



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 05:02 AM EDT

PDB ID : 7JYB
Title : Binary soak structure of alkanesulfonate monooxygenase MsuD from *Pseudomonas fluorescens* with FMN
Authors : Liew, J.J.M.; Dowling, D.P.; El Saudi, I.M.
Deposited on : 2020-08-30
Resolution : 2.76 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-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

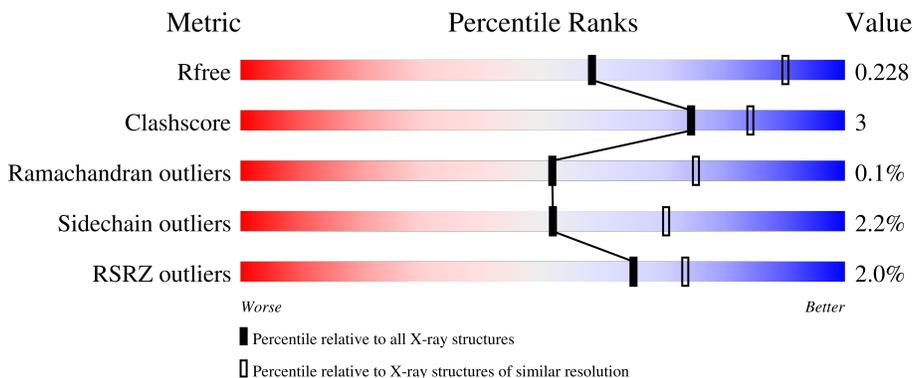
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	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 $\leq 5\%$. 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	404	79% 9% 12%
1	B	404	73% 8% 19%
1	C	404	80% 8% 12%
1	D	404	72% 8% 19%
1	E	404	79% 9% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	404	 <p>% 72% 8% 20%</p>
1	G	404	 <p>7% 70% 9% 20%</p>
1	H	404	 <p>2% 75% 10% 14%</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21381 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
			Total	C	N	O	S			
1	A	357	Total 2788	C 1771	N 496	O 517	S 4	0	1	0
1	B	327	Total 2540	C 1625	N 443	O 469	S 3	0	1	0
1	C	356	Total 2777	C 1764	N 493	O 516	S 4	0	0	0
1	D	326	Total 2525	C 1616	N 440	O 466	S 3	0	0	0
1	E	356	Total 2777	C 1764	N 493	O 516	S 4	0	0	0
1	F	323	Total 2513	C 1610	N 436	O 464	S 3	0	0	0
1	G	322	Total 2503	C 1604	N 435	O 461	S 3	0	0	0
1	H	348	Total 2706	C 1728	N 469	O 505	S 4	0	0	0

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

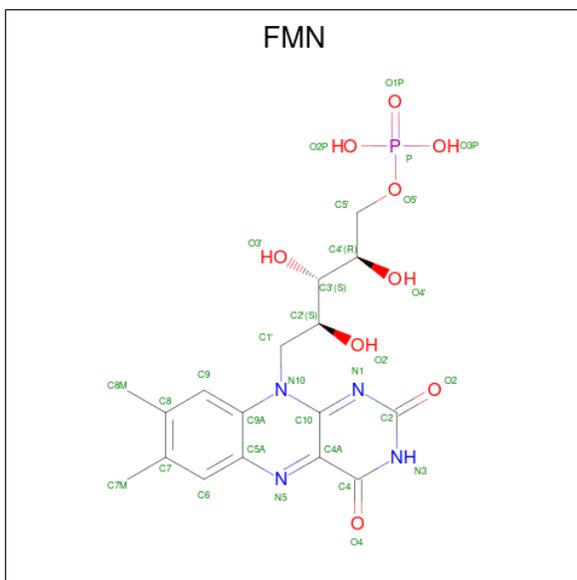
Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	GLY	-	expression tag	UNP Q3K9A1
G	-20	SER	-	expression tag	UNP Q3K9A1
G	-19	SER	-	expression tag	UNP Q3K9A1
G	-18	HIS	-	expression tag	UNP Q3K9A1
G	-17	HIS	-	expression tag	UNP Q3K9A1
G	-16	HIS	-	expression tag	UNP Q3K9A1
G	-15	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

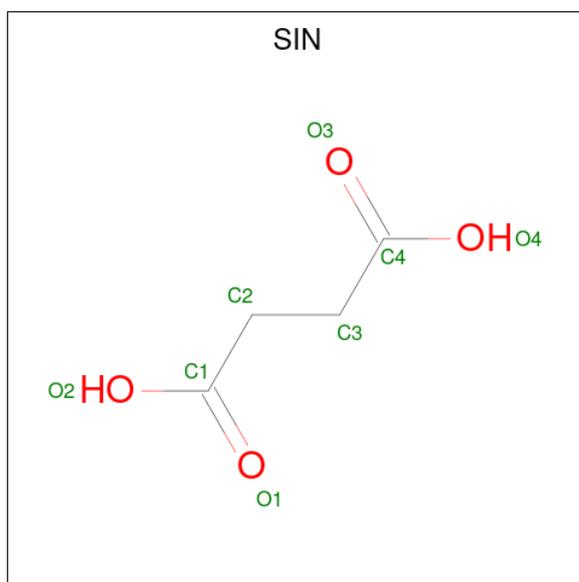
Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	MET	-	expression tag	UNP Q3K9A1
H	-1	ALA	-	expression tag	UNP Q3K9A1
H	0	SER	-	expression tag	UNP Q3K9A1

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



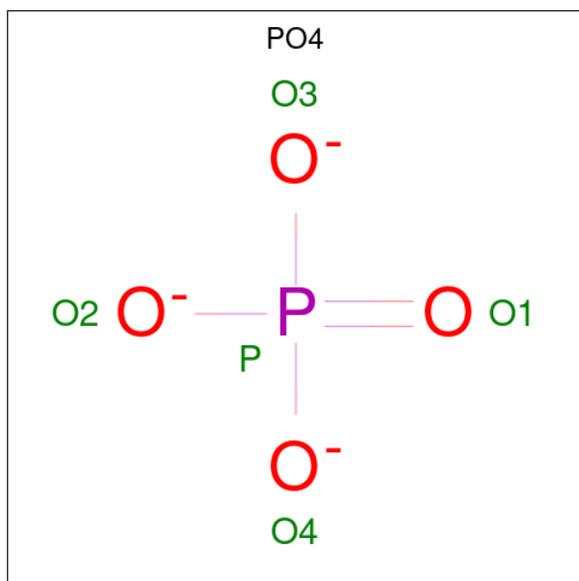
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).



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

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	6	Total O 6 6	0	0
5	C	8	Total O 8 8	0	0
5	D	1	Total O 1 1	0	0
5	E	15	Total O 15 15	0	0
5	F	3	Total O 3 3	0	0
5	G	3	Total O 3 3	0	0
5	H	2	Total O 2 2	0	0

PHE
GLY
GLU
MET
MET
ILE
ALA
ALA
ASN
ASP
VAL
VAL
LEU
PRO
ALA
LYS
ALA
ALA
ASN
ALA

● Molecule 1: Alkanesulfonate monooxygenase

Chain H:  2% 75% 10% 14%

MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
SER
SER
SER
GLY
LEU
VAL
PRO
ARG
GLY
SER
SER
HIS
MET
MET
ALA
S0
L7
G11
Y15
Q20
V25
I47
I59
R77
I80
V85
L96
S97
R100
V105
S122
H123
Y127
D131
K135

E149
K154
I224
H227
R231
E235
K243
L244
L245
E246
H247
I248
S249
E250
E251
T252
R262
PHE
ASP
SER
GLU
GLY
GLN
ARG
ARG
MET
ALA
ALA
LEU
HIS
ASP
GLY
ARG
ARG
ASP
N281
W289
A290
G291
V292
E296
GLY
GLY
S299
A302
P307
I322

E334
A340
F344
E349
F350
L354
ALA
GLY
ARG
GLY
VAL
THR
N361
L362
F365
F366
G367
E368
N369
I370
A371
N372
D373
VAL
LEU
LEU
PRO
ALA
ALA
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	94.20Å 214.38Å 95.20Å 90.00° 119.13° 90.00°	Depositor
Resolution (Å)	83.16 – 2.76 83.16 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.4 (83.16-2.76) 98.4 (83.16-2.76)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.180 , 0.224 0.184 , 0.228	Depositor DCC
R_{free} test set	4179 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-l,k,h 0.000 for l,k,-h-l 0.011 for h,-k,-h-l 0.008 for -h-l,-k,l 0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21381	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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: PO4, FMN, 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	0.25	0/2860	0.44	0/3886
1	B	0.25	0/2608	0.44	0/3551
1	C	0.25	0/2845	0.44	0/3866
1	D	0.25	0/2589	0.44	0/3525
1	E	0.26	0/2845	0.45	0/3866
1	F	0.25	0/2576	0.44	0/3507
1	G	0.24	0/2566	0.43	0/3495
1	H	0.25	0/2771	0.44	0/3768
All	All	0.25	0/21660	0.44	0/29464

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 [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	2788	0	2745	20	0
1	B	2540	0	2505	19	0
1	C	2777	0	2735	15	0
1	D	2525	0	2494	17	0
1	E	2777	0	2735	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2513	0	2482	16	0
1	G	2503	0	2468	21	0
1	H	2706	0	2662	25	0
2	A	31	0	19	0	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
3	E	8	0	4	0	0
4	F	5	0	0	0	0
4	H	5	0	0	1	0
5	A	10	0	0	0	0
5	B	6	0	0	0	0
5	C	8	0	0	0	0
5	D	1	0	0	0	0
5	E	15	0	0	0	0
5	F	3	0	0	0	0
5	G	3	0	0	0	0
5	H	2	0	0	0	0
All	All	21381	0	20944	137	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.

The worst 5 of 137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:PHE:HD2	1:E:268:GLN:HG2	1.50	0.76
1:E:85:VAL:HG21	1:F:80:ILE:HD13	1.72	0.69
1:B:227[A]:HIS:HD2	1:B:299:SER:HB3	1.57	0.69
1:E:80:ILE:HD12	1:F:85:VAL:HG21	1.74	0.69
1:C:131:ASP:OD1	1:C:135:LYS:NZ	2.26	0.64

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	356/404 (88%)	344 (97%)	12 (3%)	0	100	100
1	B	324/404 (80%)	314 (97%)	10 (3%)	0	100	100
1	C	354/404 (88%)	344 (97%)	9 (2%)	1 (0%)	41	60
1	D	322/404 (80%)	311 (97%)	10 (3%)	1 (0%)	41	60
1	E	354/404 (88%)	345 (98%)	9 (2%)	0	100	100
1	F	317/404 (78%)	310 (98%)	7 (2%)	0	100	100
1	G	316/404 (78%)	309 (98%)	7 (2%)	0	100	100
1	H	340/404 (84%)	326 (96%)	14 (4%)	0	100	100
All	All	2683/3232 (83%)	2603 (97%)	78 (3%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	297	GLY
1	C	295	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/321 (89%)	278 (97%)	8 (3%)	43	63
1	B	261/321 (81%)	255 (98%)	6 (2%)	50	69
1	C	285/321 (89%)	278 (98%)	7 (2%)	47	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	259/321 (81%)	254 (98%)	5 (2%)	57	73
1	E	285/321 (89%)	281 (99%)	4 (1%)	67	79
1	F	259/321 (81%)	251 (97%)	8 (3%)	40	60
1	G	257/321 (80%)	252 (98%)	5 (2%)	57	73
1	H	280/321 (87%)	274 (98%)	6 (2%)	53	71
All	All	2172/2568 (85%)	2123 (98%)	49 (2%)	52	69

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	254	GLU
1	F	205	LYS
1	E	354	LEU
1	F	124	SER
1	F	315	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	308	GLN
1	C	281	ASN
1	E	247	HIS
1	H	123	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	B	401	-	33,33,33	1.06	1 (3%)	48,50,50	1.29	8 (16%)
2	FMN	G	401	-	33,33,33	1.06	2 (6%)	48,50,50	1.31	8 (16%)
2	FMN	A	401	-	33,33,33	1.06	2 (6%)	48,50,50	1.26	8 (16%)
4	PO4	H	401	-	4,4,4	0.89	0	6,6,6	0.48	0
2	FMN	D	401	-	33,33,33	1.07	1 (3%)	48,50,50	1.29	8 (16%)
2	FMN	E	401	-	33,33,33	1.07	2 (6%)	48,50,50	1.29	8 (16%)
3	SIN	E	402	-	7,7,7	1.02	0	8,8,8	1.71	2 (25%)
2	FMN	C	401	-	33,33,33	1.07	1 (3%)	48,50,50	1.31	9 (18%)
4	PO4	F	501	-	4,4,4	0.90	0	6,6,6	0.44	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
2	FMN	B	401	-	-	8/18/18/18	0/3/3/3
2	FMN	G	401	-	-	7/18/18/18	0/3/3/3
2	FMN	A	401	-	-	8/18/18/18	0/3/3/3
2	FMN	D	401	-	-	5/18/18/18	0/3/3/3
2	FMN	E	401	-	-	9/18/18/18	0/3/3/3
3	SIN	E	402	-	-	1/5/5/5	-
2	FMN	C	401	-	-	9/18/18/18	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	FMN	C5A-N5	-2.65	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	FMN	C5A-N5	-2.64	1.34	1.39
2	A	401	FMN	C5A-N5	-2.63	1.34	1.39
2	D	401	FMN	C5A-N5	-2.62	1.34	1.39
2	C	401	FMN	C5A-N5	-2.59	1.34	1.39

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FMN	C4-C4A-N5	2.96	122.45	118.23
2	D	401	FMN	C4-C4A-N5	2.93	122.39	118.23
2	C	401	FMN	C4-C4A-N5	2.87	122.32	118.23
2	G	401	FMN	C4A-C10-N1	-2.81	118.21	124.73
2	E	401	FMN	C4-C4A-N5	2.69	122.06	118.23

There are no chirality outliers.

5 of 47 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	B	401	FMN	N10-C1'-C2'-O2'
2	B	401	FMN	N10-C1'-C2'-C3'
2	B	401	FMN	C2'-C3'-C4'-O4'

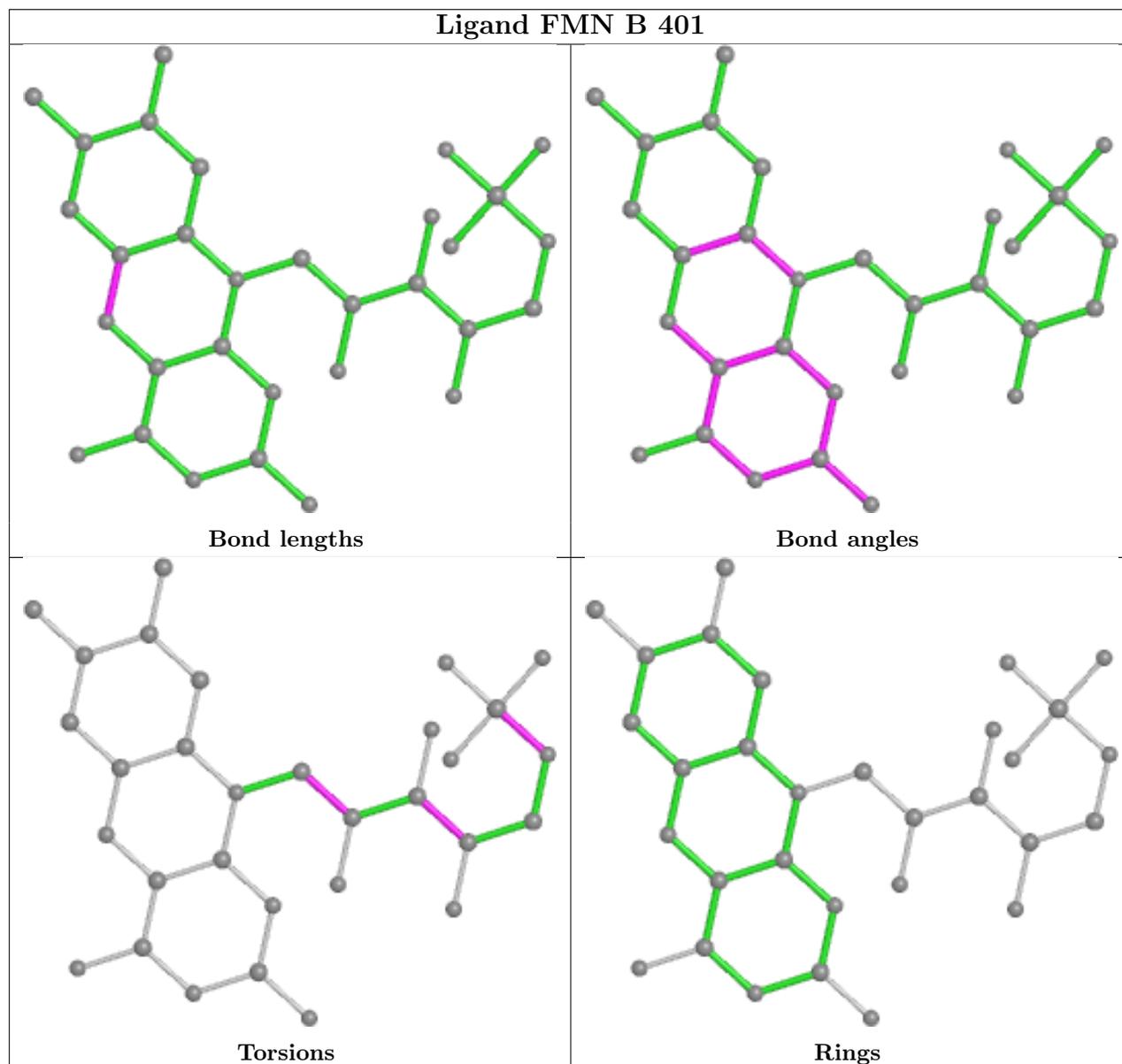
There are no ring outliers.

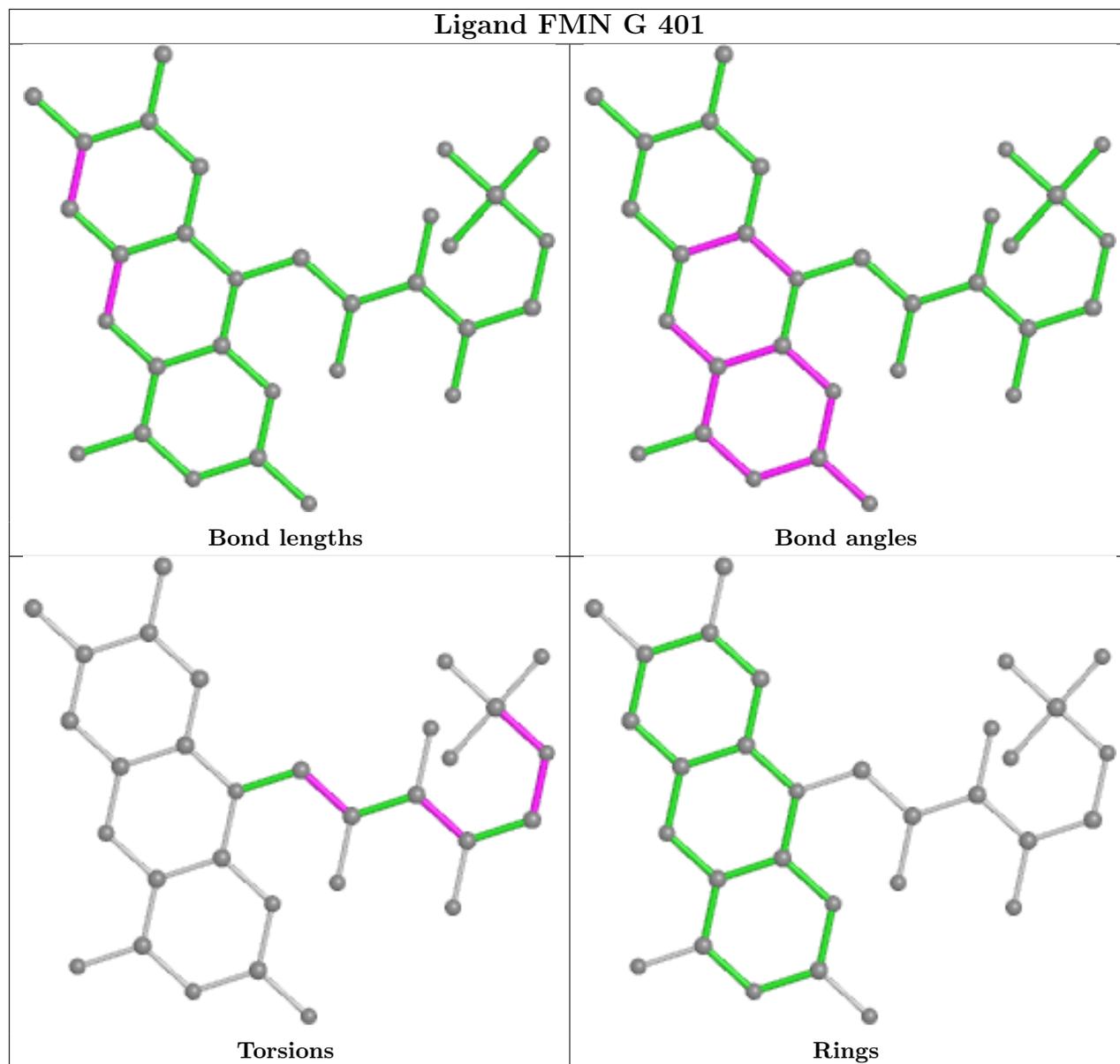
4 monomers are involved in 4 short contacts:

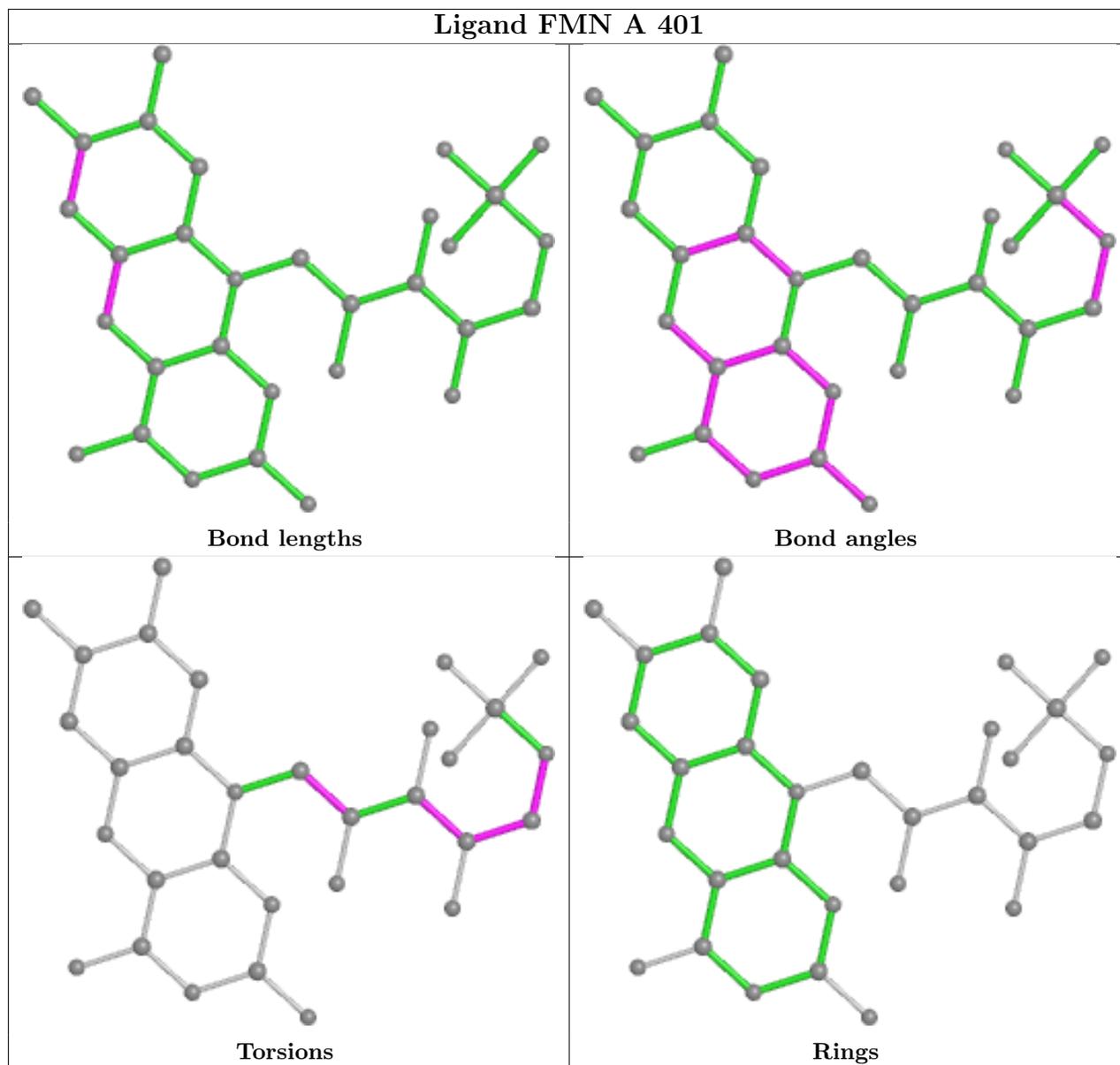
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FMN	1	0
2	G	401	FMN	1	0
4	H	401	PO4	1	0
2	E	401	FMN	1	0

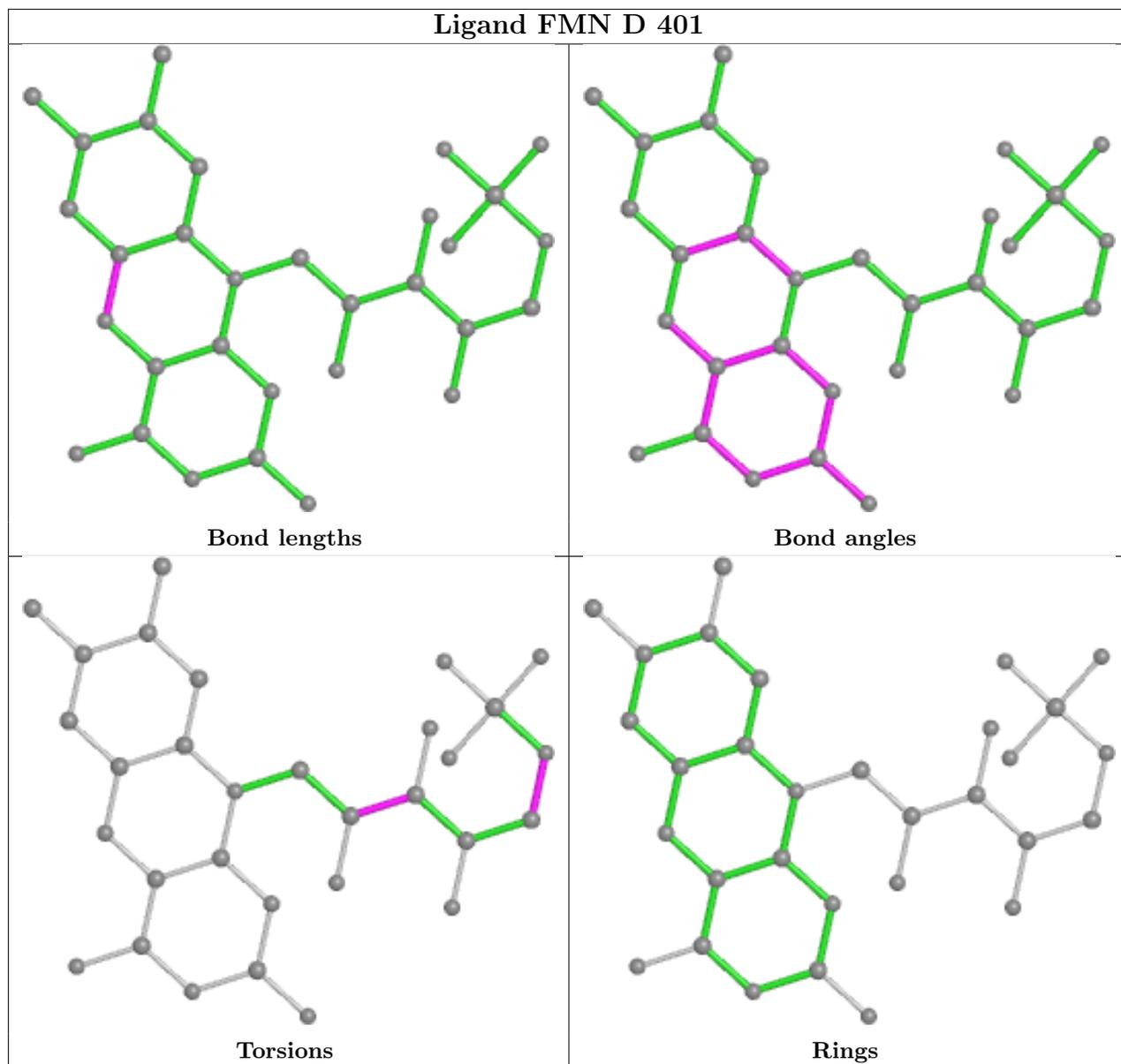
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

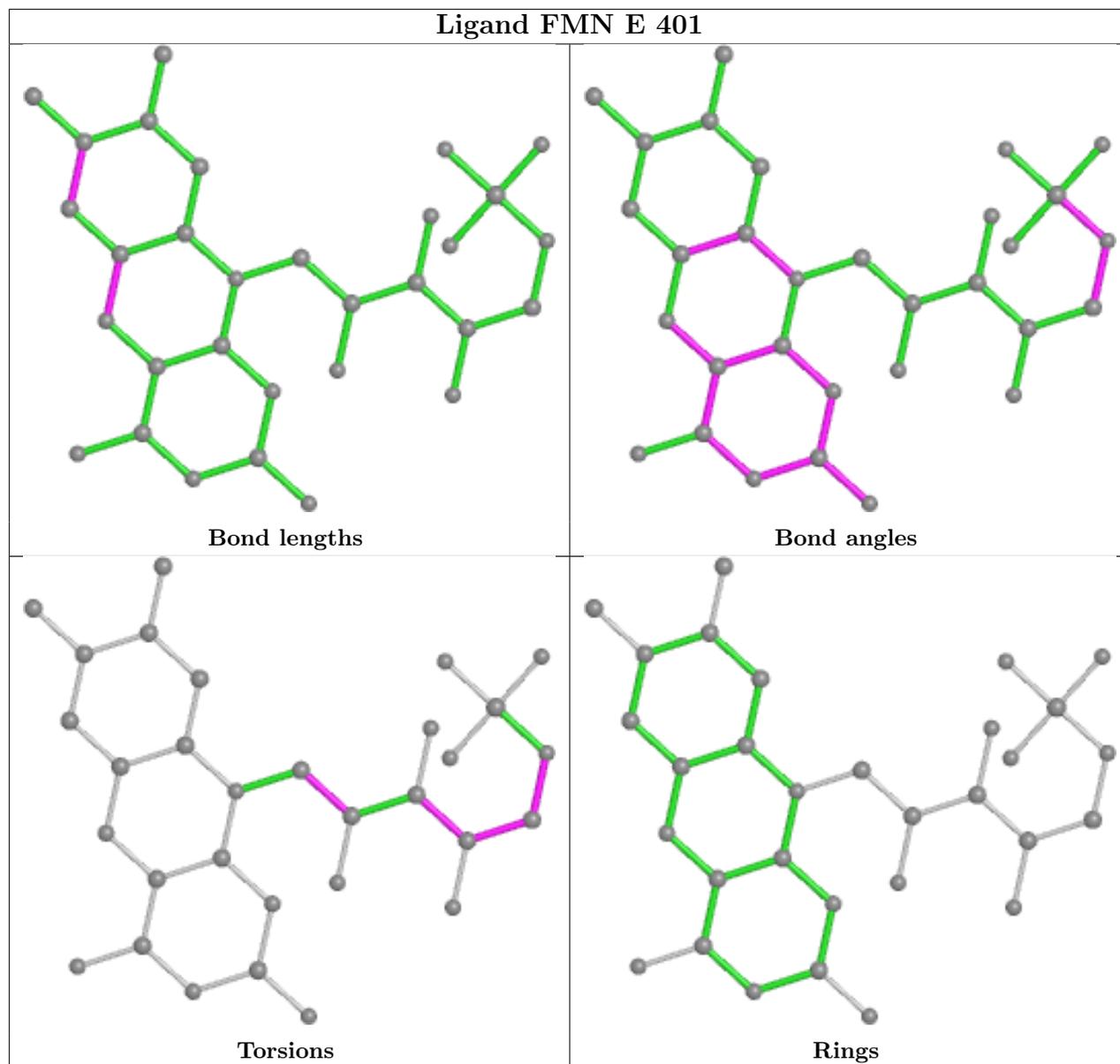
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

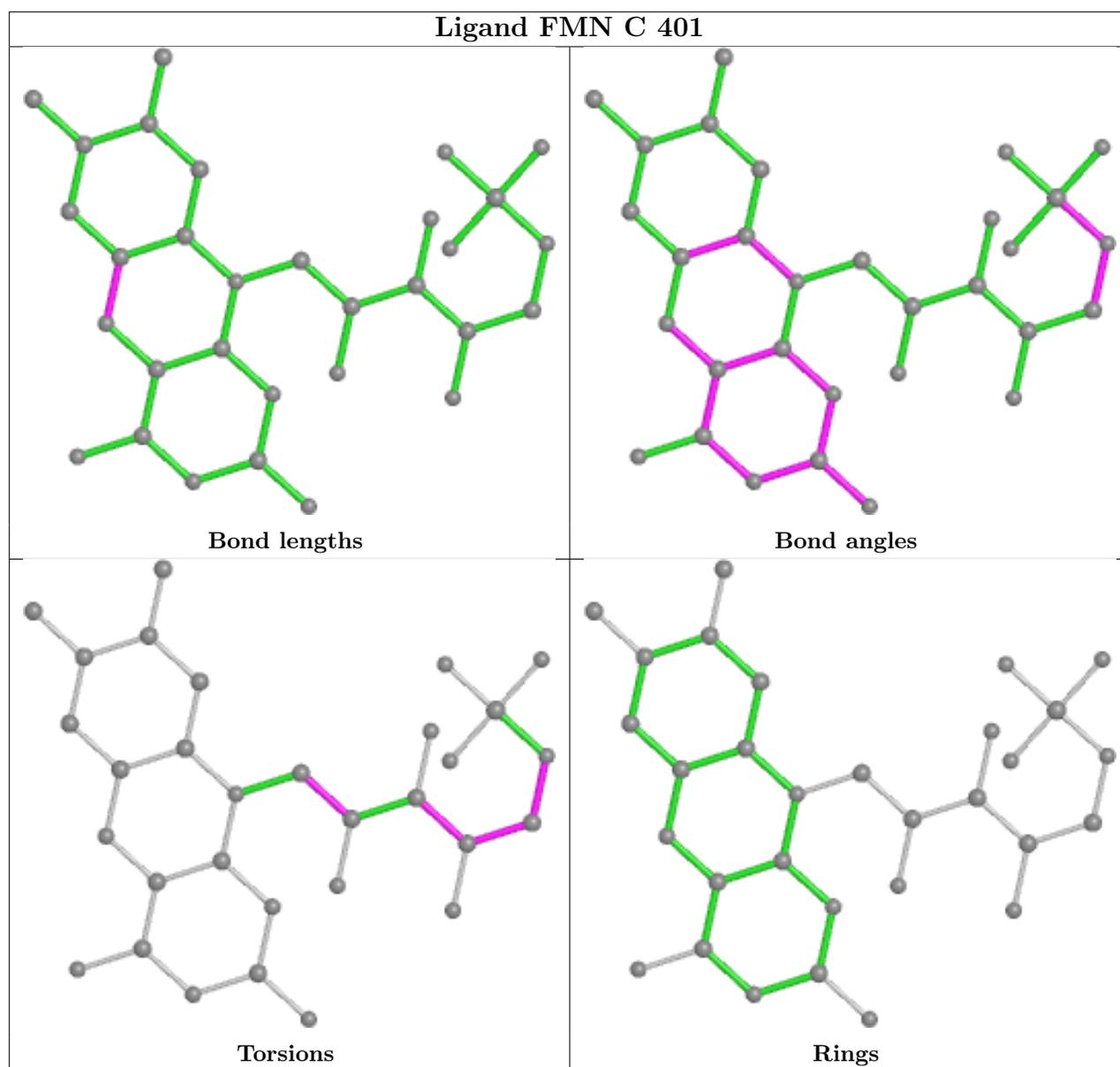












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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(Å ²)	Q<0.9
1	A	357/404 (88%)	0.06	6 (1%) 70 78	44, 72, 137, 202	0
1	B	327/404 (80%)	-0.04	1 (0%) 94 96	40, 73, 111, 164	0
1	C	356/404 (88%)	0.09	5 (1%) 75 82	43, 68, 125, 170	0
1	D	326/404 (80%)	0.04	2 (0%) 89 92	45, 73, 120, 142	0
1	E	356/404 (88%)	-0.06	0 100 100	43, 59, 110, 156	0
1	F	323/404 (79%)	-0.08	3 (0%) 84 89	44, 68, 108, 206	0
1	G	322/404 (79%)	0.39	27 (8%) 11 13	54, 96, 132, 170	0
1	H	348/404 (86%)	0.09	10 (2%) 51 61	50, 75, 133, 171	0
All	All	2715/3232 (84%)	0.06	54 (1%) 65 73	40, 72, 127, 206	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	126	ARG	5.9
1	C	254	GLU	5.3
1	H	372	ASN	5.1
1	B	17	GLY	4.7
1	G	122	SER	4.7

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](#)

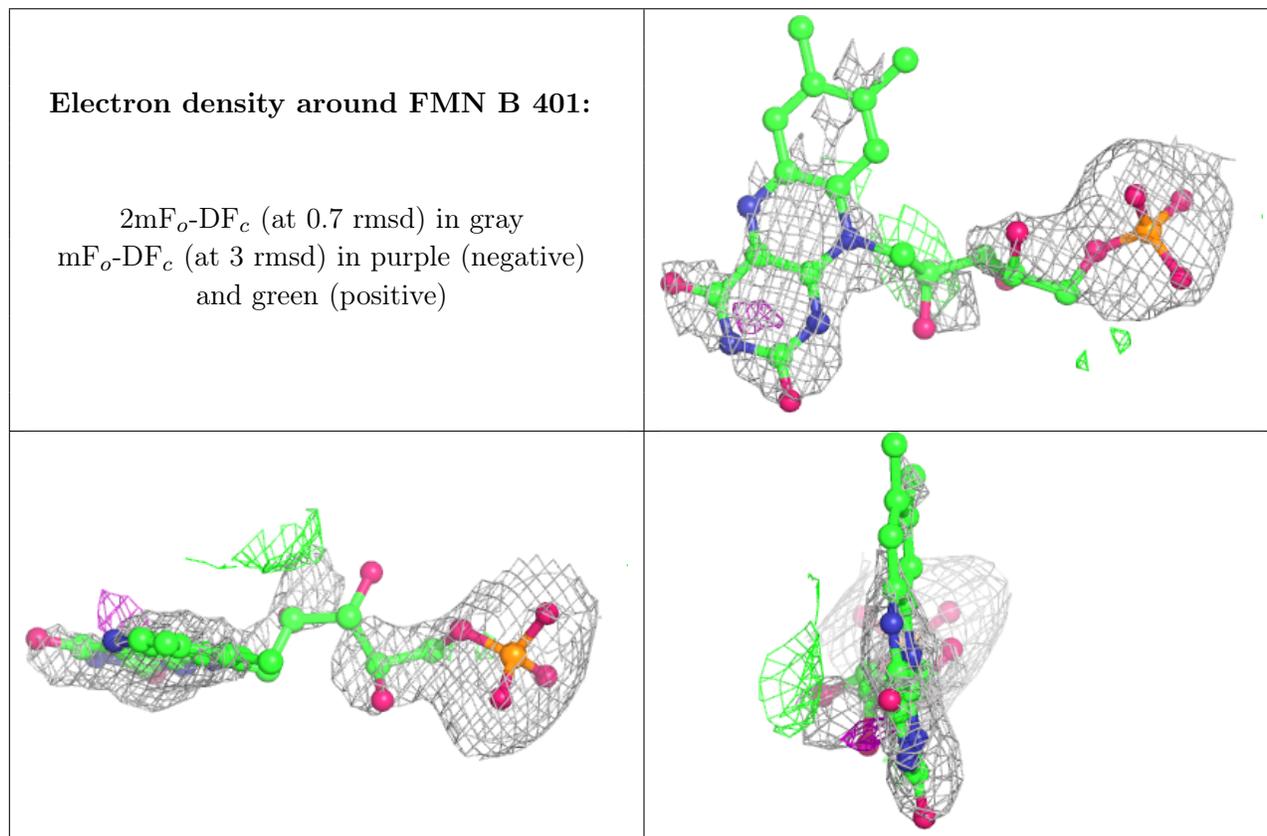
There are no monosaccharides in this entry.

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.

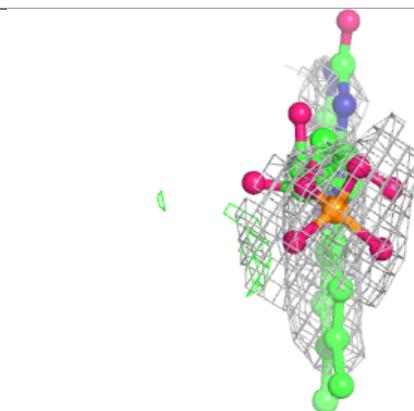
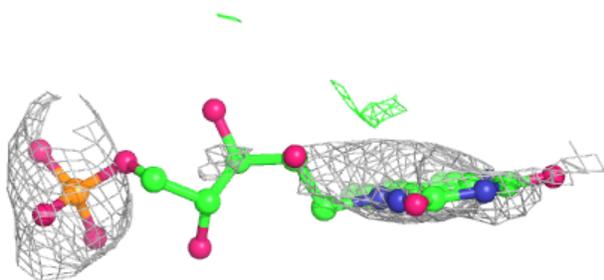
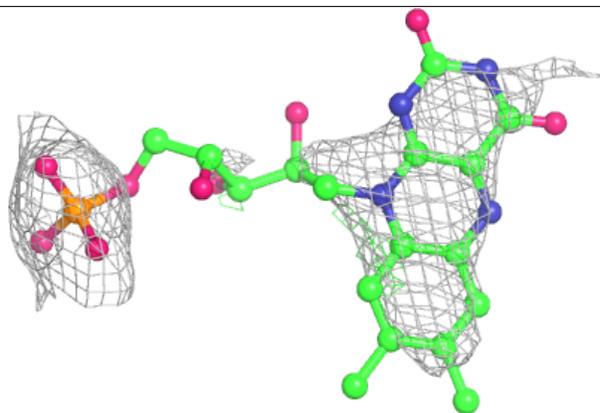
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	B	401	31/31	0.82	0.41	77,95,104,110	31
2	FMN	G	401	31/31	0.84	0.42	90,105,118,127	31
2	FMN	D	401	31/31	0.90	0.24	75,98,109,113	0
3	SIN	E	402	8/8	0.90	0.33	80,87,99,102	8
4	PO4	H	401	5/5	0.92	0.15	78,95,106,113	0
2	FMN	A	401	31/31	0.94	0.15	61,78,94,97	0
2	FMN	E	401	31/31	0.95	0.16	53,66,76,85	0
2	FMN	C	401	31/31	0.95	0.18	69,80,92,94	0
4	PO4	F	501	5/5	0.96	0.14	64,72,81,89	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.

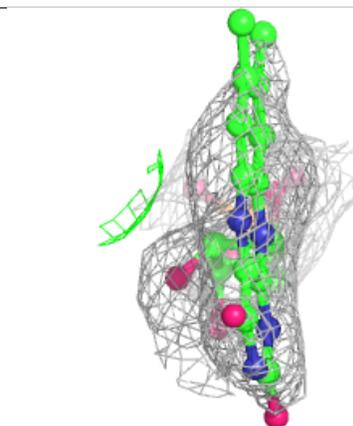
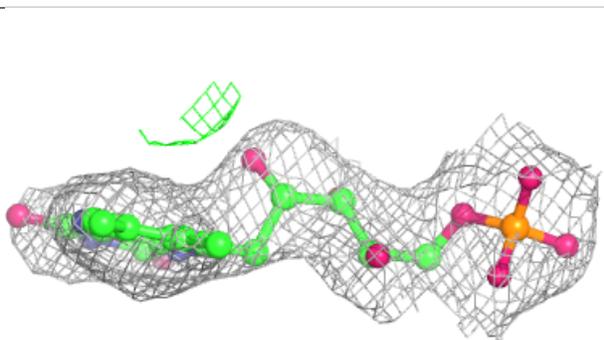
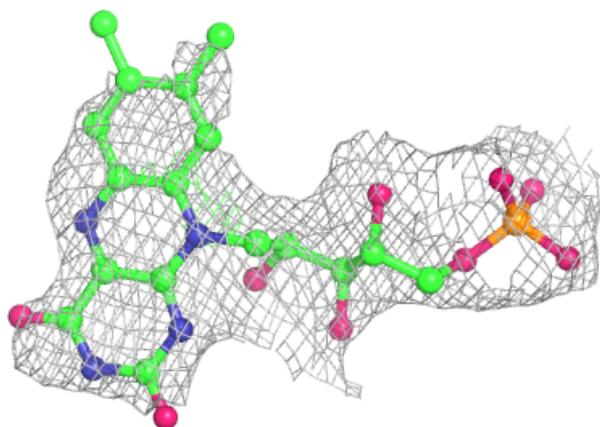


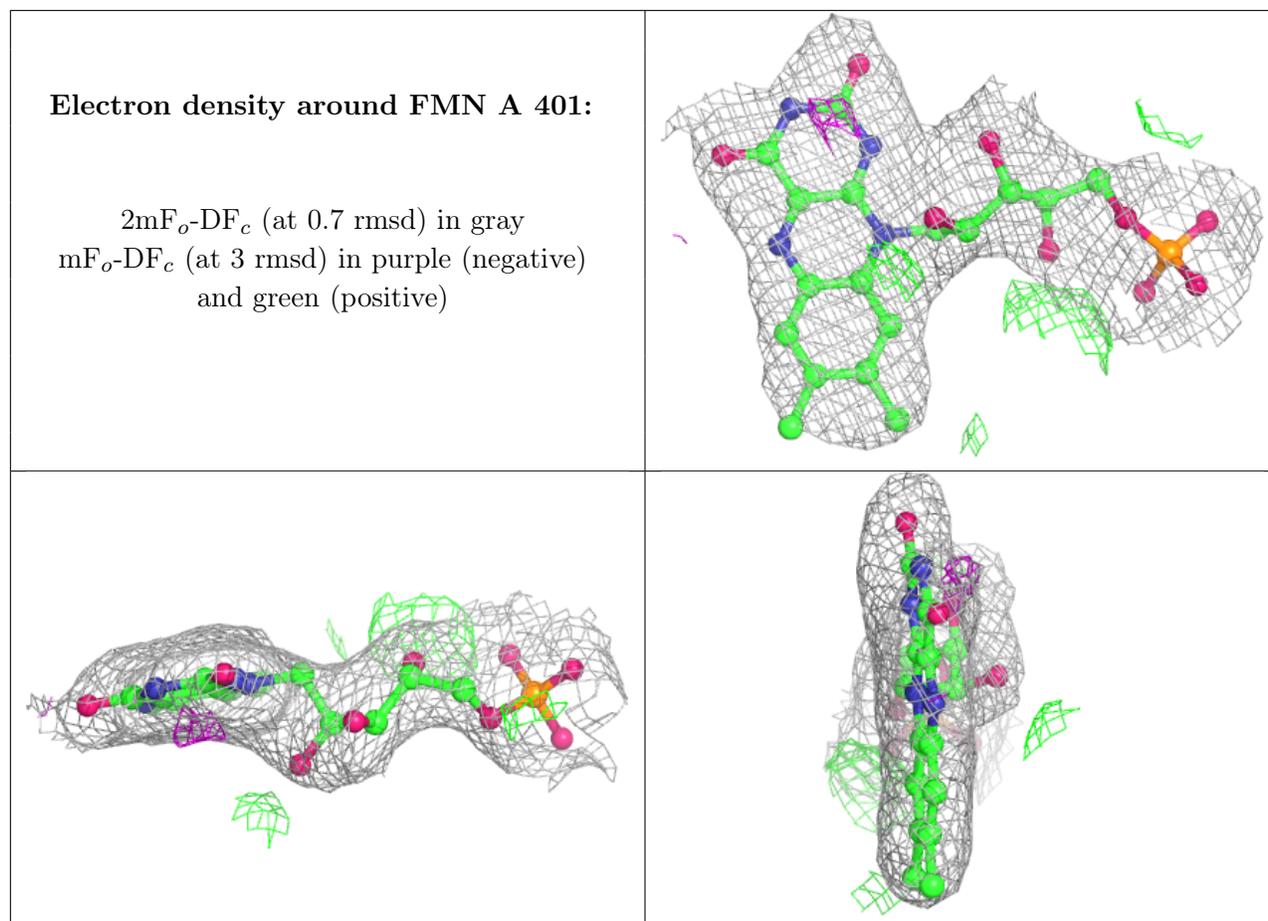
Electron density around FMN G 401:

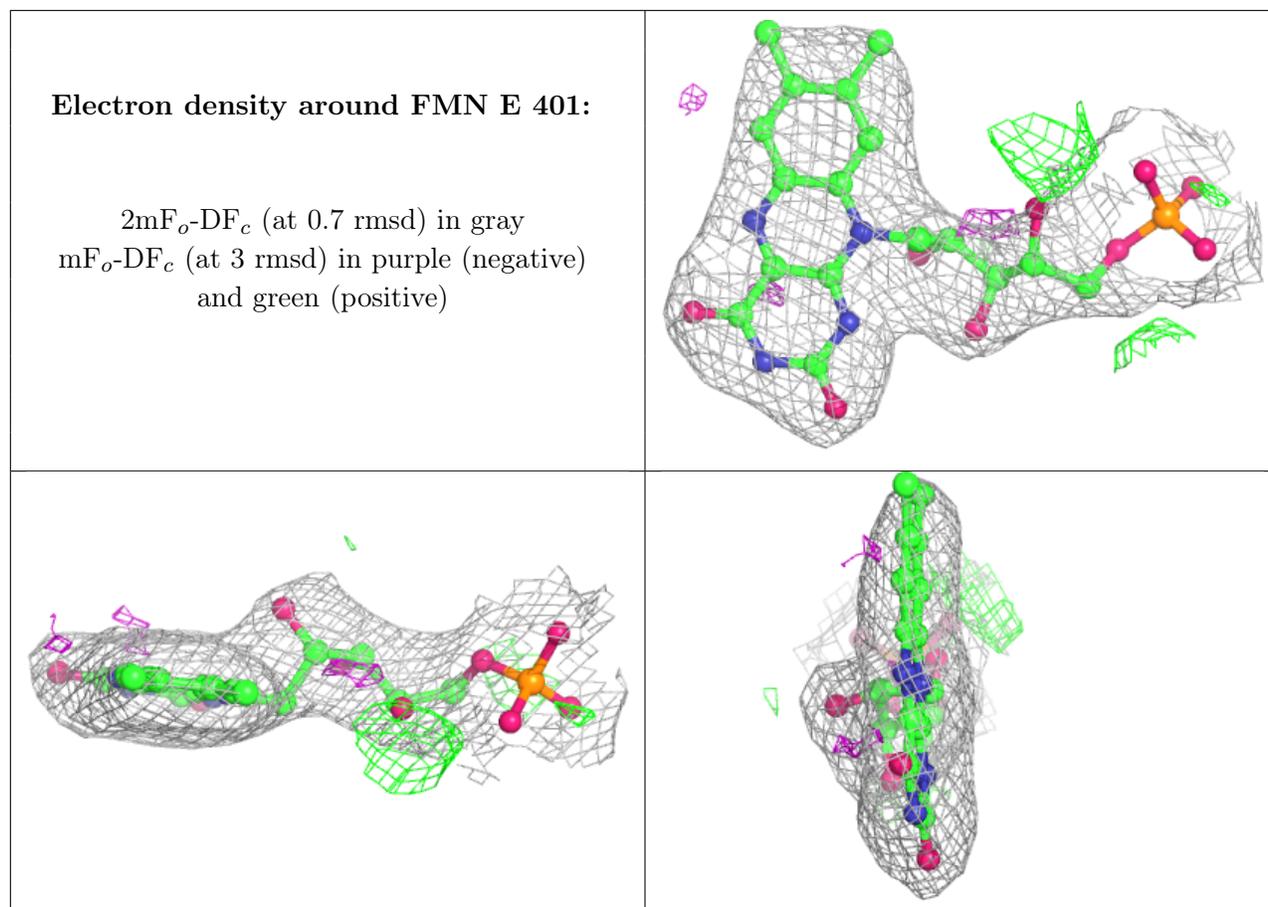
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

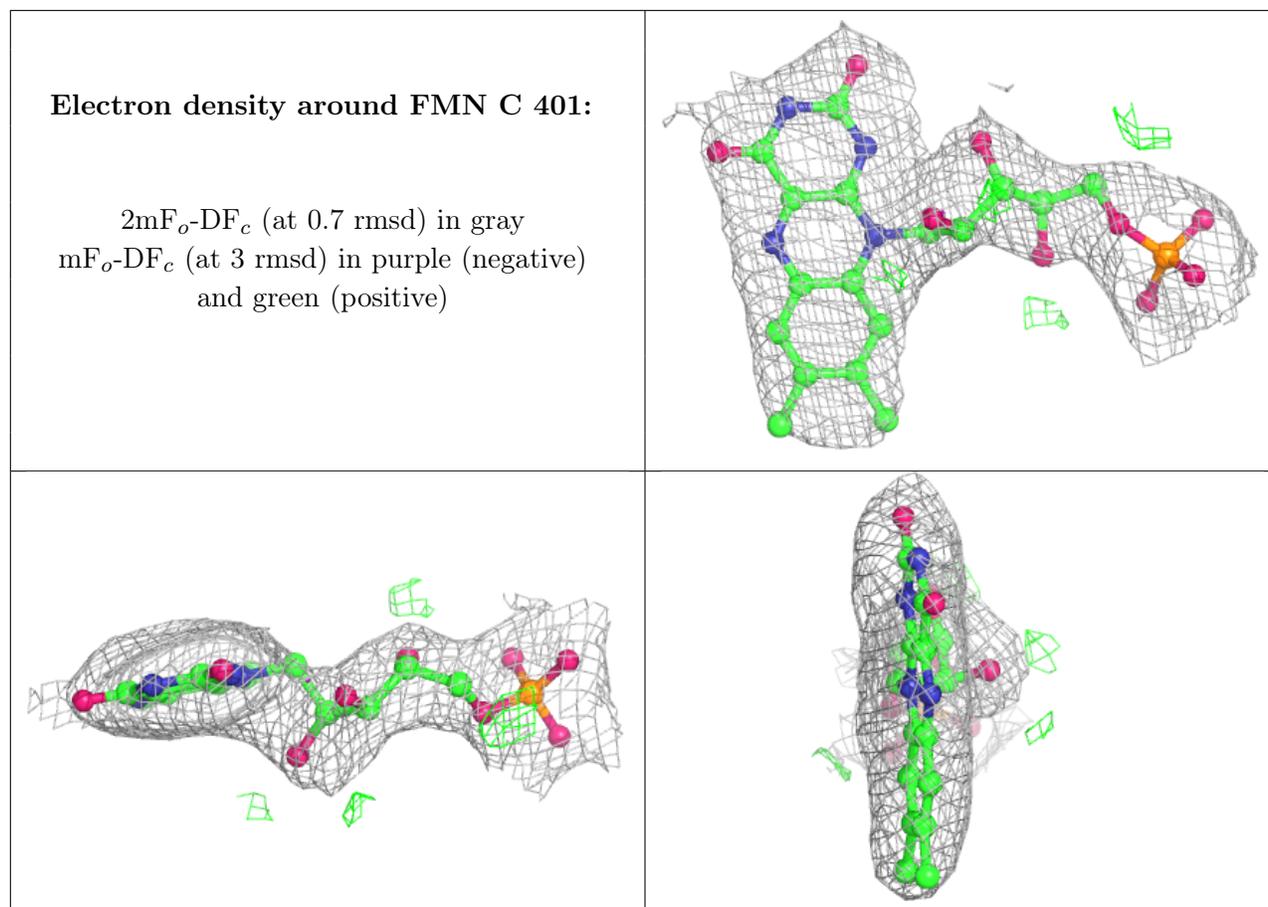
**Electron density around FMN D 401:**

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









6.5 Other polymers [i](#)

There are no such residues in this entry.