WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 02:22 AM EDT

PDB ID	:	7K14
Title	:	Ternary soak structure of alkanesulfonate monooxygenase MsuD from Pseudomonas fluorescens with FMN and methanesulfonate
Authors	:	Liew, J.J.M.; Dowling, D.P.; El Saudi, I.M.
Deposited on	:	2020-09-07
Resolution	:	2.75 Å(reported)

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

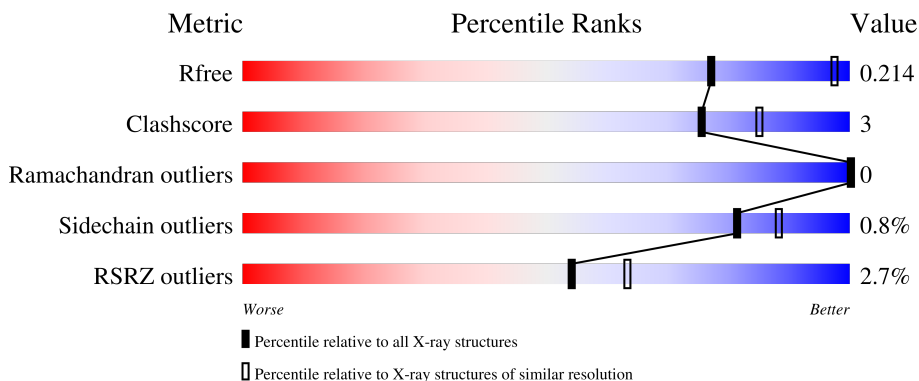|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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		0.214
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		2.7%

Worse   *Better*

■ 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	2% · 78% · 10% · 12%
1	B	404	5% · 79% · 8% · 12%
1	C	404	·% · 81% · 7% · 12%
1	D	404	·% · 80% · 8% · 12%
1	E	404	79% · 9% · 12%

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Mol	Chain	Length	Quality of chain
1	F	404	72% 8% 21%
1	G	404	6% 78% 8% 14%
1	H	404	3% 80% 6% 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
3	03S	A	402	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21777 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	356	Total	C	N	O	S	0	0	0
			2755	1750	487	514	4			
1	B	354	Total	C	N	O	S	0	1	0
			2732	1740	481	507	4			
1	C	356	Total	C	N	O	S	0	0	0
			2748	1747	487	510	4			
1	D	356	Total	C	N	O	S	0	0	0
			2703	1721	472	506	4			
1	E	356	Total	C	N	O	S	0	1	0
			2764	1757	491	512	4			
1	F	321	Total	C	N	O	S	0	0	0
			2476	1589	429	455	3			
1	G	346	Total	C	N	O	S	0	0	0
			2670	1701	470	495	4			
1	H	347	Total	C	N	O	S	0	0	0
			2664	1698	464	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).
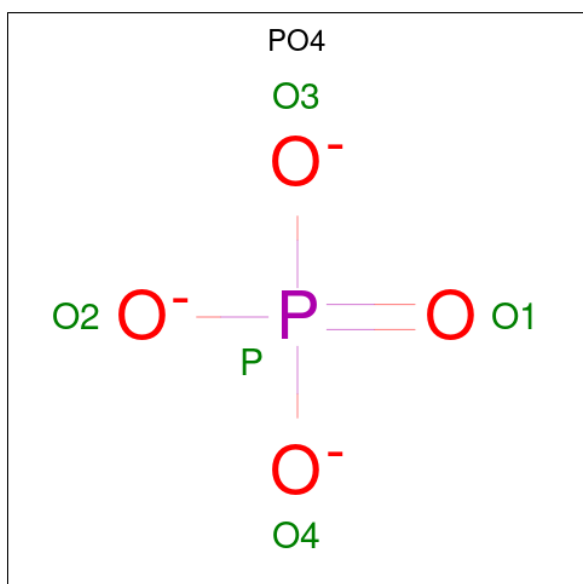

FMN
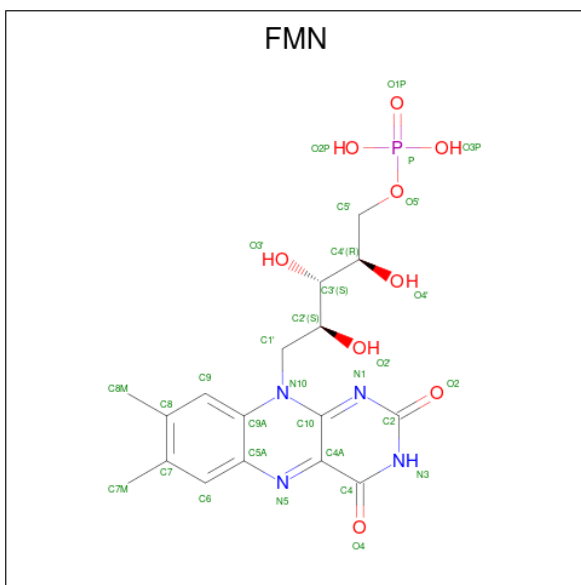
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total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

- Molecule 3 is methanesulfonic acid (three-letter code: 03S) (formula: CH_4O_3S).
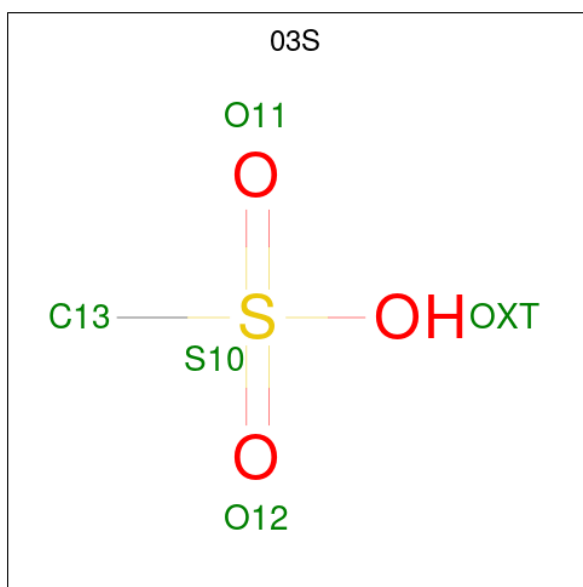
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 5	C 1	O 3	S 1	0	0
3	B	1	Total 5	C 1	O 3	S 1	0	0
3	C	1	Total 5	C 1	O 3	S 1	0	0
3	D	1	Total 5	C 1	O 3	S 1	0	0
3	E	1	Total 5	C 1	O 3	S 1	0	0

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

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Cl 1	0	0
5	H	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	O 3	0	0
6	B	5	Total 5	O 5	0	0
6	C	1	Total 1	O 1	0	0
6	D	3	Total 3	O 3	0	0
6	E	1	Total 1	O 1	0	0
6	F	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.
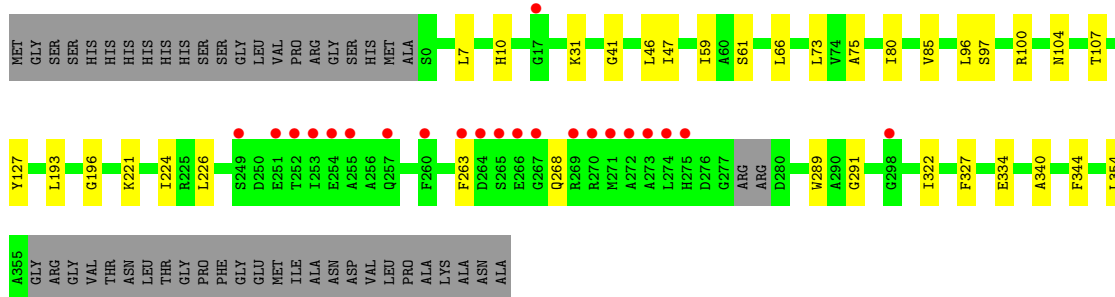
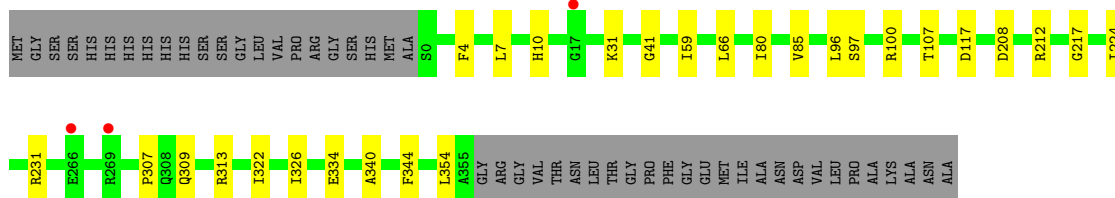• Molecule 1: Alkanesulfonate monooxygenase

Chain A:
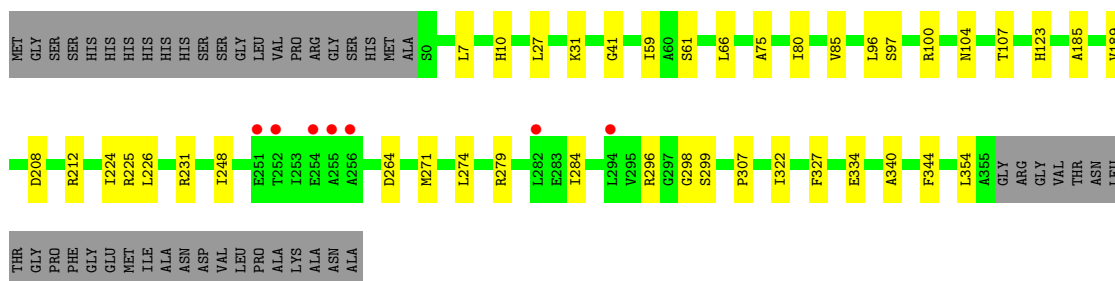
• Molecule 1: Alkanesulfonate monooxygenase

Chain B:

• Molecule 1: Alkanesulfonate monooxygenase

Chain C:

• Molecule 1: Alkanesulfonate monooxygenase

Chain D:

• Molecule 1: Alkanesulfonate monooxygenase

Chain E:

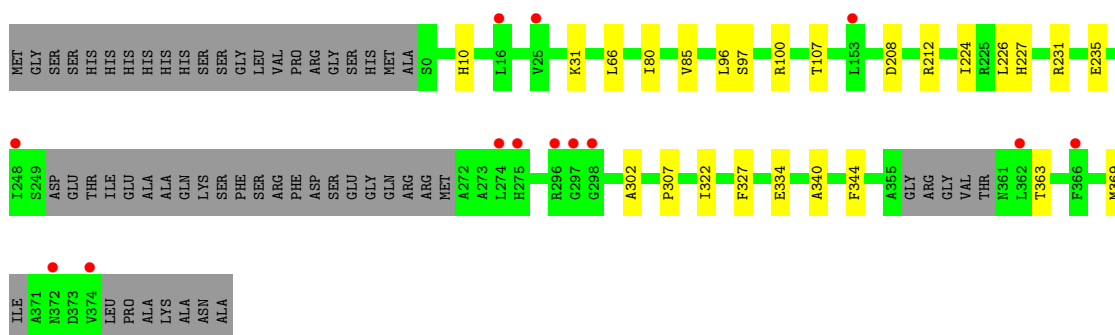• Molecule 1: Alkanesulfonate monooxygenase

Chain F:

• Molecule 1: Alkanesulfonate monooxygenase

Chain G:

• Molecule 1: Alkanesulfonate monooxygenase

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.00Å 211.93Å 94.35Å 90.00° 119.05° 90.00°	Depositor
Resolution (Å)	81.16 – 2.75 82.18 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (81.16-2.75) 99.1 (82.18-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.172 , 0.214 0.172 , 0.214	Depositor DCC
R_{free} test set	4125 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	82.0	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.018 for h,-k,-h-l 0.013 for -h-l,-k,l 0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21777	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: CL, 03S, PO4, FMN

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	0.36	0/2823	0.54	0/3842
1	B	0.34	0/2803	0.52	0/3816
1	C	0.36	0/2816	0.52	0/3833
1	D	0.33	0/2771	0.50	0/3782
1	E	0.39	0/2835	0.56	0/3856
1	F	0.33	0/2539	0.52	0/3463
1	G	0.31	0/2735	0.48	0/3722
1	H	0.33	0/2729	0.50	0/3718
All	All	0.34	0/22051	0.52	0/30032

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	2755	0	2687	26	0
1	B	2732	0	2658	22	0
1	C	2748	0	2681	17	0
1	D	2703	0	2594	18	0
1	E	2764	0	2709	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2476	0	2424	18	0
1	G	2670	0	2608	17	0
1	H	2664	0	2586	14	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	1	0
2	G	31	0	19	1	0
2	H	31	0	19	0	0
3	A	5	0	3	2	0
3	B	5	0	3	0	0
3	C	5	0	3	0	0
3	D	5	0	3	0	0
3	E	5	0	3	0	0
4	F	5	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	3	0	0	0	0
6	B	5	0	0	0	0
6	C	1	0	0	0	0
6	D	3	0	0	0	0
6	E	1	0	0	0	0
6	F	3	0	0	0	0
All	All	21777	0	21095	132	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 3.

All (132) 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:C:85:VAL:HG21	1:D:80:ILE:HD13	1.66	0.78
1:A:85:VAL:HG21	1:B:80:ILE:HD13	1.66	0.77
1:E:85:VAL:HG21	1:F:80:ILE:HD13	1.67	0.76
1:C:80:ILE:HD13	1:D:85:VAL:HG21	1.70	0.73
1:D:77:ARG:NH1	1:D:78:PRO:O	2.23	0.72
1:E:80:ILE:HD13	1:F:85:VAL:HG21	1.71	0.72
1:G:80:ILE:HD13	1:H:85:VAL:HG21	1.74	0.69
1:G:85:VAL:HG21	1:H:80:ILE:HD13	1.75	0.69
1:C:31:LYS:HD2	1:C:66:LEU:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:PHE:HD2	1:E:268:GLN:HG2	1.63	0.63
1:H:31:LYS:HD2	1:H:66:LEU:HD13	1.79	0.63
1:A:97:SER:O	1:A:100:ARG:HD3	1.98	0.63
1:G:31:LYS:HD2	1:G:66:LEU:HD13	1.81	0.63
1:A:248:ILE:O	1:A:279:ARG:NH2	2.32	0.62
1:B:41:GLY:HA3	1:B:354:LEU:HD13	1.81	0.62
1:D:97:SER:O	1:D:100:ARG:HD3	2.00	0.61
1:F:97:SER:O	1:F:100:ARG:HD3	2.02	0.60
1:E:248:ILE:O	1:E:279:ARG:NH2	2.35	0.60
1:B:31:LYS:HD2	1:B:66:LEU:HD13	1.84	0.59
1:C:97:SER:O	1:C:100:ARG:HD3	2.02	0.59
1:A:334:GLU:HG3	1:D:334:GLU:HG3	1.84	0.59
1:A:31:LYS:HD2	1:A:66:LEU:HD13	1.83	0.59
1:E:52:SER:HB2	1:H:369:MET:HG3	1.83	0.59
1:D:248:ILE:O	1:D:279:ARG:NH2	2.36	0.58
1:B:97:SER:O	1:B:100:ARG:HD3	2.02	0.58
1:C:59:ILE:HD13	1:D:96:LEU:HD11	1.85	0.58
1:F:41:GLY:HA3	1:F:354:LEU:HD13	1.86	0.58
1:B:193:LEU:HD13	2:B:401:FMN:HM73	1.86	0.58
1:G:97:SER:O	1:G:100:ARG:HD3	2.04	0.57
1:G:263:PHE:HD2	1:G:268:GLN:HG2	1.70	0.57
1:F:227:HIS:CE1	1:F:329:GLY:HA2	2.40	0.56
1:A:80:ILE:HD13	1:B:85:VAL:HG21	1.86	0.56
1:A:96:LEU:HD11	1:B:59:ILE:HD13	1.88	0.56
1:E:97:SER:O	1:E:100:ARG:HD3	2.07	0.55
1:F:7:LEU:HD12	1:F:47:ILE:HG12	1.87	0.55
1:A:75:ALA:HA	1:A:104:ASN:O	2.07	0.55
1:E:334:GLU:HG3	1:H:334:GLU:HG3	1.88	0.55
1:F:224:ILE:HB	1:F:322:ILE:HD13	1.90	0.55
1:E:96:LEU:HD11	1:F:59:ILE:HD13	1.89	0.54
1:F:334:GLU:HG3	1:G:334:GLU:HG3	1.89	0.54
1:H:97:SER:O	1:H:100:ARG:HD3	2.07	0.54
1:C:224:ILE:HB	1:C:322:ILE:HD13	1.91	0.53
1:A:59:ILE:HD13	1:B:96:LEU:HD11	1.90	0.52
1:D:208:ASP:O	1:D:212:ARG:HG3	2.09	0.52
1:G:59:ILE:HD13	1:H:96:LEU:HD11	1.93	0.51
1:G:75:ALA:HA	1:G:104:ASN:O	2.09	0.51
1:B:46:LEU:HA	1:B:73:LEU:HB3	1.92	0.51
1:E:41:GLY:HA3	1:E:354:LEU:HD13	1.92	0.51
1:E:59:ILE:HD13	1:F:96:LEU:HD11	1.92	0.51
1:H:227:HIS:HB3	1:H:302:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:PHE:CD2	1:E:268:GLN:HG2	2.42	0.51
1:H:231:ARG:O	1:H:307:PRO:HD3	2.12	0.50
1:H:235:GLU:OE1	1:H:235:GLU:N	2.44	0.50
1:D:31:LYS:HD2	1:D:66:LEU:HD13	1.92	0.50
1:E:46:LEU:HA	1:E:73:LEU:HB3	1.94	0.50
1:A:231:ARG:O	1:A:307:PRO:HD3	2.12	0.49
1:B:226:LEU:O	1:B:327:PHE:HA	2.13	0.49
1:E:31:LYS:HD2	1:E:66:LEU:HD13	1.93	0.49
1:C:231:ARG:O	1:C:307:PRO:HD3	2.13	0.48
1:G:311:ALA:O	1:G:315:LYS:HG2	2.12	0.48
1:E:274:LEU:HD22	1:E:284:ILE:HD12	1.95	0.48
1:E:231:ARG:O	1:E:307:PRO:HD3	2.13	0.48
1:D:41:GLY:HA3	1:D:354:LEU:HD13	1.94	0.48
1:A:41:GLY:HA3	1:A:354:LEU:HD13	1.95	0.48
1:D:224:ILE:HB	1:D:322:ILE:HD13	1.95	0.48
1:E:210[A]:ARG:NH2	1:E:320:LEU:O	2.47	0.48
1:H:226:LEU:O	1:H:327:PHE:HA	2.14	0.48
1:C:4:PHE:HB2	1:C:326:ILE:HA	1.96	0.47
1:H:224:ILE:HB	1:H:322:ILE:HD13	1.96	0.47
1:B:224:ILE:HB	1:B:322:ILE:HD13	1.97	0.47
1:A:296:ARG:NH2	3:A:402:03S:O11	2.39	0.47
1:H:208:ASP:O	1:H:212:ARG:HG3	2.15	0.47
1:A:27:LEU:HB2	1:B:96:LEU:HD22	1.97	0.47
1:B:340:ALA:O	1:B:344:PHE:HB2	2.15	0.46
1:F:227:HIS:HB3	1:F:302:ALA:HB2	1.96	0.46
1:C:217:GLY:O	1:E:313:ARG:NH2	2.44	0.46
1:G:46:LEU:HA	1:G:73:LEU:HB3	1.96	0.46
1:G:224:ILE:HB	1:G:322:ILE:HD13	1.97	0.46
1:G:340:ALA:O	1:G:344:PHE:HB2	2.16	0.46
1:C:208:ASP:O	1:C:212:ARG:HG3	2.16	0.45
1:C:96:LEU:HD11	1:D:59:ILE:HD13	1.98	0.45
1:A:185:ALA:O	1:A:189:VAL:HG22	2.16	0.45
1:C:340:ALA:O	1:C:344:PHE:HB2	2.15	0.45
1:F:68:GLU:OE1	1:F:69:ARG:NH1	2.49	0.45
1:B:263:PHE:HD2	1:B:268:GLN:HG2	1.82	0.45
1:D:340:ALA:O	1:D:344:PHE:HB2	2.17	0.45
1:G:47:ILE:HD12	1:G:60:ALA:HB2	1.99	0.44
1:F:340:ALA:O	1:F:344:PHE:HB2	2.18	0.44
1:B:75:ALA:HA	1:B:104:ASN:O	2.17	0.44
1:B:289:TRP:CZ2	1:B:291:GLY:HA3	2.53	0.44
1:A:224:ILE:HB	1:A:322:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ALA:O	1:A:344:PHE:HB2	2.17	0.44
1:C:41:GLY:HA3	1:C:354:LEU:HD13	2.00	0.44
1:C:80:ILE:HG21	1:C:117:ASP:HB3	2.00	0.43
1:F:226:LEU:O	1:F:327:PHE:HA	2.18	0.43
1:D:15:TYR:HA	1:D:244:LEU:HD12	1.99	0.43
1:E:123:HIS:HB2	1:E:264:ASP:OD2	2.19	0.43
1:A:271:MET:HG2	1:A:298:GLY:O	2.18	0.43
1:E:224:ILE:HB	1:E:322:ILE:HD13	2.00	0.43
1:H:340:ALA:O	1:H:344:PHE:HB2	2.18	0.43
1:D:227:HIS:HB3	1:D:302:ALA:HB2	2.01	0.42
1:E:289:TRP:CZ2	1:E:291:GLY:HA3	2.54	0.42
1:A:225:ARG:NE	3:A:402:03S:O12	2.50	0.42
1:D:226:LEU:O	1:D:327:PHE:HA	2.18	0.42
1:E:30:LEU:HD13	1:E:59:ILE:HD12	2.01	0.42
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.90	0.42
1:A:123:HIS:HE1	2:A:401:FMN:O3P	2.03	0.42
1:F:4:PHE:HB2	1:F:326:ILE:HA	2.01	0.42
1:B:196:GLY:HA2	1:B:224:ILE:HD11	2.01	0.42
1:A:61:SER:HB2	1:B:61:SER:HB2	2.01	0.42
1:B:7:LEU:HD12	1:B:47:ILE:HG12	2.01	0.42
1:D:289:TRP:CZ2	1:D:291:GLY:HA3	2.54	0.42
1:F:75:ALA:HA	1:F:104:ASN:O	2.20	0.42
1:G:127:TYR:OH	2:G:401:FMN:O5'	2.38	0.42
1:G:231:ARG:O	1:G:307:PRO:HD3	2.20	0.42
1:A:208:ASP:O	1:A:212:ARG:HG3	2.20	0.42
1:B:334:GLU:HG3	1:C:334:GLU:HG3	2.01	0.41
1:A:123:HIS:HB2	1:A:264:ASP:OD2	2.20	0.41
1:A:226:LEU:O	1:A:327:PHE:HA	2.20	0.41
1:B:221:LYS:HE2	1:B:221:LYS:HB3	1.76	0.41
1:C:7:LEU:HA	1:C:7:LEU:HD23	1.80	0.41
1:D:170:PRO:HA	1:D:171:PRO:HD3	1.97	0.41
1:A:274:LEU:HD22	1:A:284:ILE:HD12	2.03	0.41
1:C:309:GLN:O	1:C:313:ARG:HG2	2.21	0.41
1:G:272:ALA:HA	1:G:275:HIS:NE2	2.35	0.41
1:A:296:ARG:NH1	1:A:299:SER:HB3	2.35	0.41
1:F:31:LYS:HD2	1:F:66:LEU:HD13	2.02	0.40
1:G:285:ALA:HB3	1:G:288:LEU:HB3	2.02	0.40
1:B:107:THR:HG21	1:B:127:TYR:CE1	2.56	0.40
1:E:134:LEU:HD23	1:E:134:LEU:HA	1.85	0.40
1:E:193:LEU:HD13	2:E:401:FMN:HM73	2.04	0.40
1:F:243:LYS:O	1:F:246:GLU:HG2	2.21	0.40

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	354/404 (88%)	349 (99%)	5 (1%)	0	100	100
1	B	351/404 (87%)	347 (99%)	4 (1%)	0	100	100
1	C	354/404 (88%)	349 (99%)	5 (1%)	0	100	100
1	D	354/404 (88%)	347 (98%)	7 (2%)	0	100	100
1	E	355/404 (88%)	349 (98%)	6 (2%)	0	100	100
1	F	315/404 (78%)	312 (99%)	3 (1%)	0	100	100
1	G	340/404 (84%)	334 (98%)	6 (2%)	0	100	100
1	H	339/404 (84%)	335 (99%)	4 (1%)	0	100	100
All	All	2762/3232 (86%)	2722 (99%)	40 (1%)	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	280/321 (87%)	278 (99%)	2 (1%)	84	89
1	B	276/321 (86%)	275 (100%)	1 (0%)	91	93
1	C	278/321 (87%)	276 (99%)	2 (1%)	84	89
1	D	269/321 (84%)	267 (99%)	2 (1%)	84	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	281/321 (88%)	277 (99%)	4 (1%)	67	79
1	F	251/321 (78%)	250 (100%)	1 (0%)	91	93
1	G	271/321 (84%)	269 (99%)	2 (1%)	84	89
1	H	270/321 (84%)	267 (99%)	3 (1%)	73	84
All	All	2176/2568 (85%)	2159 (99%)	17 (1%)	81	88

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

Mol	Chain	Res	Type
1	A	10	HIS
1	A	107	THR
1	B	10	HIS
1	C	10	HIS
1	C	107	THR
1	D	10	HIS
1	D	107	THR
1	E	10	HIS
1	E	77	ARG
1	E	107	THR
1	E	156	GLN
1	F	10	HIS
1	G	10	HIS
1	G	107	THR
1	H	10	HIS
1	H	107	THR
1	H	363	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	C	257	GLN
1	D	257	GLN
1	F	227	HIS
1	G	156	GLN
1	H	361	ASN

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	E	401	-	33,33,33	1.09	2 (6%)	48,50,50	1.25	6 (12%)
2	FMN	G	401	-	33,33,33	1.06	2 (6%)	48,50,50	1.26	8 (16%)
3	03S	D	402	-	4,4,4	0.38	0	5,6,6	0.93	0
2	FMN	C	401	-	33,33,33	1.02	2 (6%)	48,50,50	1.27	8 (16%)
2	FMN	B	401	-	33,33,33	1.11	2 (6%)	48,50,50	1.27	7 (14%)
3	03S	A	402	-	4,4,4	0.42	0	5,6,6	1.08	1 (20%)
3	03S	E	402	-	4,4,4	0.38	0	5,6,6	0.89	0
3	03S	C	402	-	4,4,4	0.40	0	5,6,6	0.90	0
4	PO4	F	401	-	4,4,4	0.84	0	6,6,6	0.54	0
2	FMN	A	401	-	33,33,33	1.10	2 (6%)	48,50,50	1.28	7 (14%)
2	FMN	H	401	-	33,33,33	1.06	2 (6%)	48,50,50	1.25	6 (12%)
3	03S	B	402	-	4,4,4	0.45	0	5,6,6	1.12	1 (20%)
2	FMN	D	401	-	33,33,33	1.06	2 (6%)	48,50,50	1.28	7 (14%)

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	E	401	-	-	3/18/18/18	0/3/3/3
2	FMN	G	401	-	-	10/18/18/18	0/3/3/3
2	FMN	C	401	-	-	4/18/18/18	0/3/3/3
2	FMN	B	401	-	-	9/18/18/18	0/3/3/3
2	FMN	A	401	-	-	6/18/18/18	0/3/3/3
2	FMN	H	401	-	-	11/18/18/18	0/3/3/3
2	FMN	D	401	-	-	2/18/18/18	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	FMN	C5A-N5	-2.86	1.33	1.39
2	A	401	FMN	C5A-N5	-2.74	1.34	1.39
2	B	401	FMN	C5A-N5	-2.55	1.34	1.39
2	C	401	FMN	C5A-N5	-2.55	1.34	1.39
2	H	401	FMN	C5A-N5	-2.50	1.34	1.39
2	D	401	FMN	C5A-N5	-2.46	1.34	1.39
2	E	401	FMN	C6-C7	-2.40	1.36	1.39
2	G	401	FMN	C5A-N5	-2.27	1.35	1.39
2	D	401	FMN	C6-C7	-2.27	1.36	1.39
2	G	401	FMN	C6-C7	-2.19	1.36	1.39
2	B	401	FMN	C2-N3	-2.14	1.34	1.39
2	A	401	FMN	C2-N3	-2.09	1.34	1.39
2	H	401	FMN	C2-N3	-2.08	1.34	1.39
2	C	401	FMN	C6-C7	-2.04	1.36	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FMN	C4-C4A-N5	3.16	122.73	118.23
2	B	401	FMN	C4-C4A-N5	3.07	122.61	118.23
2	H	401	FMN	C4-C4A-N5	3.07	122.60	118.23
2	G	401	FMN	C4-C4A-N5	2.93	122.41	118.23
2	H	401	FMN	C4A-C10-N1	-2.76	118.32	124.73
2	A	401	FMN	C4A-C10-N1	-2.75	118.35	124.73
2	G	401	FMN	C4A-C10-N1	-2.71	118.44	124.73
2	D	401	FMN	C4A-C10-N1	-2.69	118.50	124.73
2	H	401	FMN	C10-N1-C2	2.58	122.06	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	FMN	C4-C4A-N5	2.58	121.90	118.23
2	B	401	FMN	C4A-C10-N1	-2.50	118.93	124.73
2	D	401	FMN	C10-N1-C2	2.46	121.83	116.90
2	C	401	FMN	C4A-C10-N1	-2.46	119.02	124.73
2	G	401	FMN	C10-N1-C2	2.46	121.82	116.90
2	C	401	FMN	C4-C4A-N5	2.45	121.72	118.23
2	G	401	FMN	P-O5'-C5'	2.44	125.01	118.30
2	B	401	FMN	P-O5'-C5'	2.42	124.97	118.30
2	D	401	FMN	C4-N3-C2	-2.40	121.21	125.64
2	A	401	FMN	C4-C4A-N5	2.39	121.64	118.23
2	D	401	FMN	N3-C2-N1	2.39	124.08	119.38
2	H	401	FMN	C4-N3-C2	-2.39	121.23	125.64
2	B	401	FMN	N3-C2-N1	2.38	124.05	119.38
2	E	401	FMN	N3-C2-N1	2.37	124.04	119.38
2	C	401	FMN	C5A-C9A-N10	2.35	120.38	117.95
2	A	401	FMN	N3-C2-N1	2.35	123.99	119.38
2	E	401	FMN	C4A-C10-N1	-2.34	119.30	124.73
2	C	401	FMN	C10-N1-C2	2.33	121.56	116.90
2	D	401	FMN	C10-C4A-N5	-2.33	119.92	124.86
2	H	401	FMN	N3-C2-N1	2.32	123.94	119.38
2	E	401	FMN	C5A-C9A-N10	2.31	120.34	117.95
3	B	402	03S	O12-S10-O11	-2.30	111.81	118.02
2	G	401	FMN	C4-N3-C2	-2.29	121.41	125.64
2	E	401	FMN	C4-N3-C2	-2.27	121.45	125.64
2	G	401	FMN	N3-C2-N1	2.26	123.83	119.38
2	B	401	FMN	C10-N1-C2	2.26	121.42	116.90
2	A	401	FMN	C5A-N5-C4A	2.25	121.82	118.07
3	A	402	03S	O12-S10-O11	-2.23	112.00	118.02
2	D	401	FMN	O2-C2-N1	-2.23	118.14	121.83
2	C	401	FMN	O2-C2-N1	-2.23	118.14	121.83
2	B	401	FMN	C4-N3-C2	-2.22	121.54	125.64
2	A	401	FMN	O2P-P-O5'	2.19	112.55	106.73
2	B	401	FMN	C5A-C9A-N10	2.18	120.21	117.95
2	C	401	FMN	O4-C4-C4A	-2.16	120.88	126.60
2	H	401	FMN	C10-C4A-N5	-2.14	120.31	124.86
2	A	401	FMN	C10-N1-C2	2.13	121.17	116.90
2	A	401	FMN	C10-C4A-N5	-2.11	120.38	124.86
2	G	401	FMN	C10-C4A-N5	-2.11	120.38	124.86
2	C	401	FMN	N3-C2-N1	2.09	123.49	119.38
2	C	401	FMN	C4-N3-C2	-2.09	121.79	125.64
2	G	401	FMN	O2-C2-N1	-2.08	118.38	121.83
2	E	401	FMN	C10-N1-C2	2.05	121.00	116.90

There are no chirality outliers.

All (45) 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	A	401	FMN	C5'-O5'-P-O3P
2	B	401	FMN	N10-C1'-C2'-O2'
2	B	401	FMN	N10-C1'-C2'-C3'
2	B	401	FMN	C1'-C2'-C3'-C4'
2	B	401	FMN	C3'-C4'-C5'-O5'
2	B	401	FMN	C5'-O5'-P-O2P
2	B	401	FMN	C5'-O5'-P-O3P
2	C	401	FMN	N10-C1'-C2'-O2'
2	C	401	FMN	N10-C1'-C2'-C3'
2	D	401	FMN	N10-C1'-C2'-O2'
2	D	401	FMN	N10-C1'-C2'-C3'
2	E	401	FMN	N10-C1'-C2'-O2'
2	E	401	FMN	N10-C1'-C2'-C3'
2	G	401	FMN	N10-C1'-C2'-O2'
2	G	401	FMN	N10-C1'-C2'-C3'
2	G	401	FMN	C3'-C4'-C5'-O5'
2	G	401	FMN	O4'-C4'-C5'-O5'
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	N10-C1'-C2'-O2'
2	H	401	FMN	N10-C1'-C2'-C3'
2	H	401	FMN	C1'-C2'-C3'-C4'
2	H	401	FMN	C3'-C4'-C5'-O5'
2	H	401	FMN	O4'-C4'-C5'-O5'
2	H	401	FMN	C5'-O5'-P-O1P
2	H	401	FMN	C5'-O5'-P-O2P
2	H	401	FMN	C5'-O5'-P-O3P
2	B	401	FMN	O4'-C4'-C5'-O5'
2	H	401	FMN	O2'-C2'-C3'-C4'
2	B	401	FMN	O2'-C2'-C3'-C4'
2	C	401	FMN	C3'-C4'-C5'-O5'
2	H	401	FMN	O2'-C2'-C3'-O3'
2	G	401	FMN	C2'-C3'-C4'-C5'
2	G	401	FMN	O2'-C2'-C3'-C4'
2	B	401	FMN	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	G	401	FMN	O2'-C2'-C3'-O3'
2	H	401	FMN	C2'-C3'-C4'-C5'
2	A	401	FMN	C5'-O5'-P-O2P
2	C	401	FMN	O4'-C4'-C5'-O5'
2	E	401	FMN	C3'-C4'-C5'-O5'

There are no ring outliers.
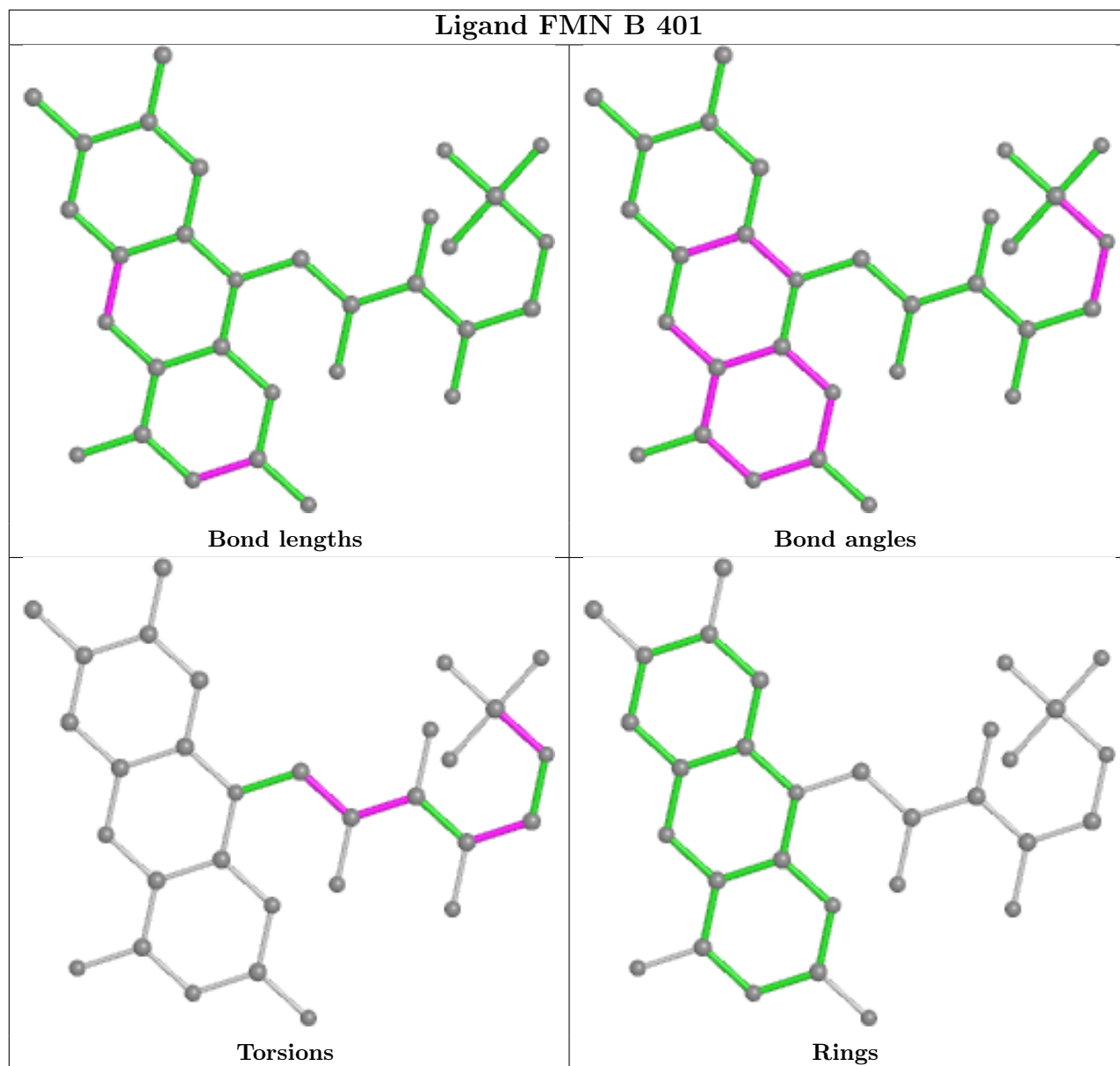
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	FMN	1	0
2	G	401	FMN	1	0
2	B	401	FMN	1	0
3	A	402	03S	2	0
2	A	401	FMN	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.
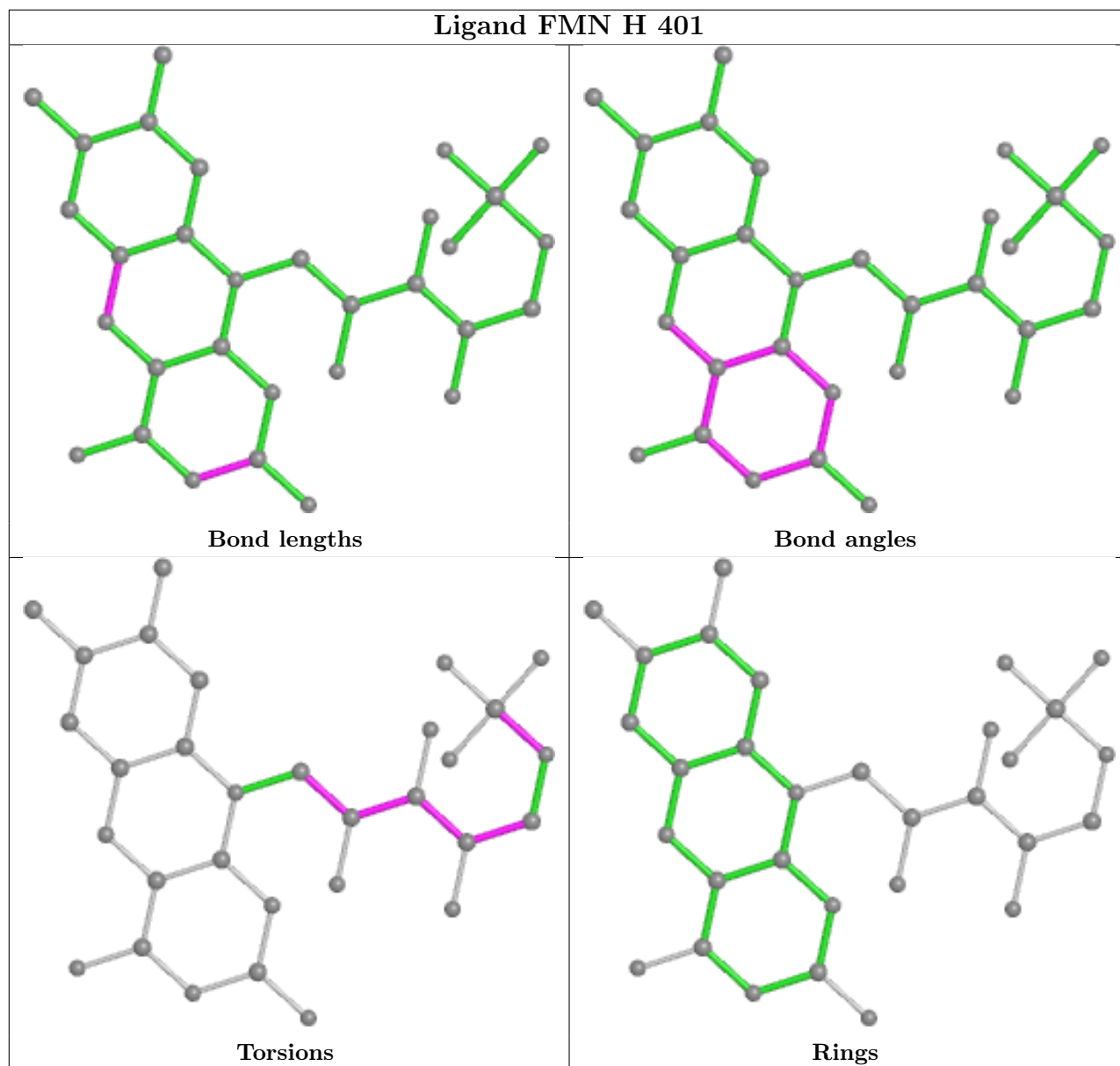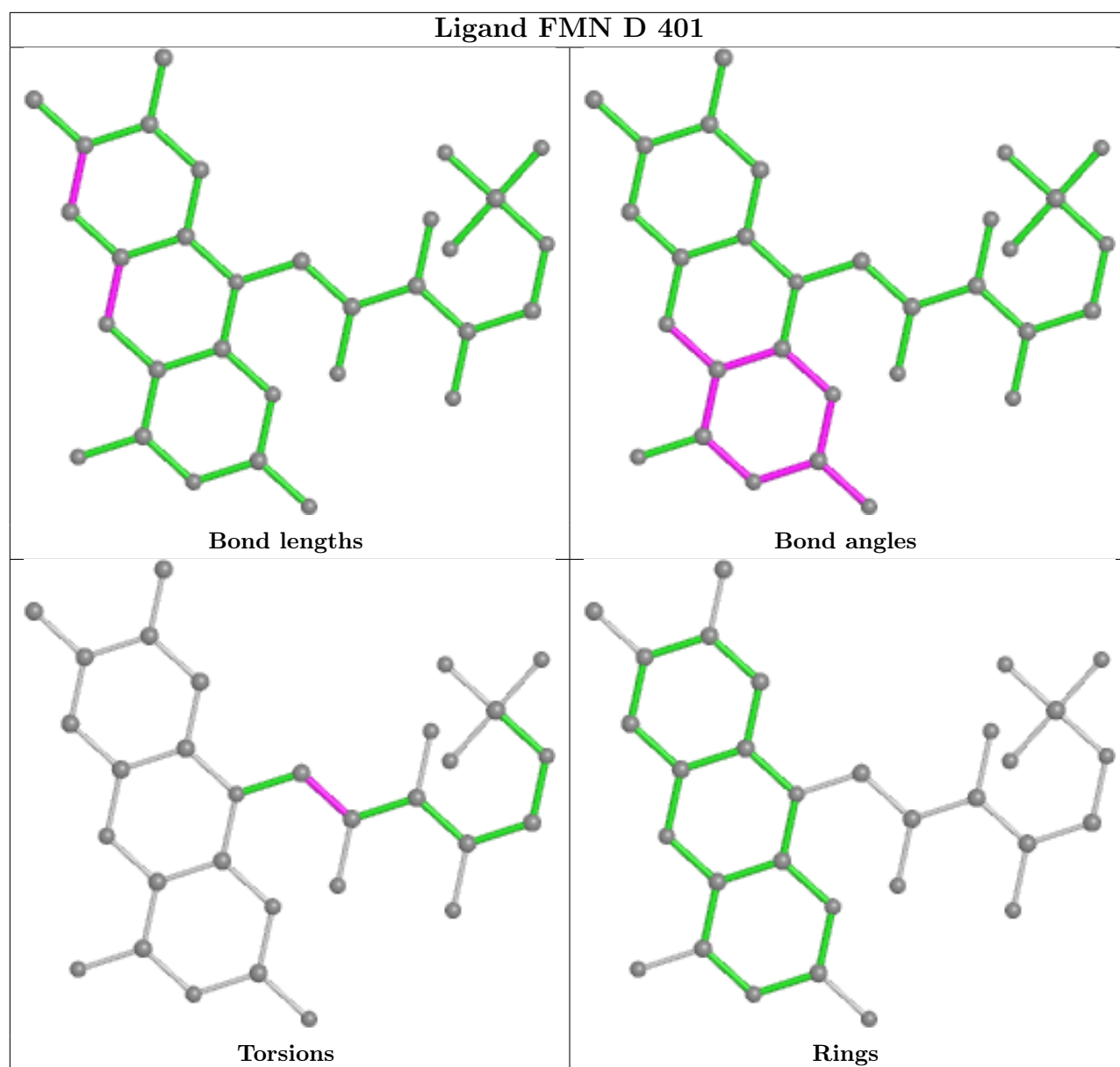
Ligand FMN E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN G 401

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand FMN C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN H 401

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN D 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 ⓘ

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	356/404 (88%)	0.16	7 (1%)	65	73	56, 88, 148, 240	0
1	B	354/404 (87%)	0.26	22 (6%)	20	25	58, 89, 163, 207	0
1	C	356/404 (88%)	0.03	3 (0%)	86	90	57, 82, 129, 171	0
1	D	356/404 (88%)	-0.02	3 (0%)	86	90	59, 91, 141, 197	0
1	E	356/404 (88%)	-0.05	2 (0%)	89	92	53, 69, 115, 146	0
1	F	321/404 (79%)	0.04	1 (0%)	94	96	56, 83, 121, 157	0
1	G	346/404 (85%)	0.34	24 (6%)	16	20	66, 113, 163, 207	0
1	H	347/404 (85%)	0.20	13 (3%)	41	49	61, 90, 140, 188	0
All	All	2792/3232 (86%)	0.12	75 (2%)	54	63	53, 87, 144, 240	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ALA	7.3
1	B	252	THR	6.0
1	B	264	ASP	5.8
1	A	256	ALA	5.6
1	G	263	PHE	5.4
1	A	254	GLU	5.0
1	B	274	LEU	5.0
1	B	265	SER	4.9
1	G	271	MET	4.6
1	G	269	ARG	4.3
1	B	269	ARG	4.2
1	A	294	LEU	4.2
1	B	275	HIS	4.2
1	A	252	THR	4.2
1	H	296	ARG	4.1
1	A	251	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	17	GLY	4.1
1	G	251	GLU	3.9
1	B	266	GLU	3.9
1	H	362	LEU	3.8
1	H	275	HIS	3.6
1	H	153	LEU	3.6
1	H	366	PHE	3.5
1	G	266	GLU	3.4
1	B	270	ARG	3.3
1	B	263	PHE	3.2
1	H	372	ASN	3.2
1	B	253	ILE	3.1
1	G	120	PHE	3.1
1	G	189	VAL	3.1
1	B	254	GLU	3.1
1	G	141	LEU	3.0
1	G	272	ALA	3.0
1	G	265	SER	3.0
1	D	232	GLU	2.9
1	D	251	GLU	2.9
1	D	294	LEU	2.8
1	G	123	HIS	2.8
1	C	269	ARG	2.8
1	C	17	GLY	2.8
1	G	248	ILE	2.7
1	B	257	GLN	2.7
1	B	251	GLU	2.7
1	E	252	THR	2.6
1	G	275	HIS	2.6
1	H	374	VAL	2.6
1	G	126	ARG	2.6
1	G	268	GLN	2.6
1	B	298	GLY	2.6
1	C	266	GLU	2.6
1	B	267	GLY	2.6
1	B	255	ALA	2.4
1	H	25	VAL	2.4
1	G	73	LEU	2.3
1	G	137	TRP	2.3
1	B	17	GLY	2.3
1	B	249	SER	2.3
1	G	121	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	282	LEU	2.2
1	A	282	LEU	2.2
1	B	272	ALA	2.2
1	H	297	GLY	2.2
1	H	248	ILE	2.1
1	H	274	LEU	2.1
1	G	16	LEU	2.1
1	B	260	PHE	2.1
1	G	281	ASN	2.1
1	H	16	LEU	2.1
1	G	264	ASP	2.1
1	E	80	ILE	2.1
1	B	273	ALA	2.0
1	G	270	ARG	2.0
1	H	298	GLY	2.0
1	G	249	SER	2.0
1	B	271	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	FMN	B	401	31/31	0.87	0.35	83,94,106,116	31
2	FMN	G	401	31/31	0.90	0.26	109,119,144,146	31
2	FMN	H	401	31/31	0.90	0.28	93,100,103,105	31
5	CL	G	402	1/1	0.93	0.10	110,110,110,110	0
4	PO4	F	401	5/5	0.95	0.10	94,105,107,113	0
2	FMN	D	401	31/31	0.95	0.17	75,85,92,97	31

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	FMN	C	401	31/31	0.96	0.16	72,79,91,96	0
2	FMN	A	401	31/31	0.96	0.16	78,84,93,98	0
3	03S	C	402	5/5	0.97	0.18	75,77,79,81	5
3	03S	E	402	5/5	0.97	0.18	66,70,71,72	5
2	FMN	E	401	31/31	0.97	0.17	62,68,73,74	0
3	03S	B	402	5/5	0.97	0.24	87,93,97,110	5
5	CL	H	402	1/1	0.98	0.17	94,94,94,94	0
3	03S	A	402	5/5	0.99	0.15	79,86,93,97	5
3	03S	D	402	5/5	0.99	0.26	80,88,88,97	5

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.
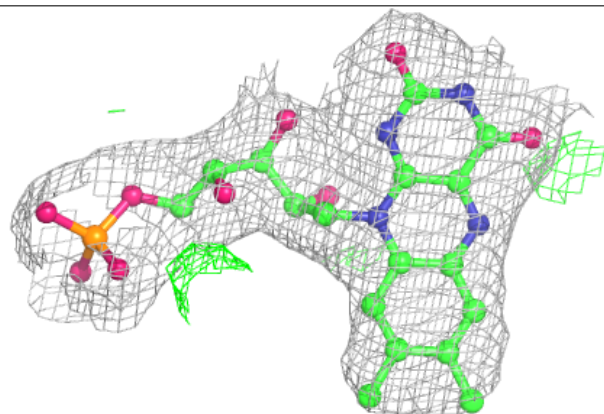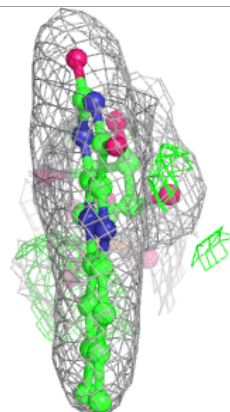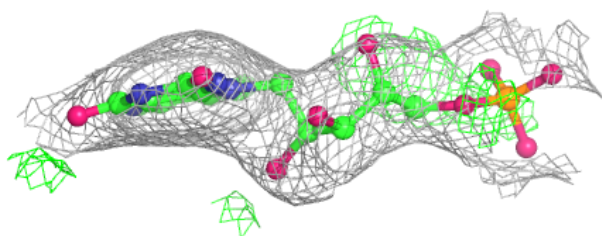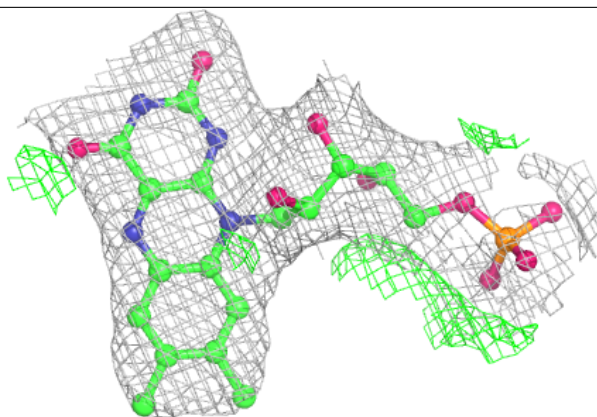

Electron density around FMN B 401:

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

Electron density around FMN G 401:

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

Electron density around FMN H 401:

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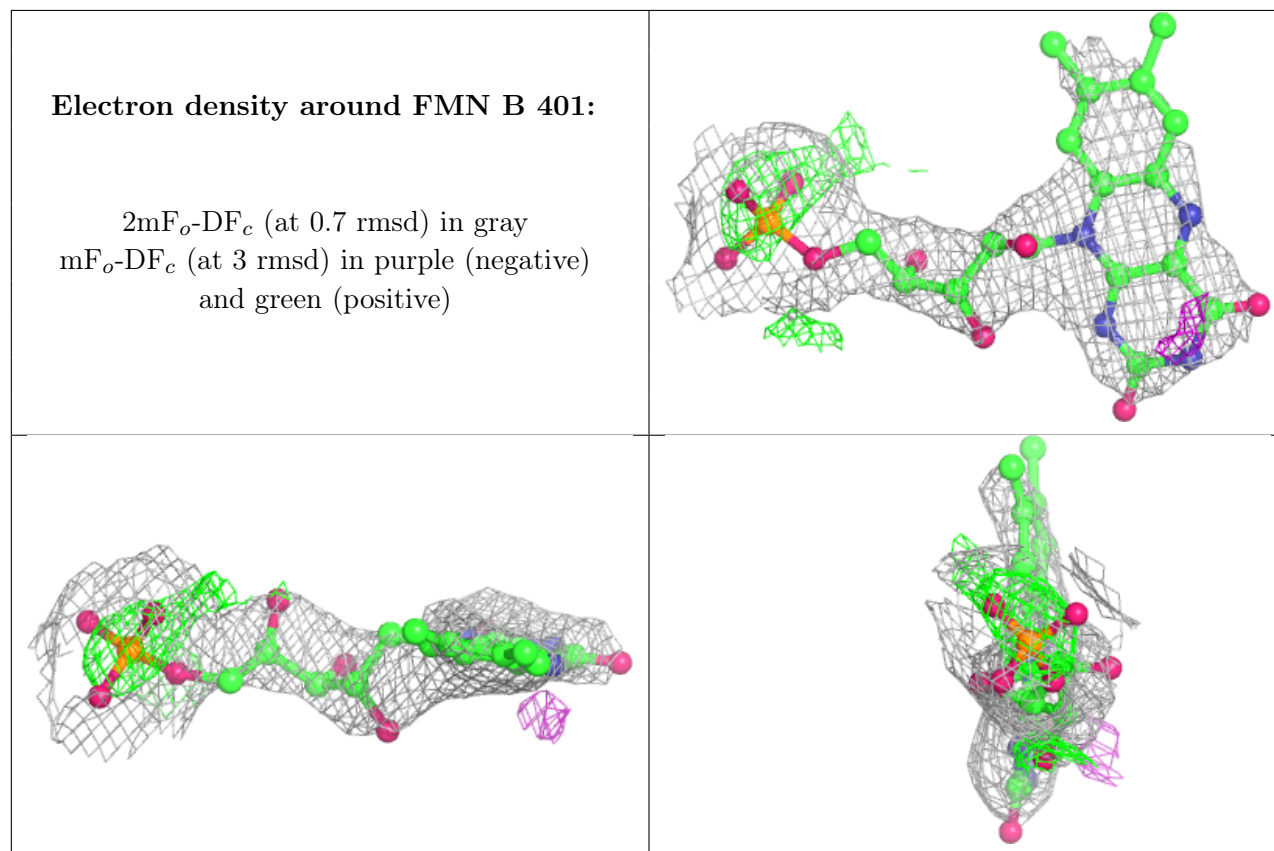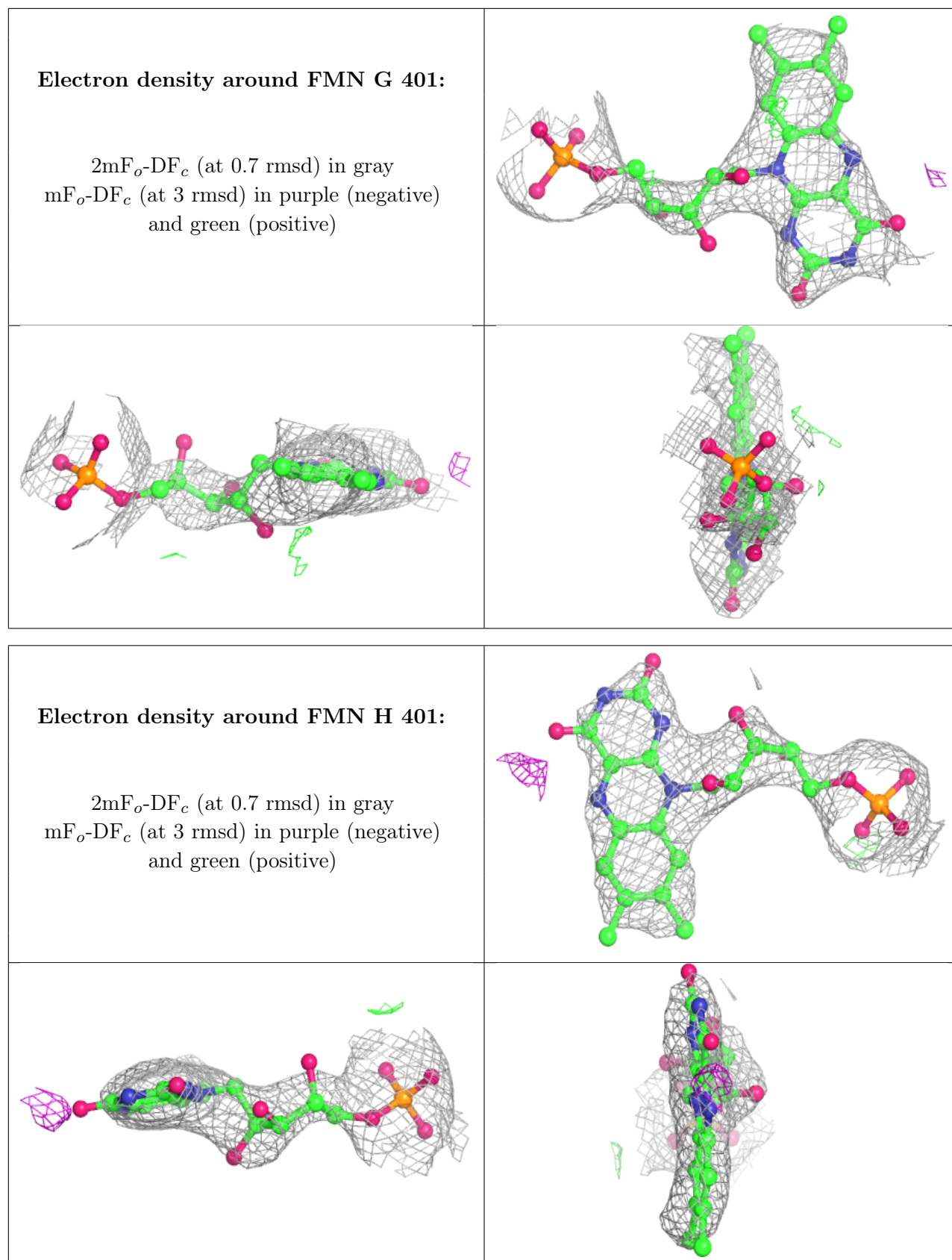
Electron density around FMN D 401:

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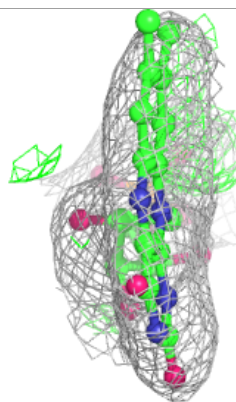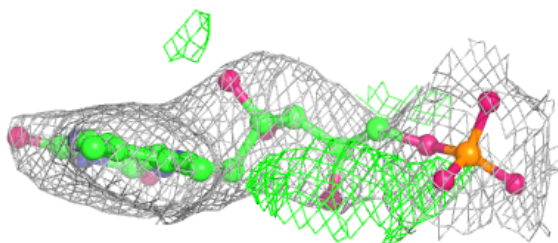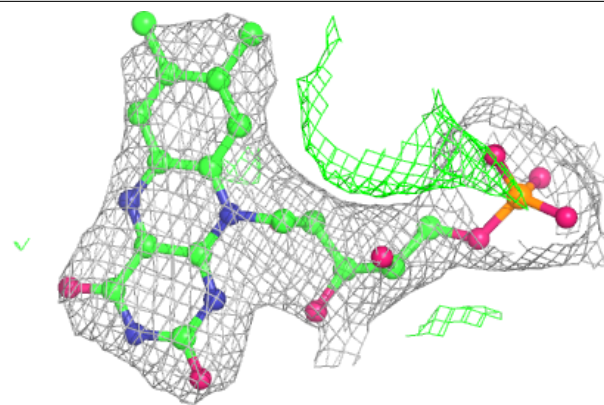
Electron density around FMN C 401:

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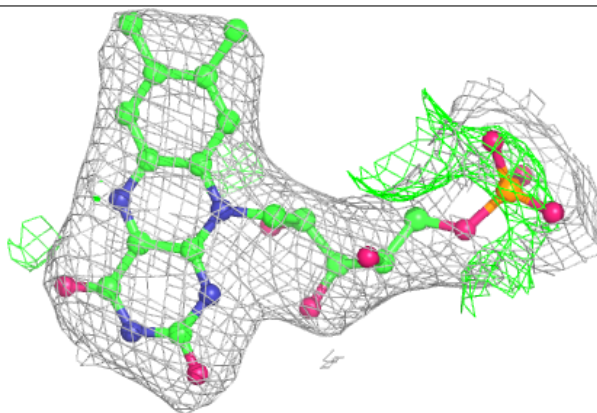$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
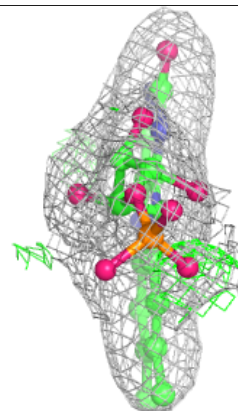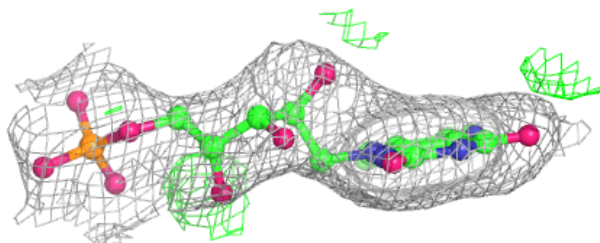
Electron density around FMN A 401:

$2mF_o$-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)
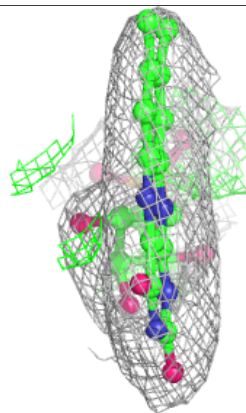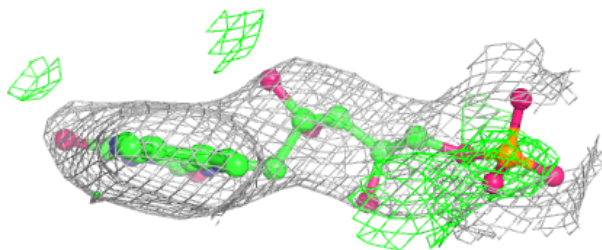
6.5 Other polymers (i)

There are no such residues in this entry.