOL	F	502	-	5,5,5	0.93	0	5,5,5	0.91	0
3	SIN	A	402	-	7,7,7	1.03	0	8,8,8	1.58	0
4	PO4	B	501	-	4,4,4	0.92	0	6,6,6	0.44	0
2	FMN	C	401	-	33,33,33	1.10	2 (6%)	48,50,50	1.38	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	H	401	-	-	1/18/18/18	0/3/3/3
3	SIN	E	402	-	-	4/5/5/5	-
6	GOL	E	404	-	-	2/4/4/4	-
2	FMN	A	401	-	-	10/18/18/18	0/3/3/3
2	FMN	G	401	-	-	7/18/18/18	0/3/3/3
2	FMN	D	401	-	-	3/18/18/18	0/3/3/3
2	FMN	E	401	-	-	9/18/18/18	0/3/3/3
3	SIN	C	402	-	-	4/5/5/5	-
6	GOL	F	502	-	-	4/4/4/4	-
3	SIN	A	402	-	-	5/5/5/5	-
2	FMN	C	401	-	-	9/18/18/18	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FMN	C5A-N5	-2.71	1.34	1.39
2	E	401	FMN	C5A-N5	-2.68	1.34	1.39
2	D	401	FMN	C5A-N5	-2.63	1.34	1.39
2	A	401	FMN	C5A-N5	-2.63	1.34	1.39
2	G	401	FMN	C5A-N5	-2.61	1.34	1.39

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	FMN	C4-C4A-N5	2.86	122.30	118.23
2	E	401	FMN	C4-C4A-N5	2.78	122.18	118.23
2	D	401	FMN	C4-C4A-N5	2.77	122.18	118.23
2	G	401	FMN	C4-C4A-N5	2.71	122.09	118.23
2	G	401	FMN	C4A-C10-N1	-2.70	118.46	124.73

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FMN	N10-C1'-C2'-O2'
2	A	401	FMN	N10-C1'-C2'-C3'
2	A	401	FMN	C3'-C4'-C5'-O5'
2	A	401	FMN	O4'-C4'-C5'-O5'
2	C	401	FMN	N10-C1'-C2'-O2'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

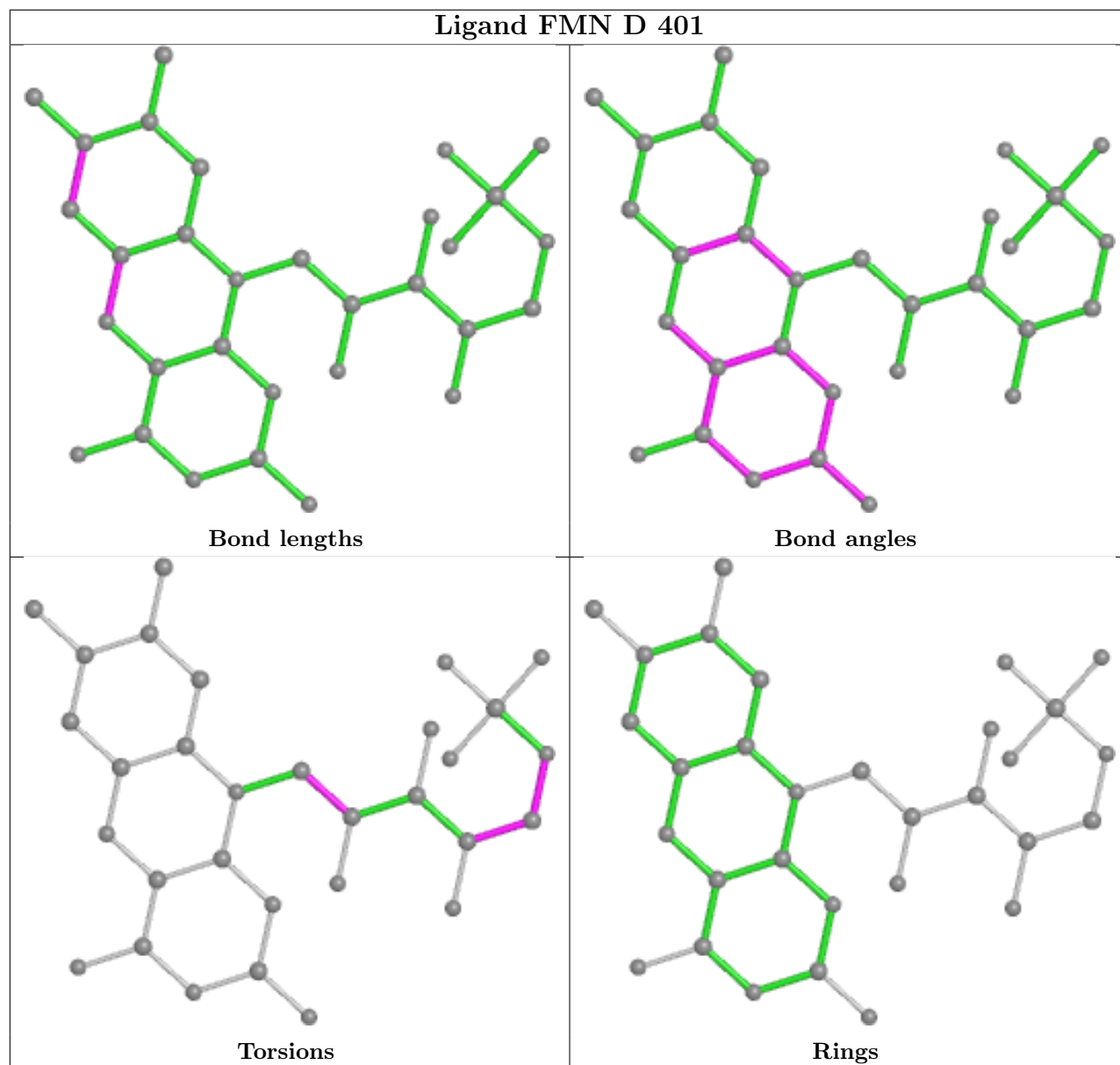| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	SIN	1	0
3	C	402	SIN	1	0
6	F	502	GOL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the
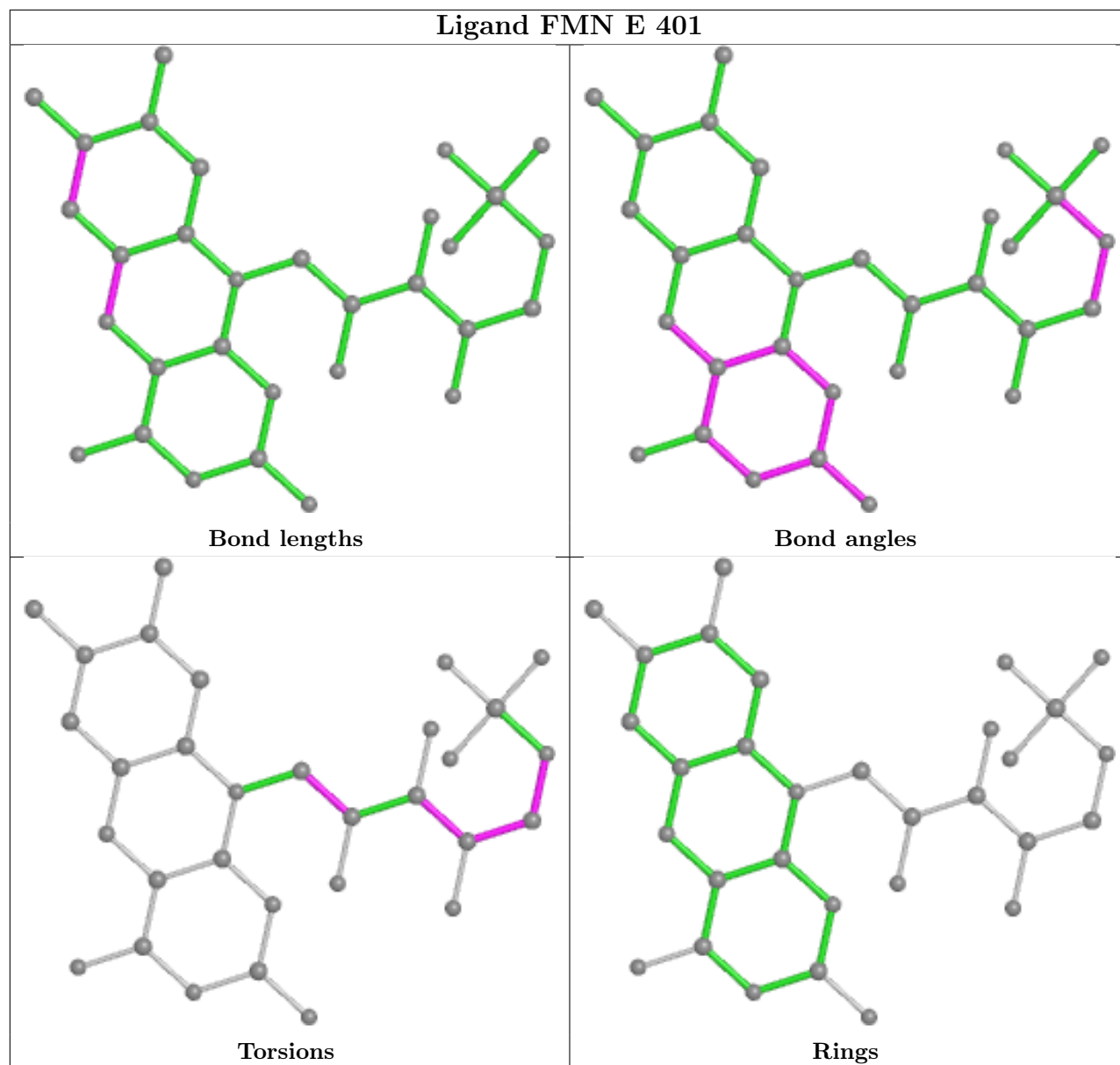
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
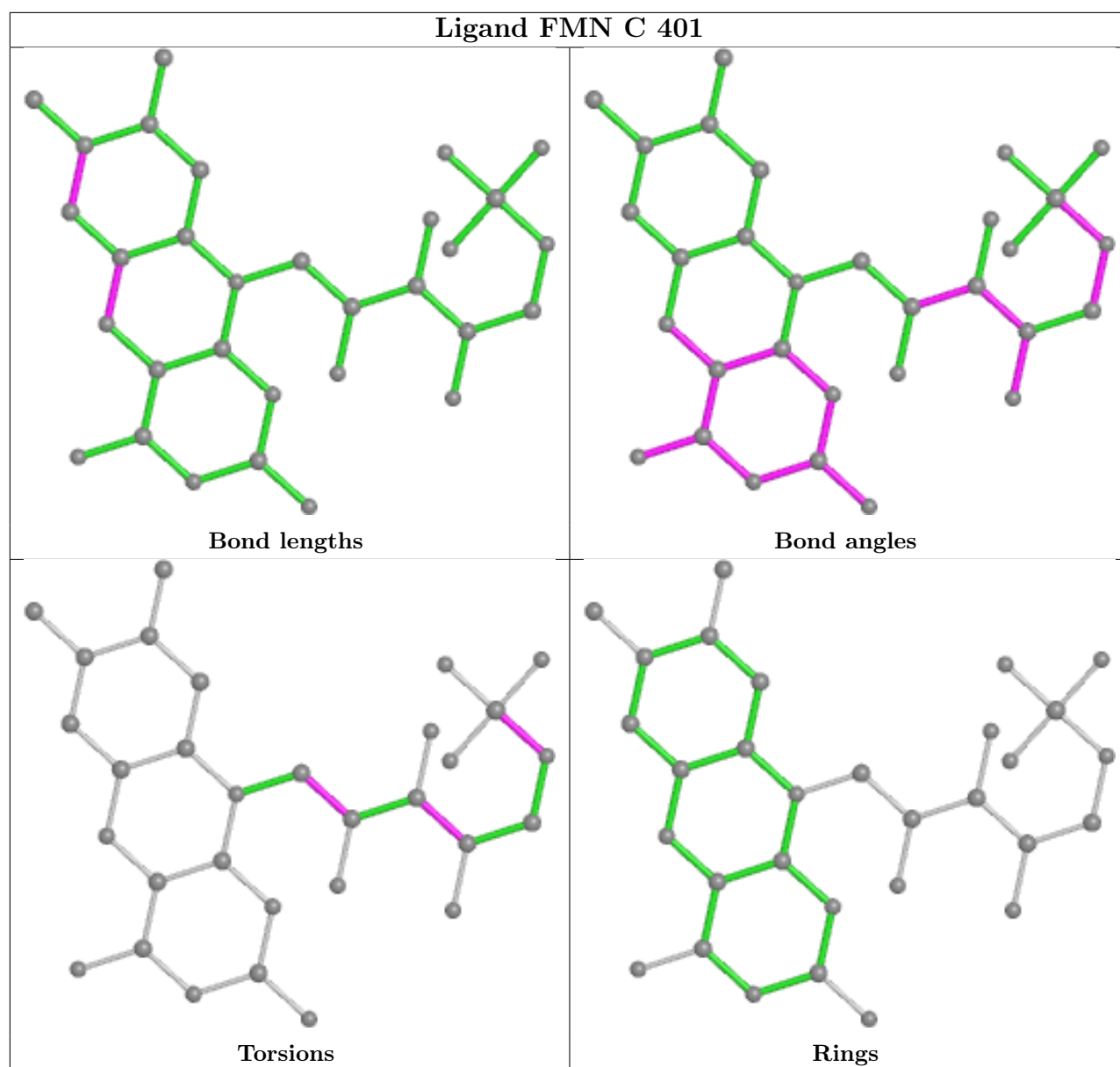
Ligand FMN H 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN G 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN C 401

Bond lengths

Bond angles

Torsions

Rings
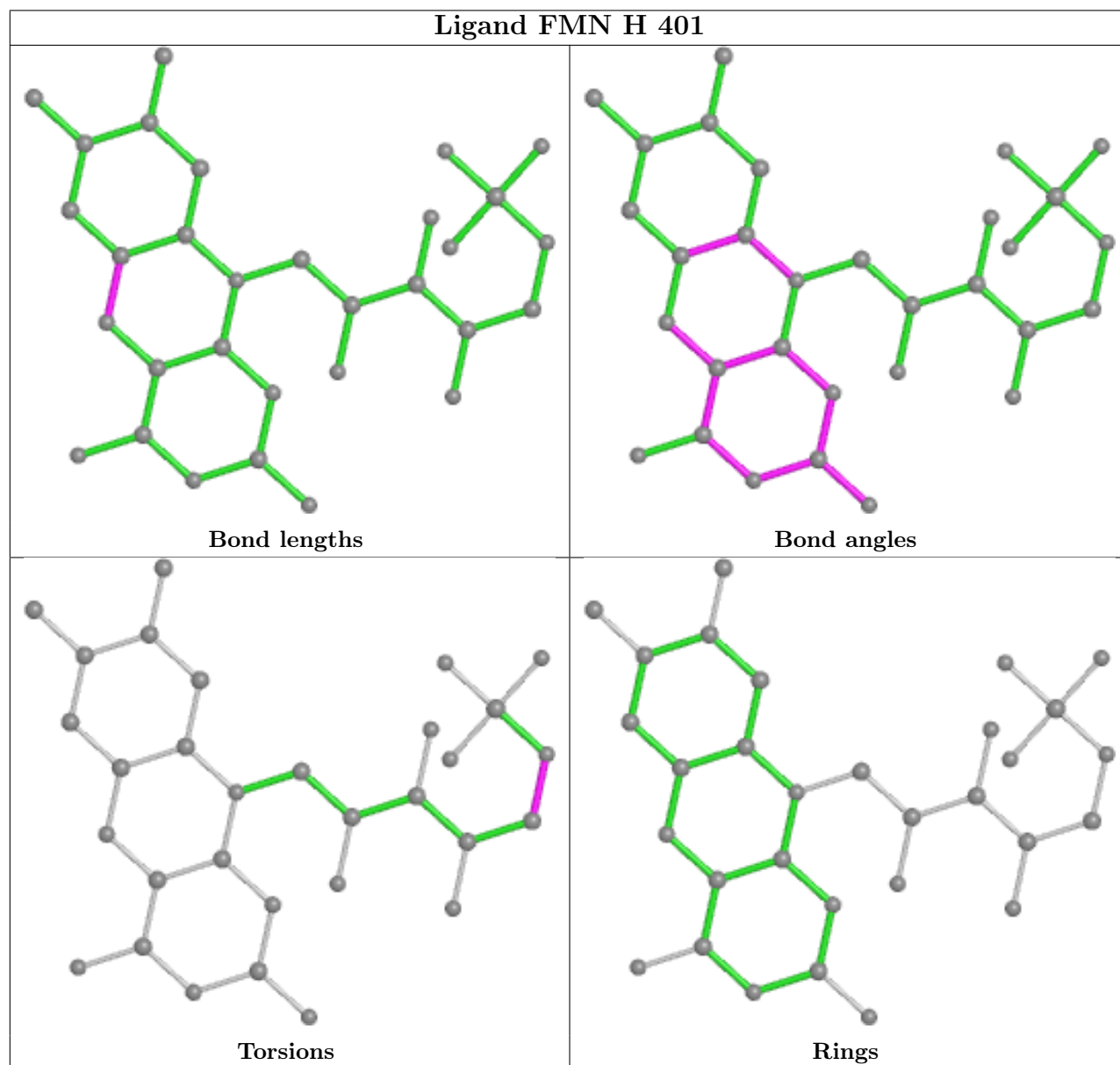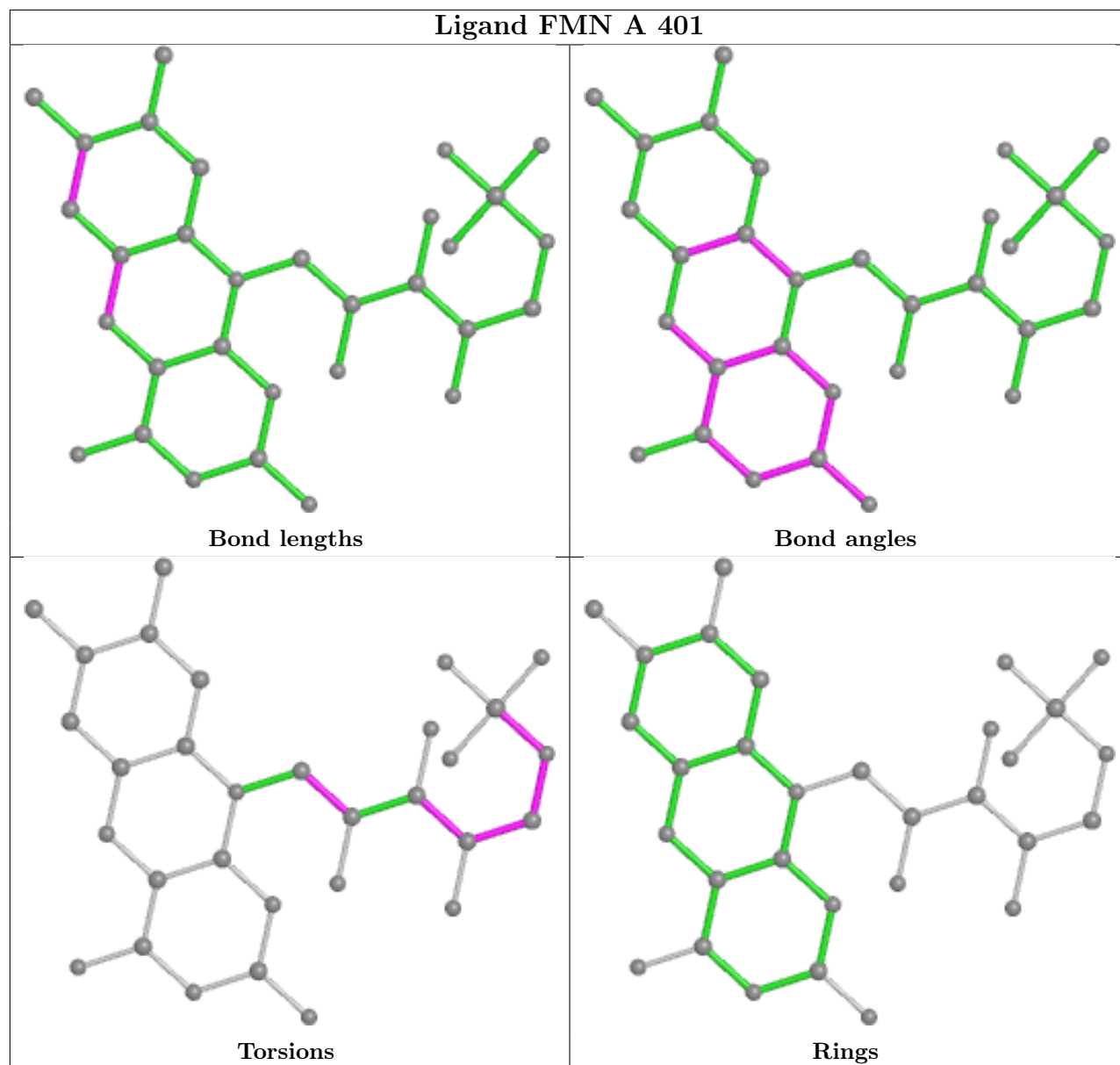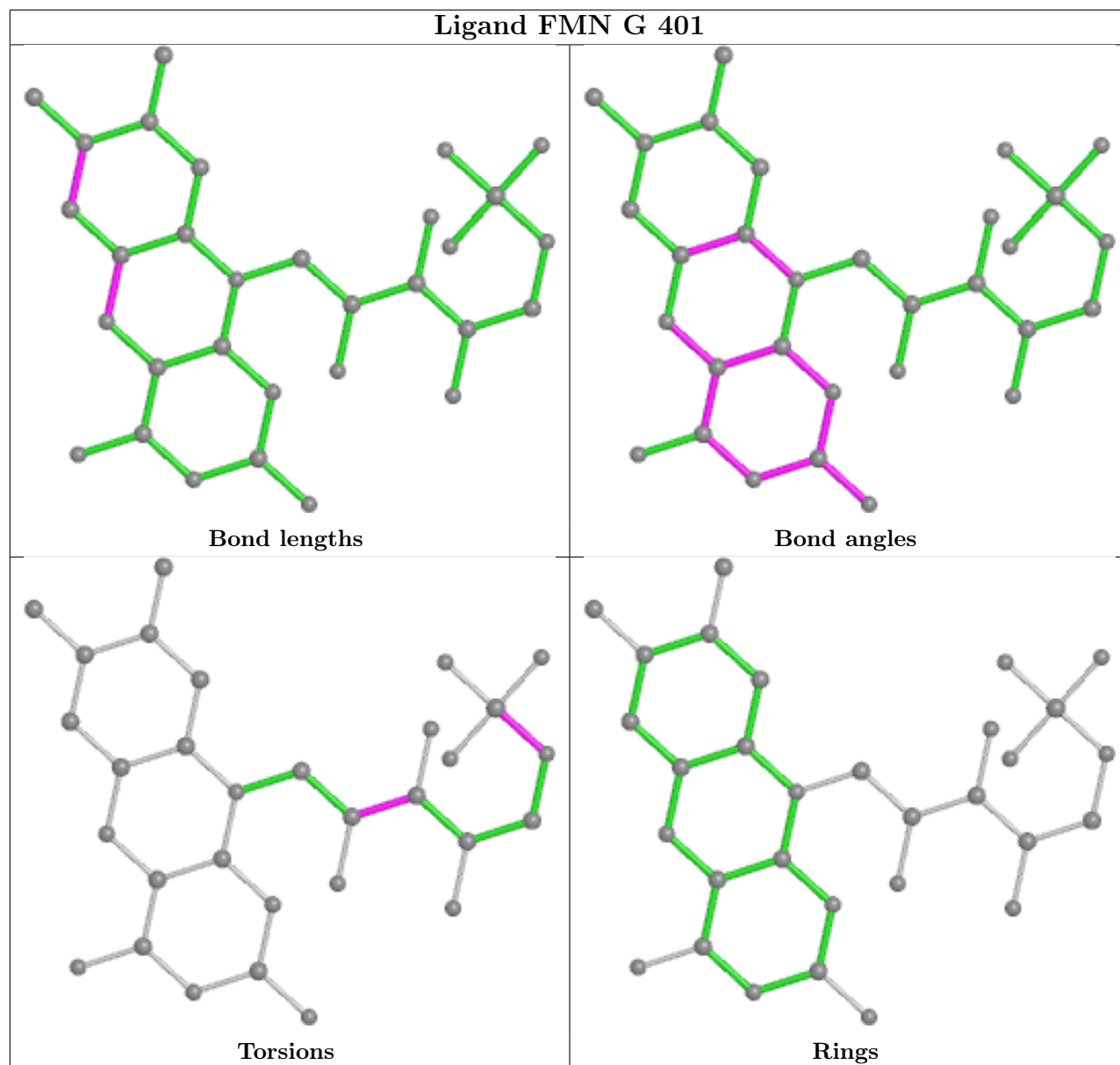
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	357/404 (88%)	-0.26	0	100	100	43, 70, 119, 171	0
1	B	338/404 (83%)	-0.11	7 (2%)	63	54	44, 69, 115, 154	0
1	C	356/404 (88%)	-0.17	1 (0%)	94	93	44, 69, 117, 171	0
1	D	342/404 (84%)	-0.06	7 (2%)	65	56	46, 76, 120, 145	0
1	E	356/404 (88%)	-0.26	0	100	100	40, 56, 89, 132	0
1	F	321/404 (79%)	-0.12	4 (1%)	79	73	43, 67, 105, 130	0
1	G	326/404 (80%)	0.05	5 (1%)	73	68	52, 89, 120, 142	0
1	H	348/404 (86%)	-0.08	12 (3%)	45	35	50, 75, 111, 161	0
All	All	2744/3232 (84%)	-0.13	36 (1%)	77	72	40, 70, 116, 171	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	GLY	6.1
1	H	295	VAL	4.7
1	F	284	ILE	4.2
1	B	375	LEU	3.9
1	B	376	PRO	3.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	FMN	H	401	31/31	0.74	0.47	83,96,104,106	31
3	SIN	C	402	8/8	0.79	0.31	91,100,111,114	0
2	FMN	G	401	31/31	0.80	0.46	77,88,104,111	31
2	FMN	D	401	31/31	0.81	0.29	68,87,96,99	31
6	GOL	E	404	6/6	0.81	0.22	75,84,96,102	0
4	PO4	F	501	5/5	0.84	0.17	77,78,84,92	5
5	NA	E	403	1/1	0.88	0.26	50,50,50,50	0
3	SIN	E	402	8/8	0.89	0.26	53,58,75,86	0
7	CL	G	402	1/1	0.89	0.08	91,91,91,91	0
2	FMN	C	401	31/31	0.90	0.27	66,79,85,90	0
6	GOL	F	502	6/6	0.91	0.27	65,73,77,80	0
4	PO4	B	501	5/5	0.93	0.18	68,77,79,81	5
2	FMN	A	401	31/31	0.93	0.18	60,72,77,82	0
3	SIN	A	402	8/8	0.93	0.17	64,71,77,78	0
2	FMN	E	401	31/31	0.97	0.16	40,58,65,72	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 FMN H 401:

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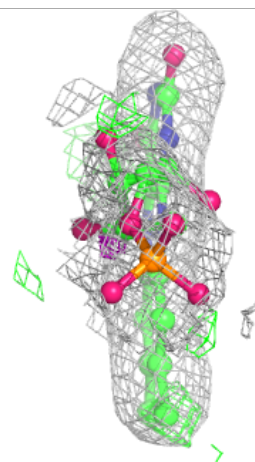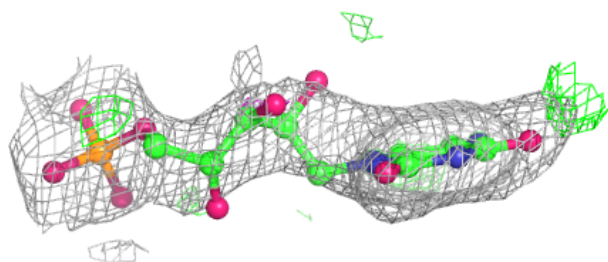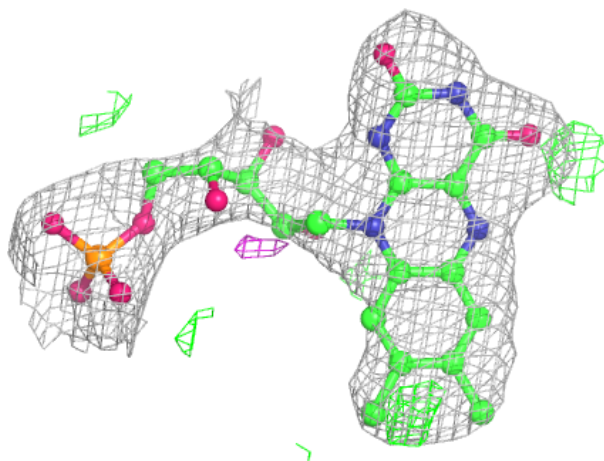mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FMN 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 D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
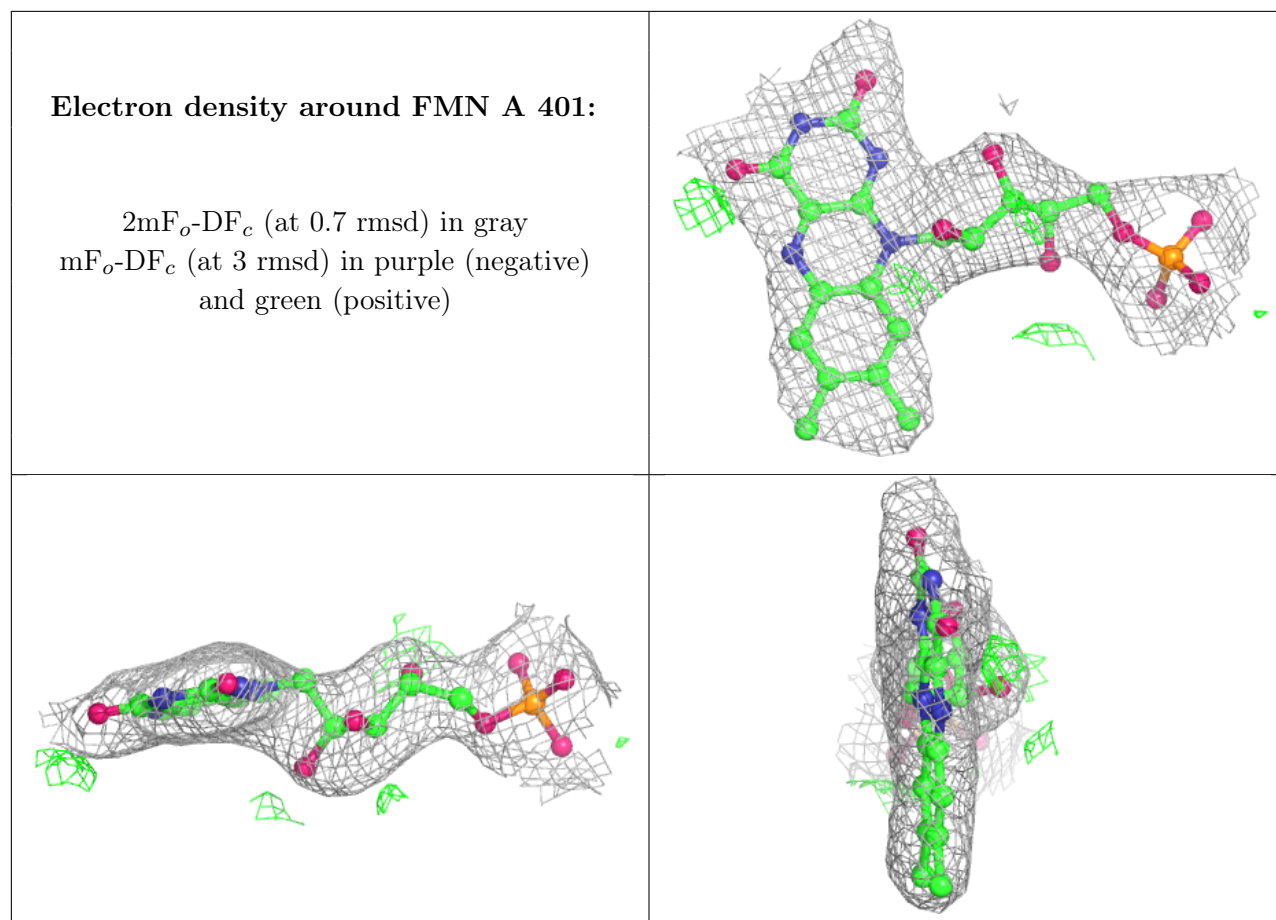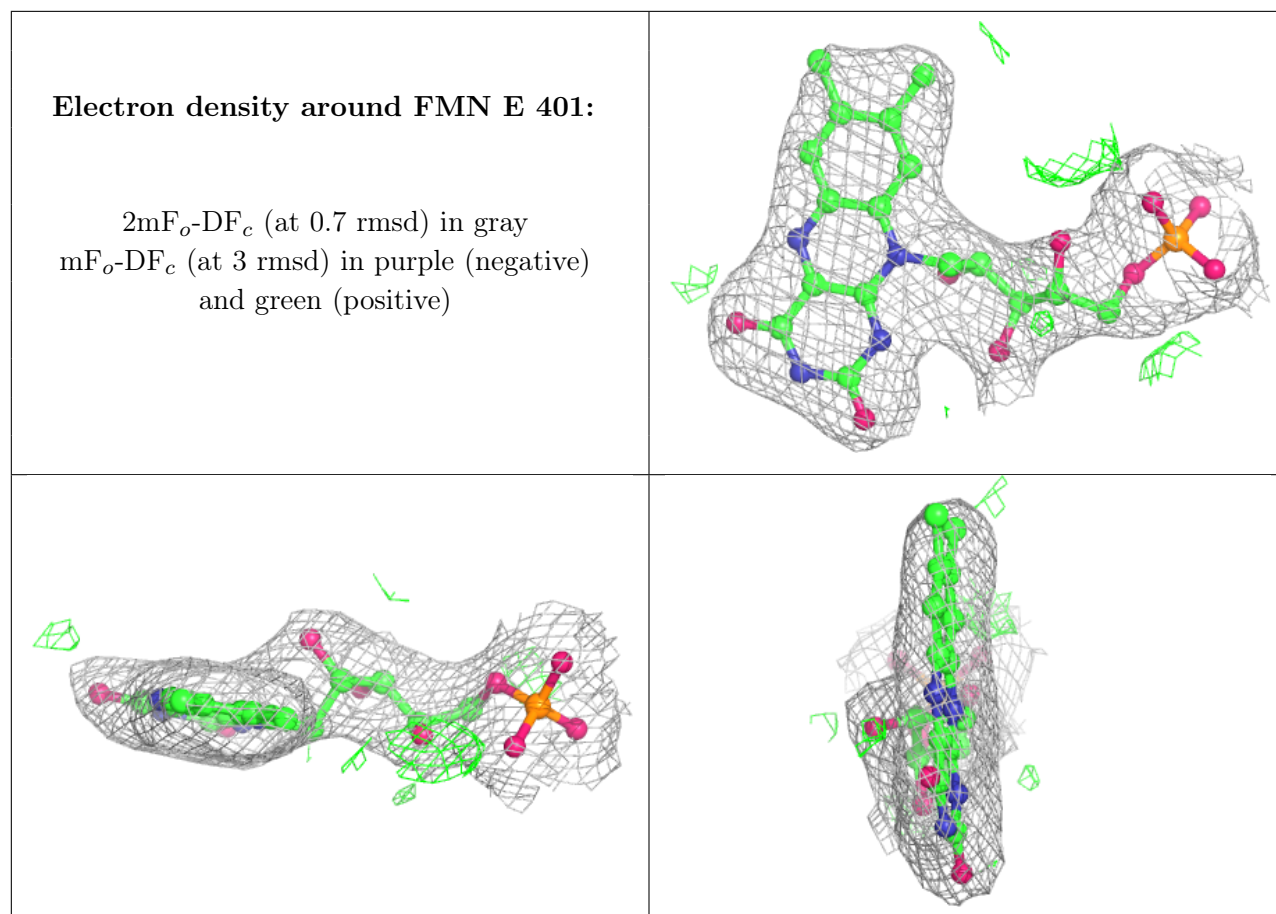mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
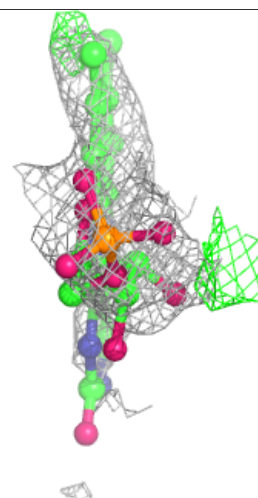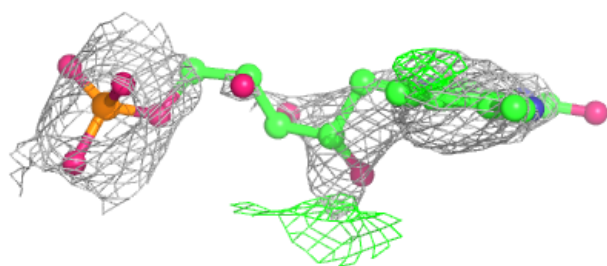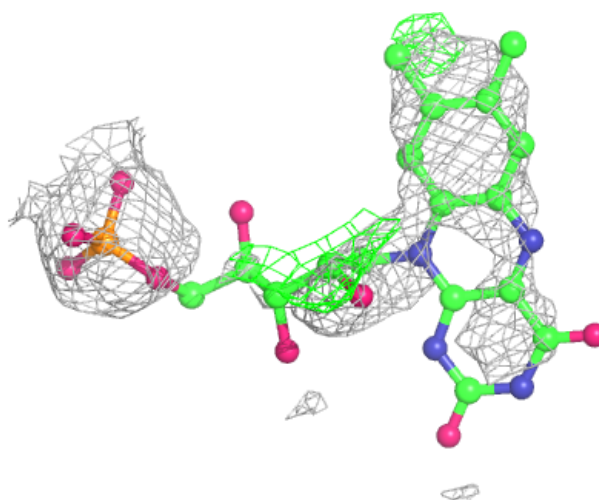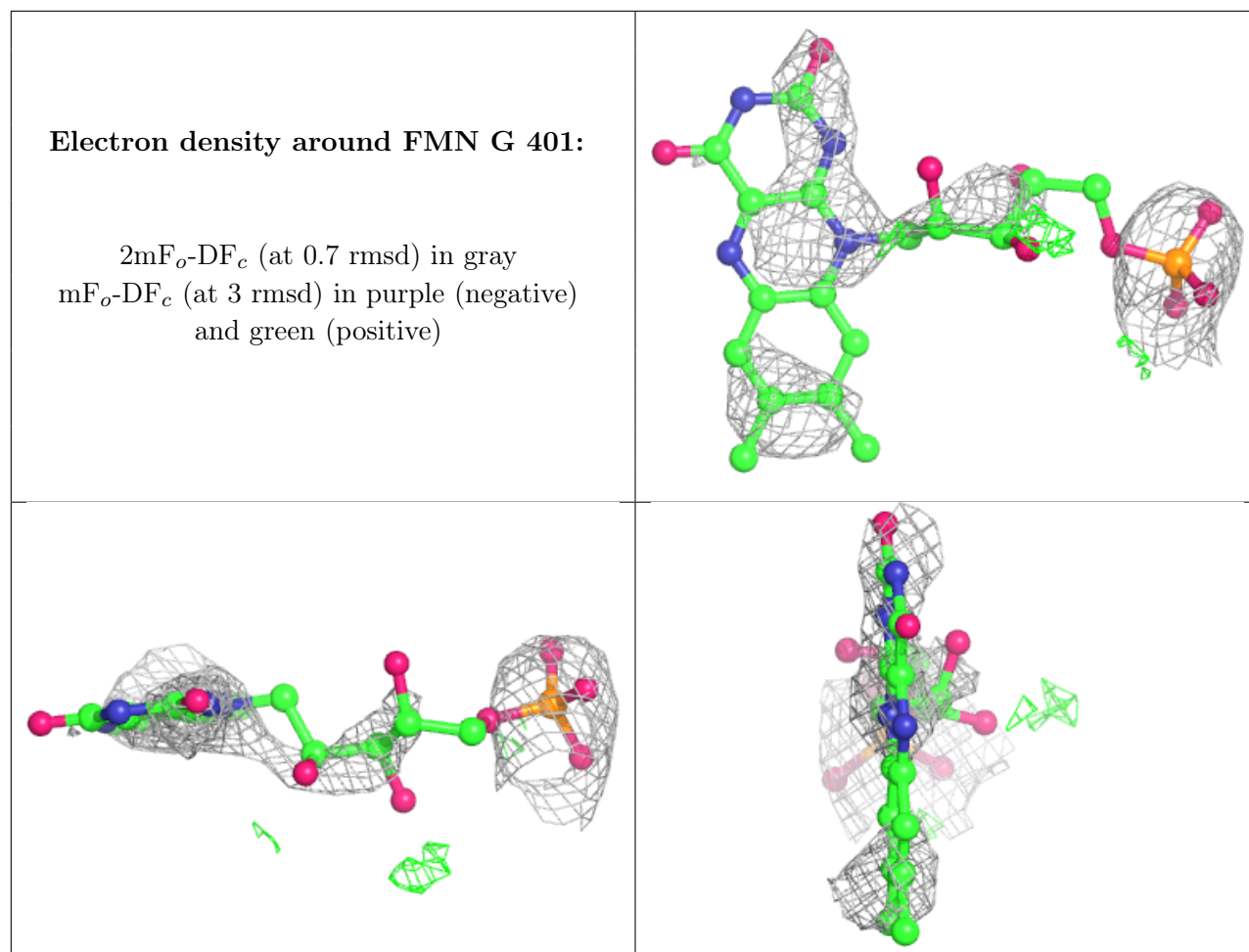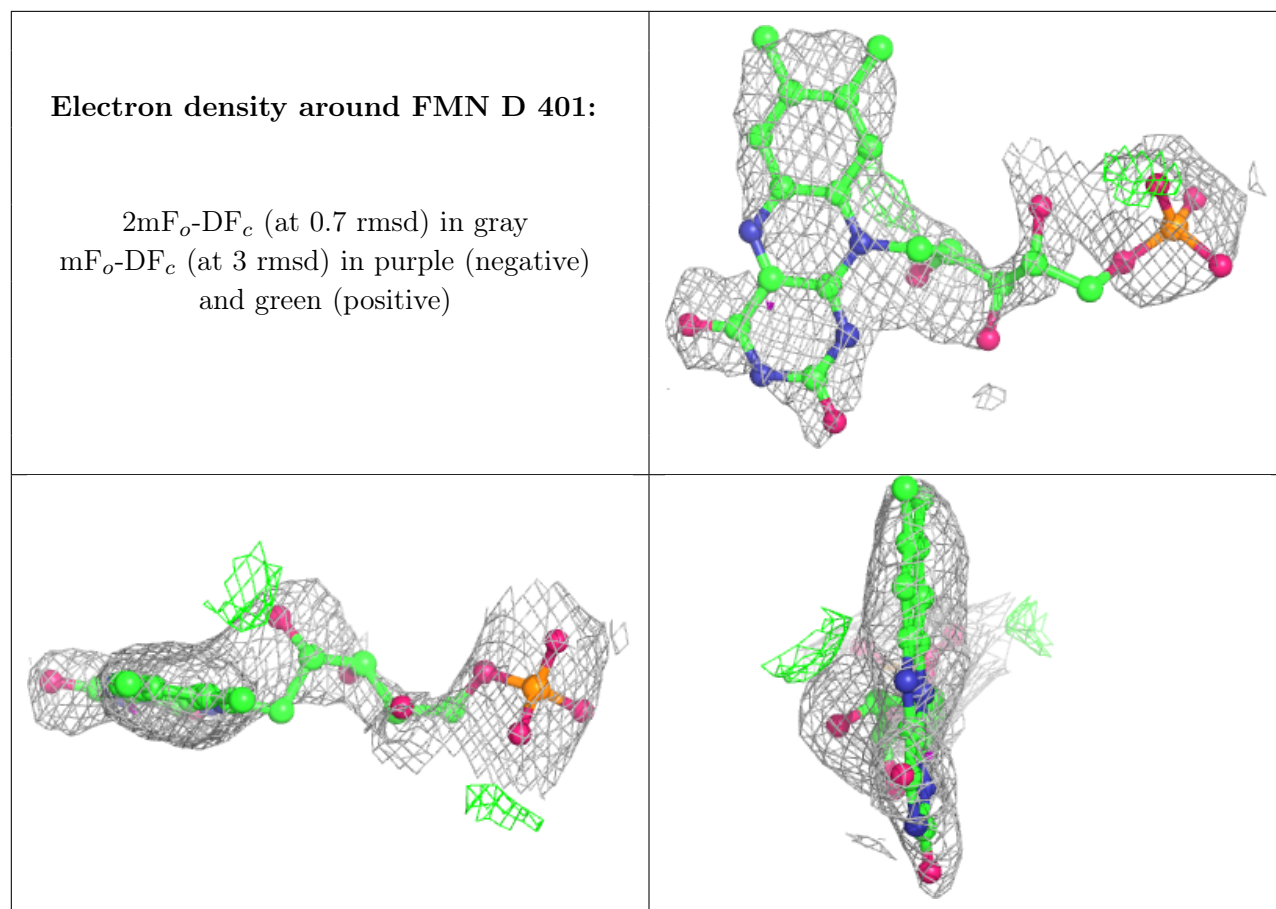
Electron density around FMN C 401:

$2mF_o$-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 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 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.