



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:53 pm BST

PDB ID : 5EBU  
Title : Aerococcus viridans L-lactate oxidase Y215F mutant  
Authors : Rainer, D.; Nidetzky, B.; Wilson, D.K.  
Deposited on : 2015-10-19  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

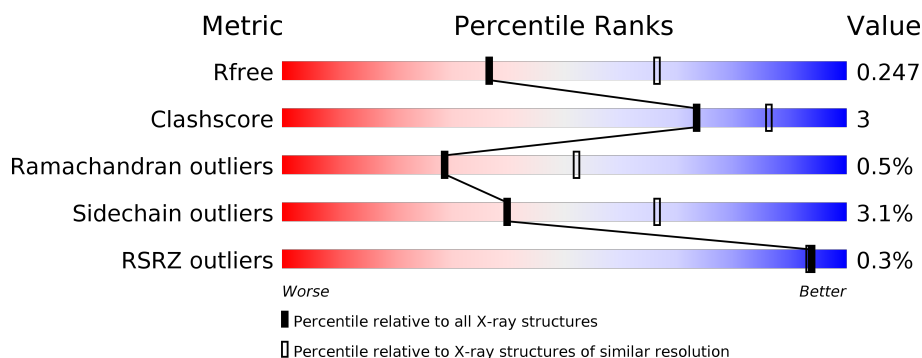
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	374	<div> <div>88%</div> <div>10% ..</div> </div>
1	B	374	<div> <div>91%</div> <div>7% ..</div> </div>
1	C	374	<div> <div>89%</div> <div>8% ..</div> </div>
1	D	374	<div> <div>82%</div> <div>12% 6%</div> </div>
1	E	374	<div> <div>88%</div> <div>9% ..</div> </div>
1	F	374	<div> <div>2%</div> <div>85%</div> <div>12% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	374	<div><div></div><div>89%</div><div>9% ..</div></div>
1	H	374	<div><div></div><div>85%</div><div>8% • 6%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22897 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 L-lactate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2822	1785	490	540	7			
1	B	367	Total	C	N	O	S	0	0	0
			2822	1785	490	540	7			
1	C	367	Total	C	N	O	S	0	0	0
			2822	1785	490	540	7			
1	D	353	Total	C	N	O	S	0	0	0
			2711	1716	468	521	6			
1	E	367	Total	C	N	O	S	0	0	0
			2822	1785	490	540	7			
1	F	367	Total	C	N	O	S	0	0	0
			2822	1785	490	540	7			
1	G	367	Total	C	N	O	S	0	0	0
			2822	1785	490	540	7			
1	H	350	Total	C	N	O	S	0	0	0
			2690	1703	465	516	6			

There are 40 discrepancies between the modelled and reference sequences:

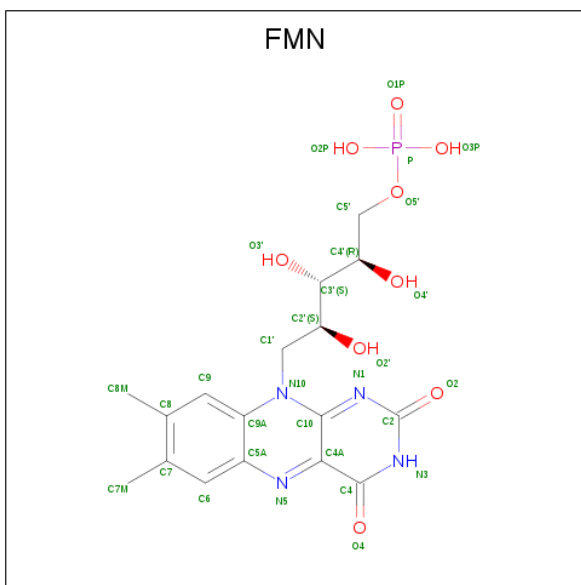
Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	THR	engineered mutation	UNP Q44467
A	163	GLY	SER	engineered mutation	UNP Q44467
A	215	PHE	TYR	engineered mutation	UNP Q44467
A	232	ALA	GLY	engineered mutation	UNP Q44467
A	255	ALA	ARG	engineered mutation	UNP Q44467
B	102	ALA	THR	engineered mutation	UNP Q44467
B	163	GLY	SER	engineered mutation	UNP Q44467
B	215	PHE	TYR	engineered mutation	UNP Q44467
B	232	ALA	GLY	engineered mutation	UNP Q44467
B	255	ALA	ARG	engineered mutation	UNP Q44467
C	102	ALA	THR	engineered mutation	UNP Q44467
C	163	GLY	SER	engineered mutation	UNP Q44467
C	215	PHE	TYR	engineered mutation	UNP Q44467

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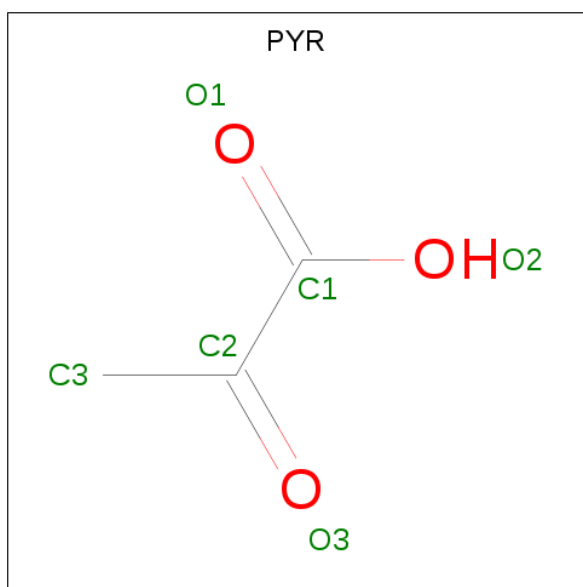
Chain	Residue	Modelled	Actual	Comment	Reference
C	232	ALA	GLY	engineered mutation	UNP Q44467
C	255	ALA	ARG	engineered mutation	UNP Q44467
D	102	ALA	THR	engineered mutation	UNP Q44467
D	163	GLY	SER	engineered mutation	UNP Q44467
D	215	PHE	TYR	engineered mutation	UNP Q44467
D	232	ALA	GLY	engineered mutation	UNP Q44467
D	255	ALA	ARG	engineered mutation	UNP Q44467
E	102	ALA	THR	engineered mutation	UNP Q44467
E	163	GLY	SER	engineered mutation	UNP Q44467
E	215	PHE	TYR	engineered mutation	UNP Q44467
E	232	ALA	GLY	engineered mutation	UNP Q44467
E	255	ALA	ARG	engineered mutation	UNP Q44467
F	102	ALA	THR	engineered mutation	UNP Q44467
F	163	GLY	SER	engineered mutation	UNP Q44467
F	215	PHE	TYR	engineered mutation	UNP Q44467
F	232	ALA	GLY	engineered mutation	UNP Q44467
F	255	ALA	ARG	engineered mutation	UNP Q44467
G	102	ALA	THR	engineered mutation	UNP Q44467
G	163	GLY	SER	engineered mutation	UNP Q44467
G	215	PHE	TYR	engineered mutation	UNP Q44467
G	232	ALA	GLY	engineered mutation	UNP Q44467
G	255	ALA	ARG	engineered mutation	UNP Q44467
H	102	ALA	THR	engineered mutation	UNP Q44467
H	163	GLY	SER	engineered mutation	UNP Q44467
H	215	PHE	TYR	engineered mutation	UNP Q44467
H	232	ALA	GLY	engineered mutation	UNP Q44467
H	255	ALA	ARG	engineered mutation	UNP Q44467

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

- Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	47	Total	O	0	0
			47	47		
4	C	25	Total	O	0	0
			25	25		
4	D	23	Total	O	0	0
			23	23		

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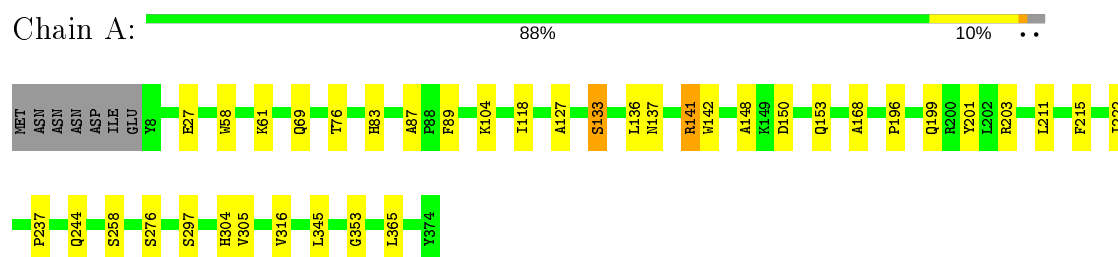
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	36	Total 36	O 36	0	0
4	F	36	Total 36	O 36	0	0
4	G	39	Total 39	O 39	0	0
4	H	30	Total 30	O 30	0	0



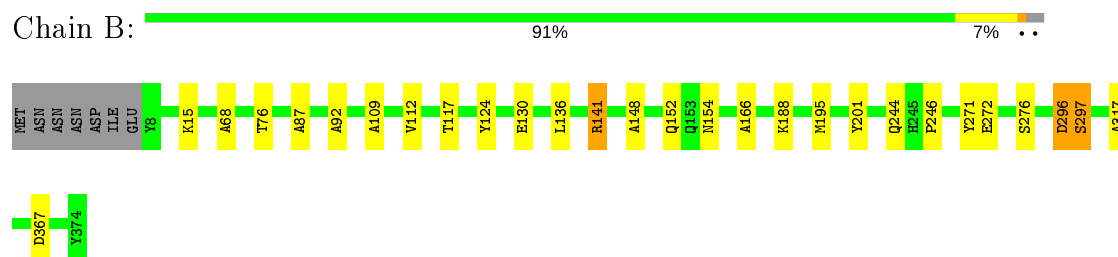
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

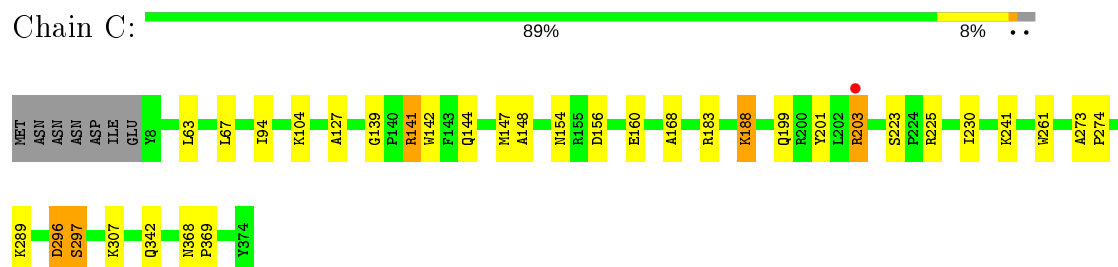
- Molecule 1: L-lactate oxidase



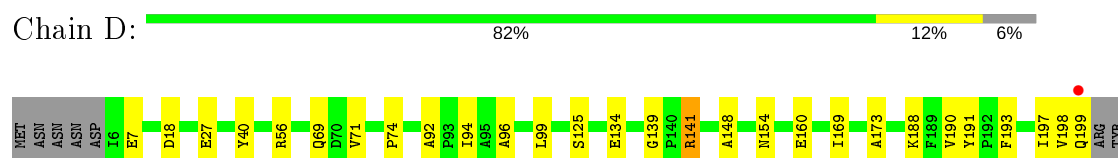
- Molecule 1: L-lactate oxidase



- Molecule 1: L-lactate oxidase



- Molecule 1: L-lactate oxidase





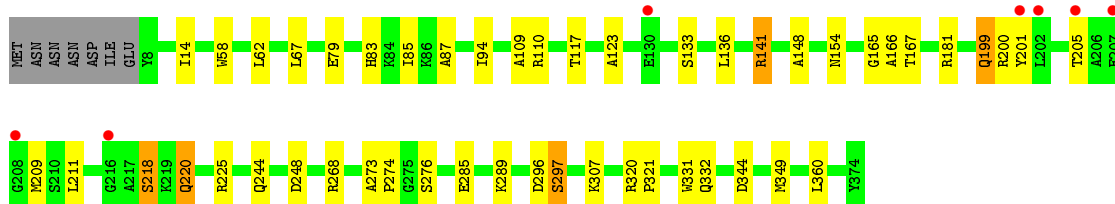
- Molecule 1: L-lactate oxidase

Chain E: 88% 9% ..



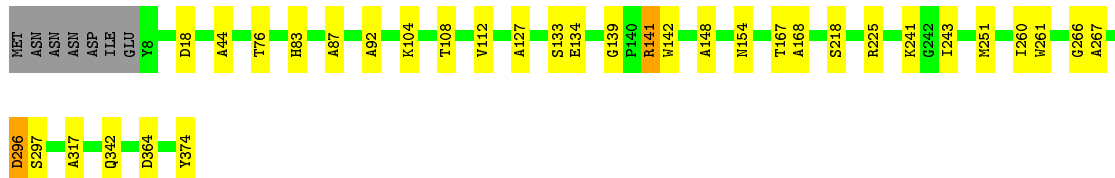
- Molecule 1: L-lactate oxidase

Chain F: 85% 12% ..



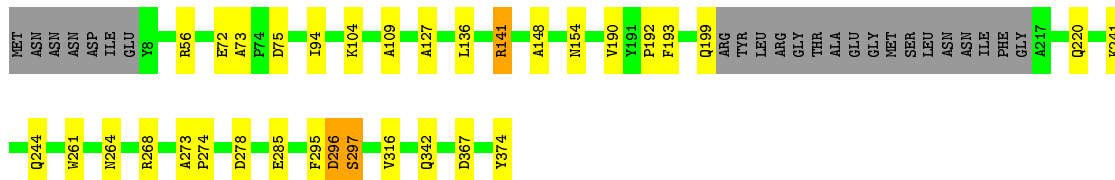
- Molecule 1: L-lactate oxidase

Chain G: 89% 9% ..



- Molecule 1: L-lactate oxidase

Chain H: 85% 8% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.35Å 119.18Å 119.56Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	39.75 – 2.60 39.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.75-2.60) 99.3 (39.75-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.182 , 0.246 0.189 , 0.247	Depositor DCC
$R_{free}$ test set	2637 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 22.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6643e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PYR

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	0.63	0/2886	0.77	0/3910
1	B	0.63	0/2886	0.76	0/3910
1	C	0.60	0/2886	0.74	2/3910 (0.1%)
1	D	0.61	0/2772	0.77	2/3756 (0.1%)
1	E	0.63	0/2886	0.78	2/3910 (0.1%)
1	F	0.63	0/2886	0.75	1/3910 (0.0%)
1	G	0.62	0/2886	0.75	1/3910 (0.0%)
1	H	0.61	0/2751	0.77	3/3728 (0.1%)
All	All	0.62	0/22839	0.76	11/30944 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	183	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	E	141	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	H	141	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	H	56	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	296	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	183	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	56	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	H	75	ASP	CB-CG-OD1	5.21	122.99	118.30
1	F	248	ASP	CB-CG-OD1	5.15	122.94	118.30
1	C	183	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	364	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2822	0	2754	18	0
1	B	2822	0	2754	15	0
1	C	2822	0	2754	17	0
1	D	2711	0	2643	21	0
1	E	2822	0	2754	19	0
1	F	2822	0	2754	29	0
1	G	2822	0	2754	16	0
1	H	2690	0	2623	16	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0
2	C	31	0	19	1	0
2	D	31	0	19	3	0
2	E	31	0	19	0	0
2	F	31	0	19	3	0
2	G	31	0	19	0	0
2	H	31	0	19	2	0
3	A	6	0	3	0	0
3	B	6	0	3	2	0
3	C	6	0	3	0	0
3	D	6	0	3	0	0
3	E	6	0	3	0	0
3	F	6	0	3	3	0
3	G	6	0	3	0	0
3	H	6	0	3	0	0
4	A	32	0	0	1	0
4	B	47	0	0	0	0
4	C	25	0	0	0	0
4	D	23	0	0	0	0
4	E	36	0	0	0	0
4	F	36	0	0	0	0
4	G	39	0	0	0	0
4	H	30	0	0	0	0
All	All	22897	0	21966	149	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 (149) 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:B:148:ALA:H	1:B:154:ASN:HD21	1.15	0.94
1:H:94:ILE:HG23	2:H:400:FMN:C6	2.18	0.73
1:F:199:GLN:HE21	1:F:199:GLN:HA	1.56	0.70
1:C:148:ALA:H	1:C:154:ASN:HD21	1.40	0.69
1:A:148:ALA:HB2	1:A:201:TYR:CD2	2.29	0.67
1:F:148:ALA:H	1:F:154:ASN:HD21	1.42	0.67
1:E:148:ALA:H	1:E:154:ASN:HD21	1.42	0.67
1:E:148:ALA:HB2	1:E:201:TYR:CD2	2.32	0.64
1:G:148:ALA:H	1:G:154:ASN:HD21	1.44	0.63
1:G:241:LYS:HA	1:G:261:TRP:HB3	1.81	0.63
1:C:241:LYS:HA	1:C:261:TRP:HB3	1.82	0.60
1:D:268:ARG:HD2	2:D:400:FMN:HM82	1.83	0.60
1:E:142:TRP:CD1	1:E:168:ALA:HB3	2.36	0.60
1:F:94:ILE:HG23	2:F:400:FMN:C6	2.32	0.60
1:A:76:THR:O	1:A:87:ALA:HA	2.01	0.60
1:D:273:ALA:HB1	1:D:274:PRO:HD2	1.82	0.60
1:B:148:ALA:N	1:B:154:ASN:HD21	1.94	0.59
1:A:142:TRP:CD1	1:A:168:ALA:HB3	2.38	0.59
1:D:40:TYR:O	1:D:268:ARG:NH2	2.35	0.58
1:A:104:LYS:HE2	1:A:127:ALA:HB2	1.83	0.58
1:D:139:GLY:O	1:D:141:ARG:NH2	2.34	0.58
1:C:142:TRP:CG	1:C:168:ALA:HB3	2.39	0.58
1:H:296:ASP:O	1:H:297:SER:HB2	2.04	0.57
1:F:14:ILE:HG22	1:F:332:GLN:OE1	2.04	0.57
1:B:148:ALA:H	1:B:154:ASN:ND2	1.96	0.57
1:B:76:THR:O	1:B:87:ALA:HA	2.05	0.56
1:G:296:ASP:C	1:G:296:ASP:OD1	2.44	0.56
1:H:241:LYS:HA	1:H:261:TRP:HB3	1.88	0.55
1:F:218:SER:O	1:F:220:GLN:NE2	2.40	0.55
1:F:148:ALA:N	1:F:154:ASN:HD21	2.05	0.54
1:D:94:ILE:HG23	2:D:400:FMN:C6	2.36	0.54
1:A:142:TRP:CG	1:A:168:ALA:HB3	2.43	0.54
1:F:148:ALA:HB2	1:F:201:TYR:CG	2.42	0.54
1:D:241:LYS:HA	1:D:261:TRP:HB3	1.91	0.53
1:E:173:ALA:HB3	1:F:67:LEU:HD23	1.90	0.53
1:E:205:THR:HG23	1:E:207:GLU:H	1.74	0.52
1:G:142:TRP:CD1	1:G:168:ALA:HB3	2.45	0.52
1:E:142:TRP:CG	1:E:168:ALA:HB3	2.45	0.52
1:D:244:GLN:HE22	1:D:276:SER:HA	1.76	0.51
1:F:181:ARG:CZ	1:F:211:LEU:HD21	2.41	0.51
1:C:142:TRP:CD1	1:C:168:ALA:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ASP:O	1:B:297:SER:HB2	2.11	0.51
1:E:76:THR:O	1:E:87:ALA:HA	2.10	0.51
1:C:296:ASP:O	1:C:297:SER:HB2	2.11	0.51
1:B:141:ARG:HG2	1:B:166:ALA:HA	1.93	0.50
2:B:400:FMN:C4A	3:B:401:PYR:O3	2.60	0.50
1:E:156:ASP:O	1:E:160:GLU:HG3	2.11	0.50
1:F:148:ALA:HB2	1:F:201:TYR:CD2	2.45	0.50
1:B:92:ALA:HB2	1:B:317:ALA:HB1	1.94	0.50
1:G:108:THR:O	1:G:112:VAL:HG23	2.12	0.49
1:D:148:ALA:H	1:D:154:ASN:HD21	1.59	0.49
1:E:191:TYR:CE2	1:E:214:ILE:HD12	2.48	0.49
1:E:203:ARG:H	1:E:203:ARG:HD3	1.77	0.49
1:B:148:ALA:HB2	1:B:201:TYR:CD2	2.47	0.49
1:C:94:ILE:HG23	2:C:400:FMN:C6	2.43	0.49
1:B:112:VAL:HG13	1:B:117:THR:HG23	1.95	0.48
1:G:76:THR:O	1:G:87:ALA:HA	2.13	0.48
1:H:148:ALA:H	1:H:154:ASN:HD21	1.60	0.48
1:F:109:ALA:HB1	1:F:136:LEU:HD23	1.95	0.48
1:C:296:ASP:C	1:C:296:ASP:OD1	2.52	0.48
1:F:296:ASP:O	1:F:297:SER:HB2	2.14	0.48
1:D:96:ALA:HB1	1:D:99:LEU:HG	1.96	0.47
1:G:44:ALA:HB1	1:G:267:ALA:O	2.14	0.47
1:E:244:GLN:HE22	1:E:276:SER:HA	1.78	0.47
1:B:124:TYR:HB3	1:B:195:MET:CE	2.44	0.47
1:E:89:PHE:CD1	1:E:318:LEU:HD11	2.49	0.47
1:H:192:PRO:HG2	1:H:193:PHE:CE2	2.49	0.47
1:C:67:LEU:HD23	1:D:173:ALA:HB3	1.96	0.47
1:A:199:GLN:HB3	4:A:503:HOH:O	2.14	0.47
1:F:273:ALA:HB1	1:F:274:PRO:HD2	1.97	0.47
1:A:305:VAL:HG11	1:A:345:LEU:HD22	1.97	0.47
1:A:150:ASP:OD2	1:A:153:GLN:HG3	2.14	0.47
1:A:61:LYS:HB3	1:A:365:LEU:HD13	1.96	0.46
1:B:296:ASP:OD1	1:B:296:ASP:C	2.53	0.46
1:G:83:HIS:NE2	1:G:167:THR:OG1	2.36	0.46
1:D:197:ILE:O	1:D:197:ILE:HG22	2.14	0.46
1:F:244:GLN:HE22	1:F:276:SER:HA	1.80	0.46
1:G:139:GLY:O	1:G:141:ARG:NH2	2.49	0.46
1:D:268:ARG:HD2	2:D:400:FMN:C8M	2.45	0.46
1:F:79:GLU:HA	1:F:83:HIS:O	2.14	0.46
1:H:148:ALA:N	1:H:154:ASN:HD21	2.14	0.46
1:G:374:TYR:OH	1:H:278:ASP:OD2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:O	1:D:199:GLN:CG	2.64	0.45
1:C:139:GLY:O	1:C:141:ARG:NH2	2.49	0.45
1:H:295:PHE:O	1:H:316:VAL:HA	2.17	0.45
1:E:320:ARG:N	1:E:321:PRO:CD	2.80	0.45
1:E:211:LEU:HD11	1:E:215:PHE:CE2	2.51	0.45
1:H:244:GLN:NE2	1:H:264:ASN:HB3	2.31	0.45
1:A:89:PHE:HA	1:A:316:VAL:O	2.17	0.45
1:D:96:ALA:HB2	1:D:191:TYR:OH	2.17	0.45
1:A:58:TRP:CZ2	1:A:304:HIS:HB3	2.52	0.45
1:G:251:MET:SD	1:G:251:MET:C	2.95	0.45
1:C:223:SER:OG	1:C:225:ARG:NH2	2.50	0.44
1:E:148:ALA:N	1:E:154:ASN:HD21	2.11	0.44
1:G:104:LYS:HE2	1:G:127:ALA:HB2	2.00	0.44
1:H:192:PRO:HG2	1:H:193:PHE:CD2	2.52	0.44
1:B:244:GLN:HE22	1:B:276:SER:HA	1.82	0.44
1:D:69:GLN:O	1:D:71:VAL:HG23	2.18	0.44
1:F:211:LEU:CD1	3:F:401:PYR:H33	2.47	0.44
1:A:136:LEU:O	1:A:137:ASN:C	2.56	0.44
1:E:35:HIS:HE1	1:E:187:ASN:OD1	2.00	0.44
1:F:349:MET:HG2	1:F:360:LEU:HD21	1.98	0.44
1:F:268:ARG:HD2	2:F:400:FMN:C8M	2.48	0.44
1:G:142:TRP:CG	1:G:168:ALA:HB3	2.53	0.44
1:F:133:SER:OG	1:F:141:ARG:NH1	2.50	0.44
1:F:85:ILE:HG22	1:F:117:THR:HA	2.00	0.43
1:F:85:ILE:HD12	1:F:87:ALA:O	2.17	0.43
1:G:243:ILE:HD12	1:G:260:ILE:HG23	2.00	0.43
1:H:109:ALA:HB1	1:H:136:LEU:HG	2.00	0.43
1:A:69:GLN:HG3	1:A:353:GLY:HA3	2.00	0.43
1:F:211:LEU:HD11	3:F:401:PYR:H33	2.00	0.43
1:A:244:GLN:HE22	1:A:276:SER:HA	1.83	0.43
1:H:104:LYS:HE2	1:H:127:ALA:HB2	2.01	0.43
1:C:104:LYS:HE2	1:C:127:ALA:HB2	1.99	0.43
1:E:274:PRO:HA	1:F:62:LEU:HD13	2.00	0.43
1:H:296:ASP:OD1	1:H:296:ASP:C	2.56	0.43
1:G:266:GLY:O	1:G:267:ALA:HB3	2.20	0.42
1:C:148:ALA:HB2	1:C:201:TYR:CD2	2.54	0.42
1:C:273:ALA:HB1	1:C:274:PRO:HD2	2.00	0.42
1:D:92:ALA:HB2	1:D:317:ALA:HB1	2.02	0.42
1:F:205:THR:O	1:F:209:MET:SD	2.78	0.42
1:F:109:ALA:HB1	1:F:136:LEU:CD2	2.49	0.42
1:H:72:GLU:O	1:H:73:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:FMN:C4	3:B:401:PYR:O3	2.68	0.41
1:E:239:PHE:HA	1:E:259:GLY:O	2.21	0.41
1:G:92:ALA:HB2	1:G:317:ALA:HB1	2.01	0.41
1:C:63:LEU:HG	1:C:307:LYS:HE2	2.03	0.41
1:F:58:TRP:O	1:F:307:LYS:NZ	2.54	0.41
1:H:273:ALA:HB1	1:H:274:PRO:HD2	2.02	0.41
1:F:320:ARG:N	1:F:321:PRO:HD2	2.36	0.41
1:B:271:TYR:CD2	1:B:272:GLU:HB2	2.55	0.41
1:A:211:LEU:HD11	1:A:215:PHE:CZ	2.55	0.41
1:C:147:MET:CE	1:C:230:ILE:HD11	2.51	0.41
1:D:74:PRO:HG2	1:D:346:THR:HG23	2.03	0.41
1:C:156:ASP:O	1:C:160:GLU:HG3	2.20	0.41
1:E:109:ALA:HB1	1:E:136:LEU:HG	2.02	0.41
1:F:110:ARG:HB3	1:F:331:TRP:HB2	2.03	0.41
1:A:83:HIS:HB2	1:A:118:ILE:HD11	2.02	0.41
1:F:165:GLY:O	1:F:166:ALA:C	2.59	0.41
1:A:222:ILE:O	1:B:68:ALA:HA	2.21	0.41
1:D:169:ILE:O	1:D:238:VAL:HA	2.20	0.40
1:D:69:GLN:HG3	1:D:353:GLY:HA3	2.02	0.40
2:F:400:FMN:C4A	3:F:401:PYR:O3	2.69	0.40
1:A:133:SER:OG	1:A:141:ARG:NH1	2.54	0.40
1:B:109:ALA:HB1	1:B:136:LEU:CD2	2.50	0.40
1:D:296:ASP:C	1:D:296:ASP:OD1	2.59	0.40
1:D:320:ARG:N	1:D:321:PRO:HD2	2.37	0.40
1:H:268:ARG:HD2	2:H:400:FMN:HM82	2.03	0.40
1:C:368:ASN:HA	1:C:369:PRO:HD2	1.91	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	365/374 (98%)	350 (96%)	14 (4%)	1 (0%)	41	64
1	B	365/374 (98%)	349 (96%)	15 (4%)	1 (0%)	41	64
1	C	365/374 (98%)	346 (95%)	16 (4%)	3 (1%)	19	39
1	D	349/374 (93%)	331 (95%)	16 (5%)	2 (1%)	25	47
1	E	365/374 (98%)	349 (96%)	15 (4%)	1 (0%)	41	64
1	F	365/374 (98%)	338 (93%)	24 (7%)	3 (1%)	19	39
1	G	365/374 (98%)	352 (96%)	12 (3%)	1 (0%)	41	64
1	H	346/374 (92%)	328 (95%)	17 (5%)	1 (0%)	41	64
All	All	2885/2992 (96%)	2743 (95%)	129 (4%)	13 (0%)	29	52

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	SER
1	B	297	SER
1	C	297	SER
1	E	297	SER
1	F	297	SER
1	G	297	SER
1	C	203	ARG
1	D	297	SER
1	H	297	SER
1	F	200	ARG
1	C	188	LYS
1	F	123	ALA
1	D	329	GLY

### 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	288/295 (98%)	281 (98%)	7 (2%)	49	74
1	B	288/295 (98%)	280 (97%)	8 (3%)	43	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	288/295 (98%)	280 (97%)	8 (3%)	43	69
1	D	277/295 (94%)	262 (95%)	15 (5%)	22	44
1	E	288/295 (98%)	282 (98%)	6 (2%)	53	77
1	F	288/295 (98%)	279 (97%)	9 (3%)	40	66
1	G	288/295 (98%)	280 (97%)	8 (3%)	43	69
1	H	275/295 (93%)	266 (97%)	9 (3%)	38	64
All	All	2280/2360 (97%)	2210 (97%)	70 (3%)	40	66

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	133	SER
1	A	141	ARG
1	A	196	PRO
1	A	203	ARG
1	A	237	PRO
1	A	258	SER
1	B	15	LYS
1	B	130	GLU
1	B	141	ARG
1	B	152	GLN
1	B	188	LYS
1	B	246	PRO
1	B	296	ASP
1	B	367	ASP
1	C	141	ARG
1	C	144	GLN
1	C	188	LYS
1	C	199	GLN
1	C	203	ARG
1	C	289	LYS
1	C	296	ASP
1	C	342	GLN
1	D	7	GLU
1	D	18	ASP
1	D	27	GLU
1	D	125	SER
1	D	134	GLU
1	D	141	ARG

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Mol	Chain	Res	Type
1	D	160	GLU
1	D	188	LYS
1	D	190	VAL
1	D	193	PHE
1	D	220	GLN
1	D	265	HIS
1	D	285	GLU
1	D	296	ASP
1	D	342	GLN
1	E	78	THR
1	E	133	SER
1	E	141	ARG
1	E	203	ARG
1	E	218	SER
1	E	344	ASP
1	F	141	ARG
1	F	167	THR
1	F	199	GLN
1	F	218	SER
1	F	220	GLN
1	F	225	ARG
1	F	285	GLU
1	F	289	LYS
1	F	344	ASP
1	G	18	ASP
1	G	133	SER
1	G	134	GLU
1	G	141	ARG
1	G	218	SER
1	G	225	ARG
1	G	296	ASP
1	G	342	GLN
1	H	141	ARG
1	H	190	VAL
1	H	199	GLN
1	H	220	GLN
1	H	285	GLU
1	H	296	ASP
1	H	342	GLN
1	H	367	ASP
1	H	374	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	199	GLN
1	A	244	GLN
1	B	154	ASN
1	B	244	GLN
1	C	144	GLN
1	C	154	ASN
1	C	199	GLN
1	D	154	ASN
1	D	220	GLN
1	D	244	GLN
1	E	35	HIS
1	E	154	ASN
1	E	244	GLN
1	F	154	ASN
1	F	220	GLN
1	F	244	GLN
1	G	154	ASN
1	H	154	ASN
1	H	244	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 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
3	PYR	A	401	-	2,5,5	0.38	0	2,6,6	0.62	0
3	PYR	F	401	-	2,5,5	0.33	0	2,6,6	0.25	0
2	FMN	F	400	-	31,33,33	2.35	6 (19%)	40,50,50	2.28	8 (20%)
2	FMN	G	400	-	31,33,33	2.12	5 (16%)	40,50,50	2.32	8 (20%)
2	FMN	D	400	-	31,33,33	2.06	4 (12%)	40,50,50	2.39	8 (20%)
2	FMN	E	400	-	31,33,33	2.00	5 (16%)	40,50,50	1.95	7 (17%)
2	FMN	B	400	-	31,33,33	2.14	6 (19%)	40,50,50	2.35	7 (17%)
2	FMN	C	400	-	31,33,33	2.22	6 (19%)	40,50,50	2.37	7 (17%)
3	PYR	C	401	-	2,5,5	0.37	0	2,6,6	0.29	0
2	FMN	A	400	-	31,33,33	1.97	5 (16%)	40,50,50	2.11	7 (17%)
2	FMN	H	400	-	31,33,33	2.13	5 (16%)	40,50,50	2.13	7 (17%)
3	PYR	G	401	-	2,5,5	0.34	0	2,6,6	0.17	0
3	PYR	H	401	-	2,5,5	0.51	0	2,6,6	0.53	0
3	PYR	D	401	-	2,5,5	0.58	0	2,6,6	0.21	0
3	PYR	E	401	-	2,5,5	0.51	0	2,6,6	0.84	0
3	PYR	B	401	-	2,5,5	0.25	0	2,6,6	0.60	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
3	PYR	A	401	-	-	0/0/4/4	-
3	PYR	F	401	-	-	0/0/4/4	-
2	FMN	F	400	-	-	1/18/18/18	0/3/3/3
2	FMN	G	400	-	-	1/18/18/18	0/3/3/3
2	FMN	D	400	-	-	1/18/18/18	0/3/3/3
2	FMN	E	400	-	-	1/18/18/18	0/3/3/3
2	FMN	B	400	-	-	1/18/18/18	0/3/3/3
2	FMN	C	400	-	-	1/18/18/18	0/3/3/3
3	PYR	C	401	-	-	0/0/4/4	-
2	FMN	A	400	-	-	3/18/18/18	0/3/3/3
2	FMN	H	400	-	-	1/18/18/18	0/3/3/3
3	PYR	G	401	-	-	0/0/4/4	-
3	PYR	H	401	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PYR	D	401	-	-	0/0/4/4	-
3	PYR	E	401	-	-	0/0/4/4	-
3	PYR	B	401	-	-	0/0/4/4	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	FMN	C4A-C10	9.70	1.48	1.38
2	G	400	FMN	C4A-C10	9.69	1.48	1.38
2	C	400	FMN	C4A-C10	9.62	1.48	1.38
2	A	400	FMN	C4A-C10	8.69	1.47	1.38
2	B	400	FMN	C4A-C10	8.55	1.47	1.38
2	H	400	FMN	C4A-C10	8.38	1.47	1.38
2	D	400	FMN	C4A-C10	8.21	1.47	1.38
2	E	400	FMN	C4A-C10	7.62	1.46	1.38
2	F	400	FMN	C4-C4A	4.90	1.49	1.41
2	H	400	FMN	C4-C4A	4.72	1.49	1.41
2	E	400	FMN	C1'-N10	-4.52	1.43	1.48
2	D	400	FMN	C9A-C5A	4.13	1.50	1.42
2	C	400	FMN	C4-C4A	3.95	1.48	1.41
2	B	400	FMN	C8-C7	3.84	1.50	1.40
2	E	400	FMN	C4-C4A	3.68	1.47	1.41
2	D	400	FMN	C8-C7	3.61	1.49	1.40
2	F	400	FMN	C9A-C5A	3.60	1.49	1.42
2	B	400	FMN	C4-C4A	3.53	1.47	1.41
2	B	400	FMN	C9A-C5A	3.49	1.49	1.42
2	G	400	FMN	C9A-N10	3.46	1.43	1.38
2	C	400	FMN	C9A-C5A	3.43	1.49	1.42
2	D	400	FMN	C4-C4A	3.33	1.47	1.41
2	H	400	FMN	C9A-C5A	3.31	1.49	1.42
2	F	400	FMN	C1'-N10	-3.27	1.44	1.48
2	B	400	FMN	C1'-N10	-3.27	1.44	1.48
2	G	400	FMN	C9A-C5A	3.26	1.49	1.42
2	H	400	FMN	C8-C7	3.20	1.48	1.40
2	E	400	FMN	C9A-C5A	3.11	1.48	1.42
2	C	400	FMN	C8-C7	2.99	1.48	1.40
2	F	400	FMN	C8-C7	2.95	1.48	1.40
2	A	400	FMN	C1'-N10	-2.71	1.45	1.48
2	A	400	FMN	C4-C4A	2.59	1.45	1.41
2	A	400	FMN	C9A-C5A	2.54	1.47	1.42
2	E	400	FMN	C8-C7	2.37	1.46	1.40
2	G	400	FMN	C4-C4A	2.33	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	FMN	C10-N1	2.33	1.36	1.33
2	A	400	FMN	C8-C7	2.30	1.46	1.40
2	G	400	FMN	C8-C7	2.27	1.46	1.40
2	C	400	FMN	C9A-N10	2.18	1.41	1.38
2	C	400	FMN	C6-C5A	-2.15	1.38	1.41
2	B	400	FMN	C2-N3	-2.11	1.34	1.38
2	H	400	FMN	C10-N1	2.10	1.36	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	FMN	C4-N3-C2	10.01	123.59	115.14
2	C	400	FMN	C4-N3-C2	9.67	123.31	115.14
2	G	400	FMN	C4-N3-C2	9.49	123.15	115.14
2	D	400	FMN	C4-N3-C2	9.30	123.00	115.14
2	A	400	FMN	C4-N3-C2	9.07	122.80	115.14
2	F	400	FMN	C4-N3-C2	8.32	122.17	115.14
2	E	400	FMN	C4-N3-C2	8.11	121.99	115.14
2	H	400	FMN	C4-N3-C2	7.33	121.33	115.14
2	D	400	FMN	C1'-N10-C9A	6.94	123.75	118.29
2	F	400	FMN	C4-C4A-C10	-6.32	115.77	119.95
2	C	400	FMN	C1'-N10-C9A	6.09	123.08	118.29
2	G	400	FMN	C1'-N10-C9A	6.03	123.04	118.29
2	H	400	FMN	C4-C4A-C10	-6.00	115.98	119.95
2	D	400	FMN	C4-C4A-C10	-5.33	116.42	119.95
2	B	400	FMN	C4A-N5-C5A	5.16	121.93	116.77
2	F	400	FMN	C4-C4A-N5	5.15	124.48	118.60
2	B	400	FMN	C1'-N10-C9A	4.79	122.06	118.29
2	C	400	FMN	C4-C4A-C10	-4.77	116.79	119.95
2	B	400	FMN	C4A-C4-N3	-4.69	117.02	123.43
2	H	400	FMN	C4-C4A-N5	4.64	123.90	118.60
2	F	400	FMN	C4A-N5-C5A	4.62	121.38	116.77
2	C	400	FMN	C4A-C4-N3	-4.53	117.23	123.43
2	H	400	FMN	C4A-N5-C5A	4.45	121.22	116.77
2	G	400	FMN	C4A-C4-N3	-4.43	117.37	123.43
2	A	400	FMN	C4A-C4-N3	-4.30	117.55	123.43
2	E	400	FMN	C4-C4A-C10	-4.21	117.16	119.95
2	C	400	FMN	C4A-N5-C5A	4.17	120.94	116.77
2	A	400	FMN	C4-C4A-C10	-4.07	117.26	119.95
2	D	400	FMN	C4A-C4-N3	-3.88	118.13	123.43
2	E	400	FMN	C4A-N5-C5A	3.78	120.55	116.77
2	C	400	FMN	C4-C4A-N5	3.72	122.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	FMN	O3P-P-O2P	3.69	121.74	107.64
2	F	400	FMN	C1'-N10-C9A	3.33	120.91	118.29
2	E	400	FMN	C4A-C4-N3	-3.23	119.01	123.43
2	D	400	FMN	C9A-N10-C10	-3.11	117.84	121.91
2	A	400	FMN	C4A-N5-C5A	3.03	119.80	116.77
2	G	400	FMN	C4A-N5-C5A	3.00	119.77	116.77
2	B	400	FMN	C4-C4A-C10	-2.96	117.99	119.95
2	H	400	FMN	C1'-N10-C9A	2.92	120.59	118.29
2	A	400	FMN	C1'-N10-C9A	2.92	120.59	118.29
2	A	400	FMN	C4-C4A-N5	2.87	121.88	118.60
2	G	400	FMN	C9A-N10-C10	-2.87	118.15	121.91
2	H	400	FMN	C4A-C4-N3	-2.80	119.60	123.43
2	G	400	FMN	C10-C4A-N5	2.64	123.08	121.26
2	D	400	FMN	C4-C4A-N5	2.61	121.58	118.60
2	D	400	FMN	C4A-N5-C5A	2.59	119.36	116.77
2	G	400	FMN	C4-C4A-C10	-2.57	118.25	119.95
2	E	400	FMN	C4-C4A-N5	2.50	121.46	118.60
2	C	400	FMN	C9A-N10-C10	-2.50	118.64	121.91
2	F	400	FMN	C4A-C4-N3	-2.37	120.18	123.43
2	E	400	FMN	O3P-P-O2P	2.37	116.68	107.64
2	E	400	FMN	O2'-C2'-C1'	-2.35	103.93	109.59
2	A	400	FMN	O3P-P-O1P	2.30	119.68	110.68
2	B	400	FMN	C4-C4A-N5	2.29	121.21	118.60
2	B	400	FMN	O3P-P-O2P	2.26	116.26	107.64
2	D	400	FMN	O3'-C3'-C4'	2.22	114.18	108.81
2	F	400	FMN	C10-C4A-N5	-2.18	119.75	121.26
2	G	400	FMN	O3P-P-O2P	2.18	115.95	107.64
2	H	400	FMN	O3P-P-O5'	2.05	112.20	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	FMN	C4'-C5'-O5'-P
2	G	400	FMN	C4'-C5'-O5'-P
2	E	400	FMN	C4'-C5'-O5'-P
2	C	400	FMN	C4'-C5'-O5'-P
2	H	400	FMN	C4'-C5'-O5'-P
2	F	400	FMN	C4'-C5'-O5'-P
2	D	400	FMN	C4'-C5'-O5'-P
2	B	400	FMN	C4'-C5'-O5'-P
2	A	400	FMN	O3'-C3'-C4'-O4'

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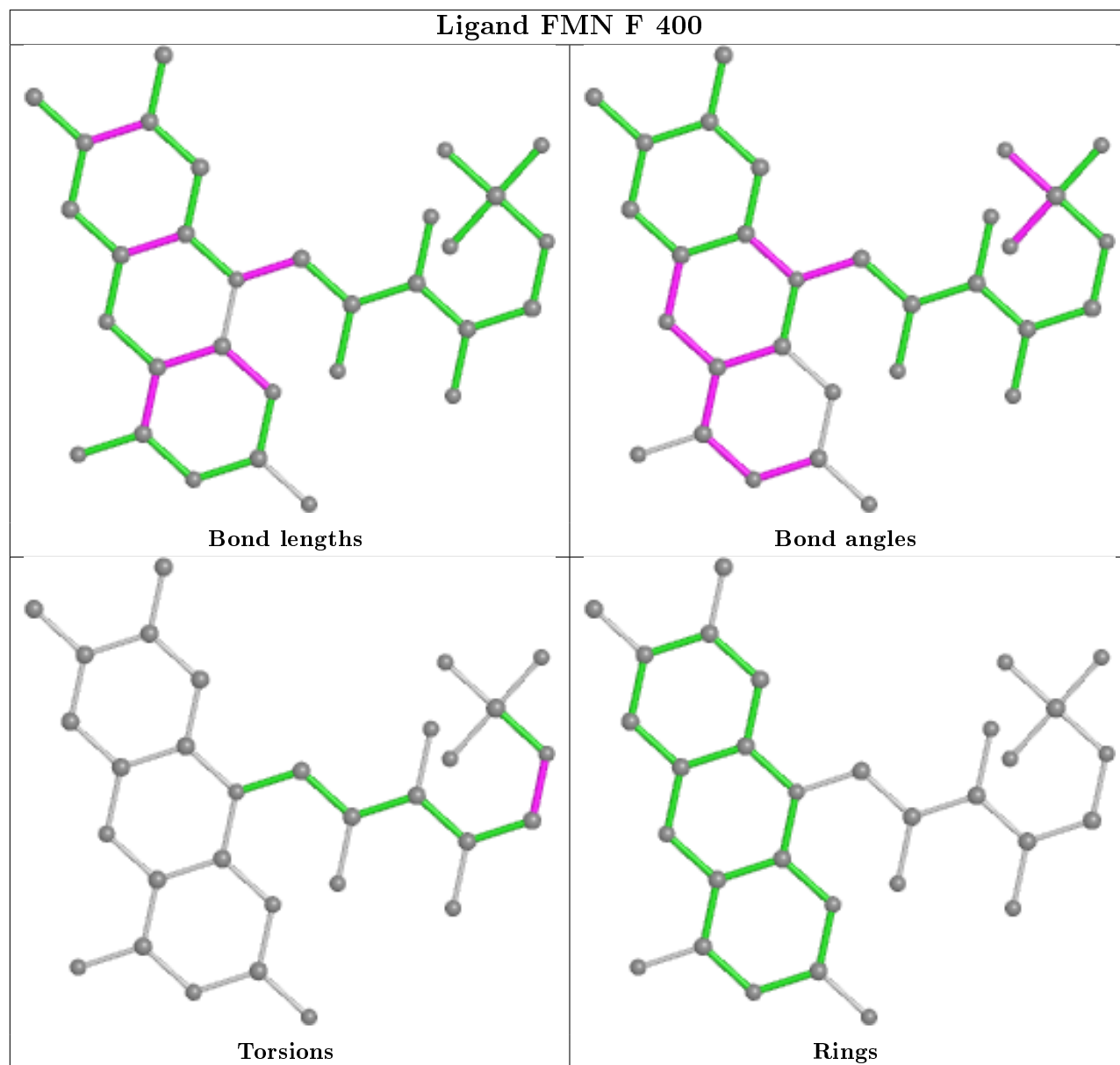
Mol	Chain	Res	Type	Atoms
2	A	400	FMN	C2'-C3'-C4'-O4'

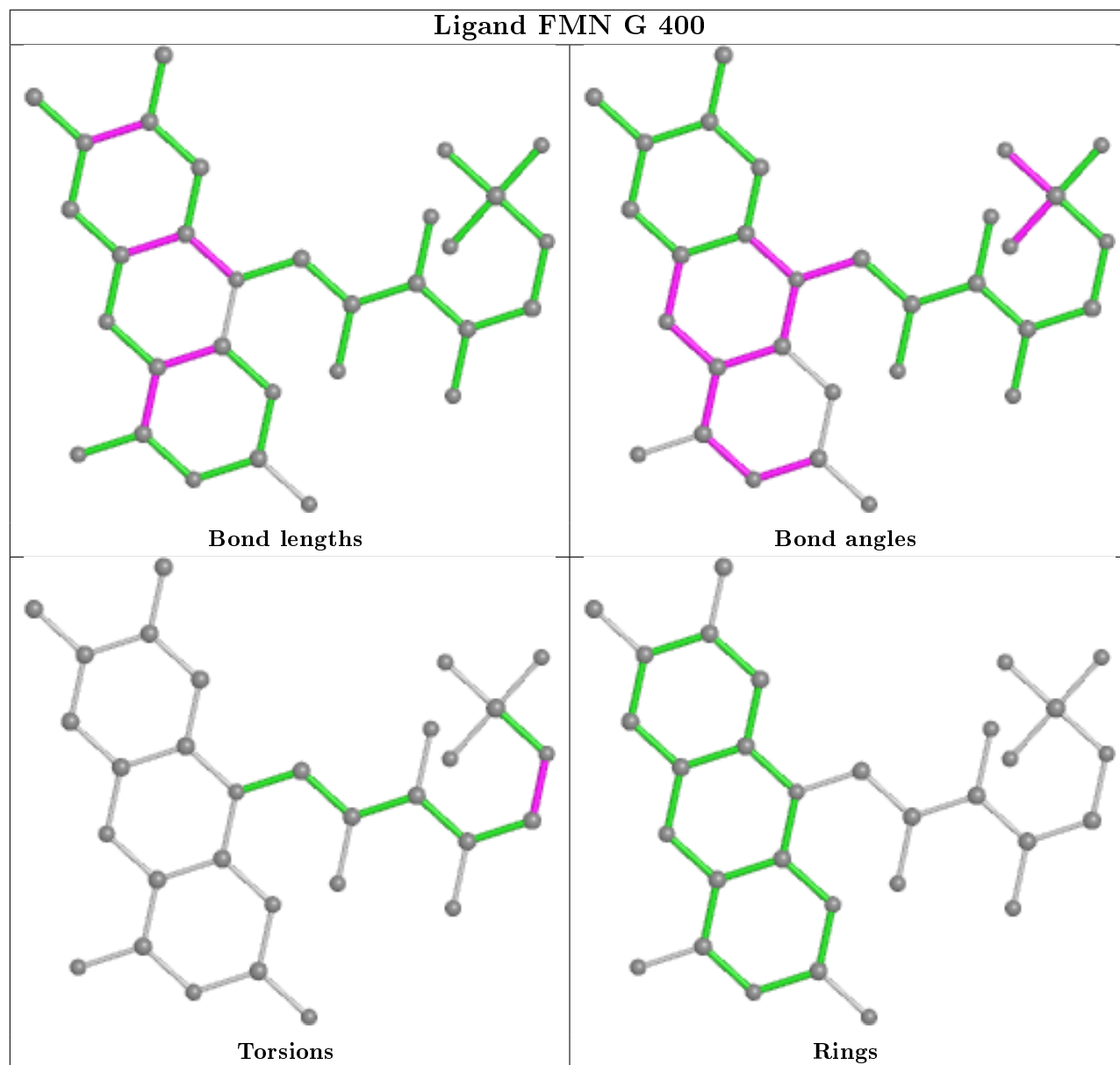
There are no ring outliers.

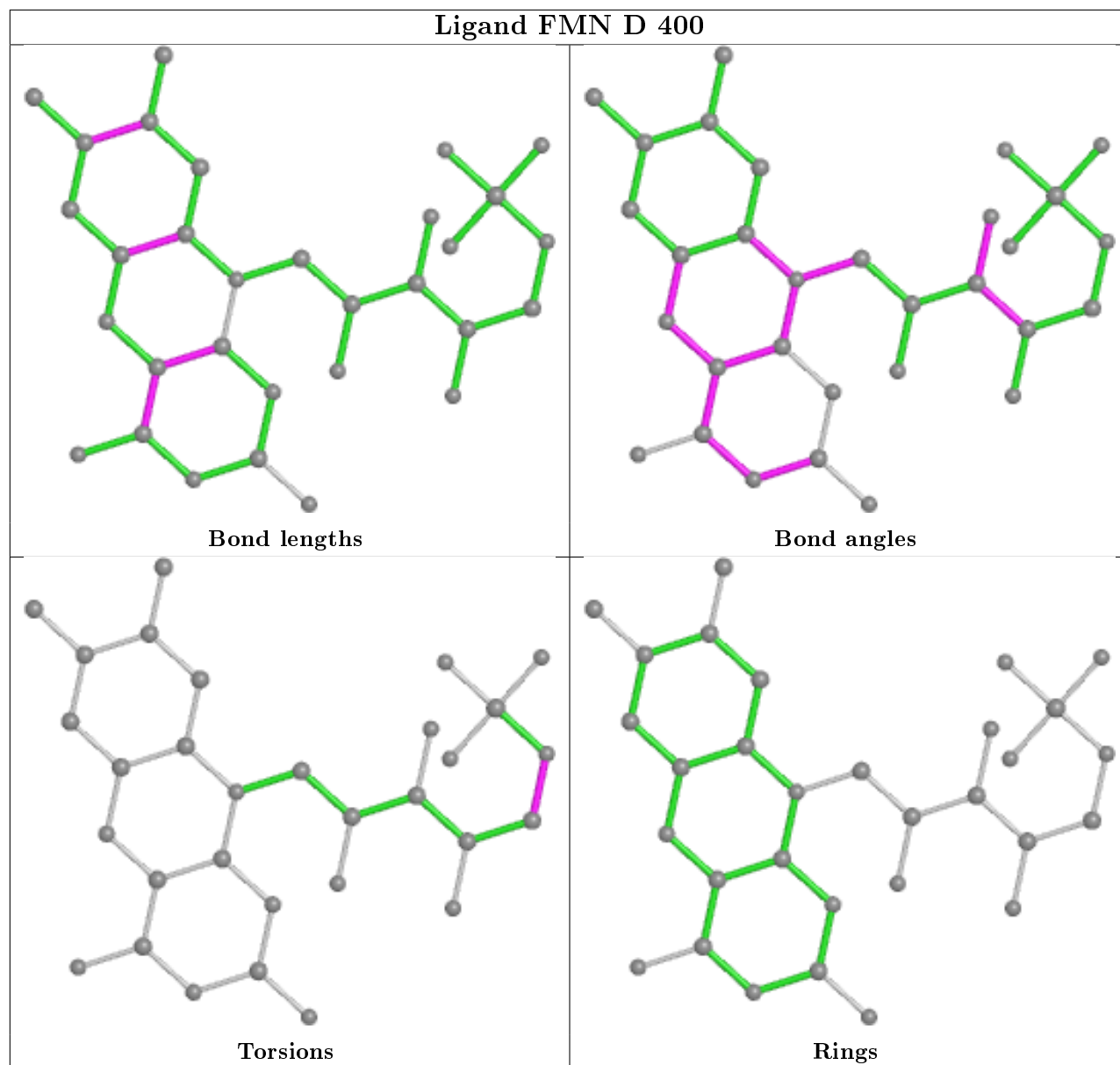
7 monomers are involved in 13 short contacts:

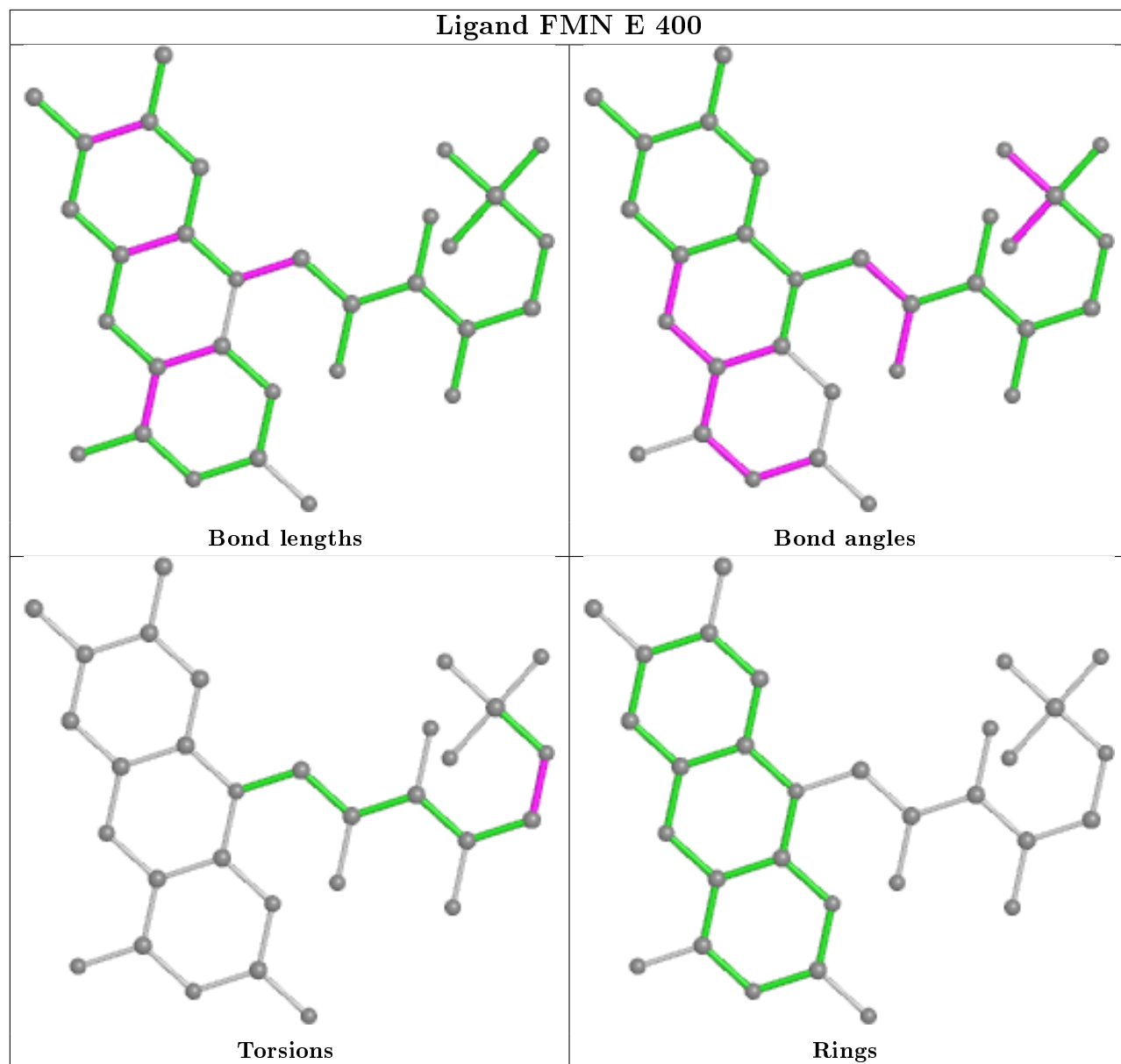
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	PYR	3	0
2	F	400	FMN	3	0
2	D	400	FMN	3	0
2	B	400	FMN	2	0
2	C	400	FMN	1	0
2	H	400	FMN	2	0
3	B	401	PYR	2	0

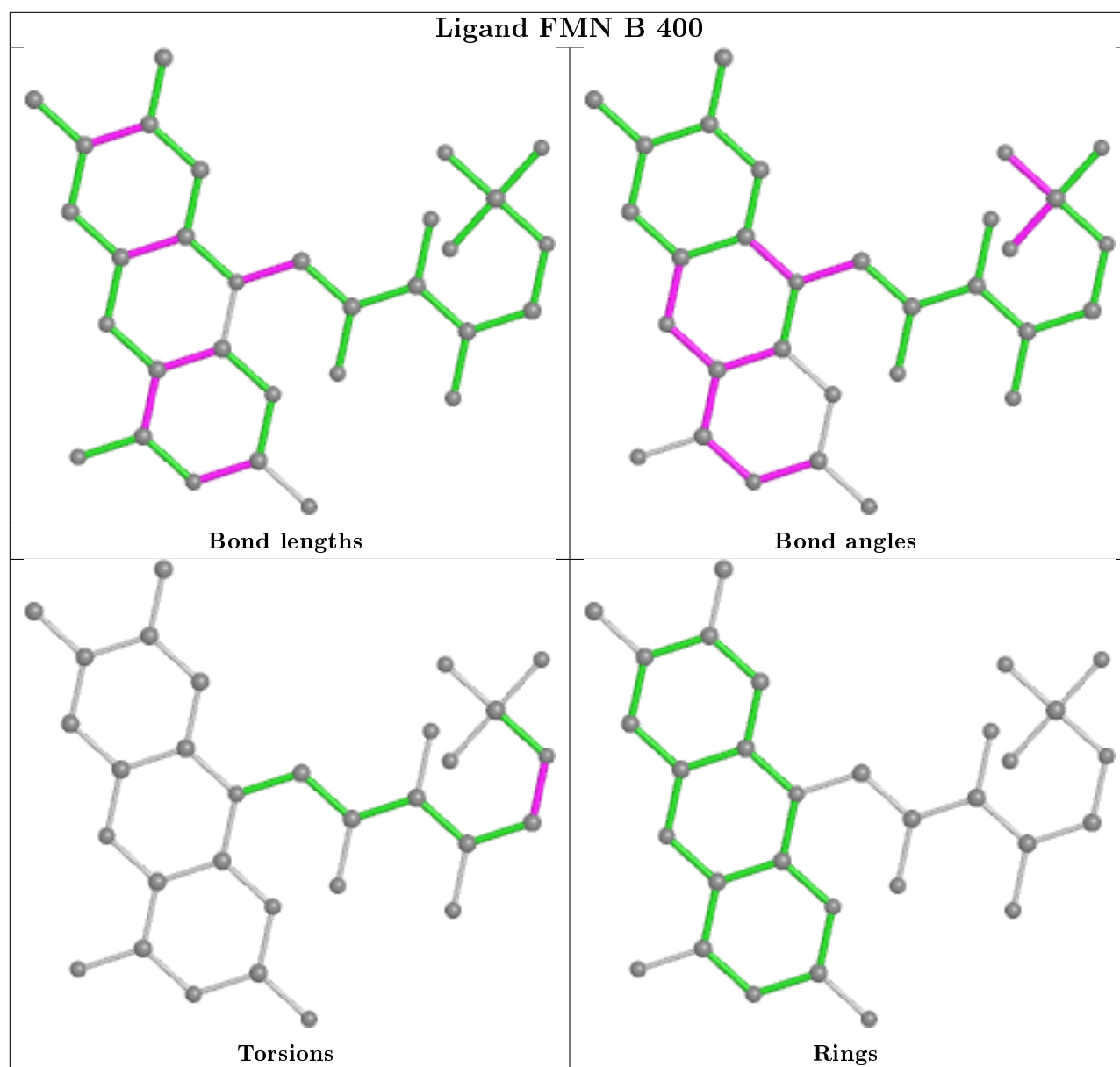
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

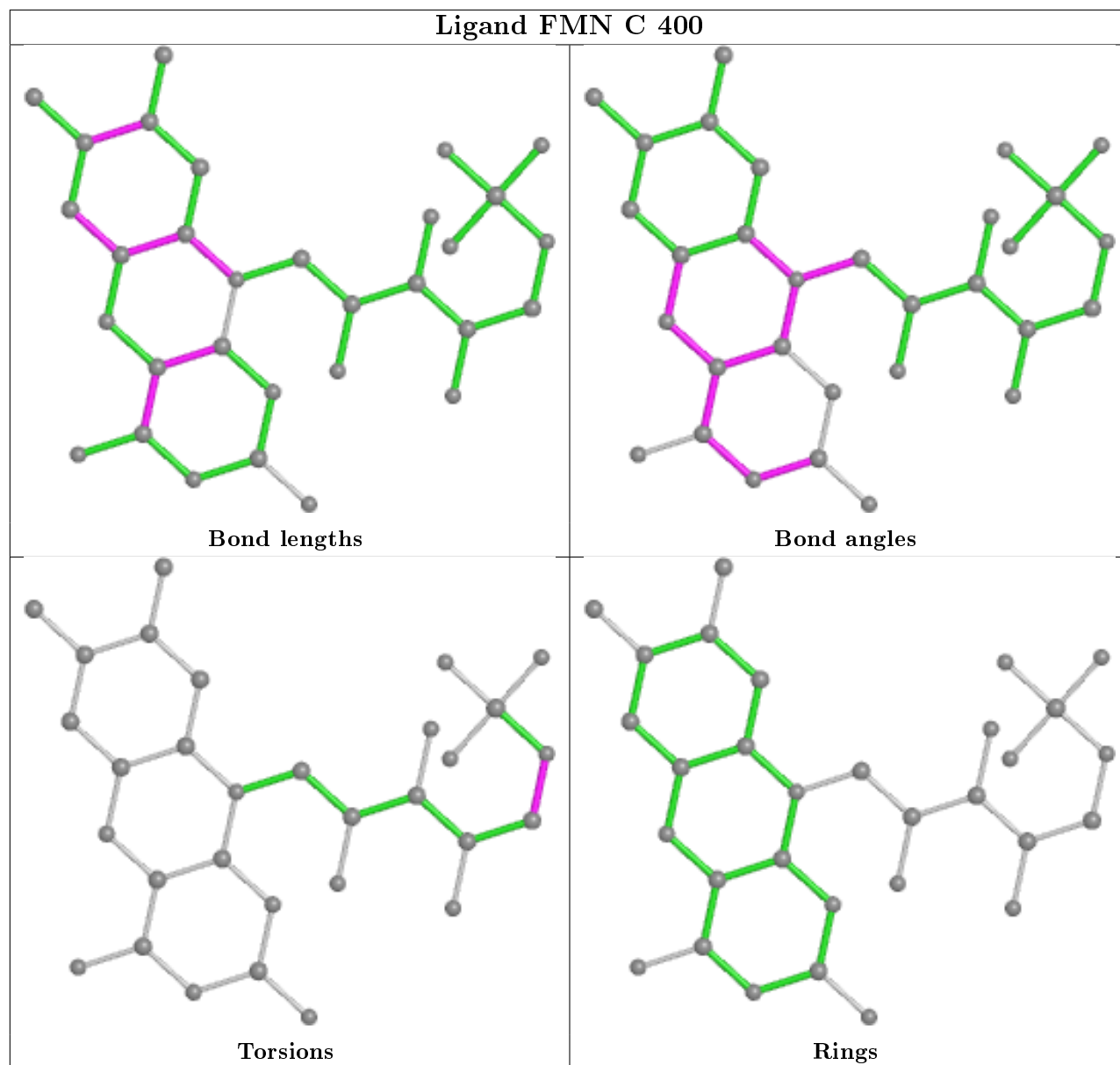




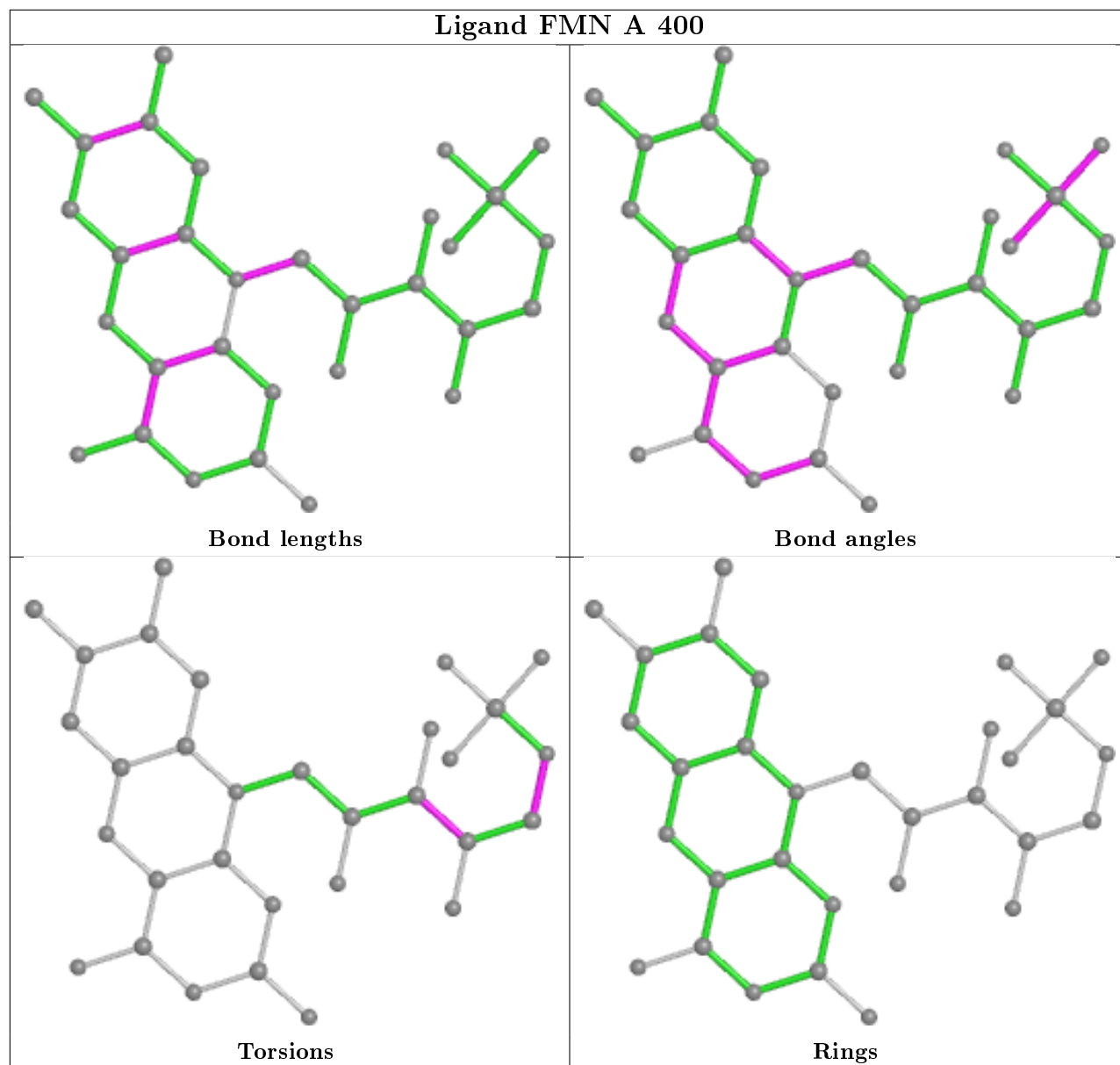


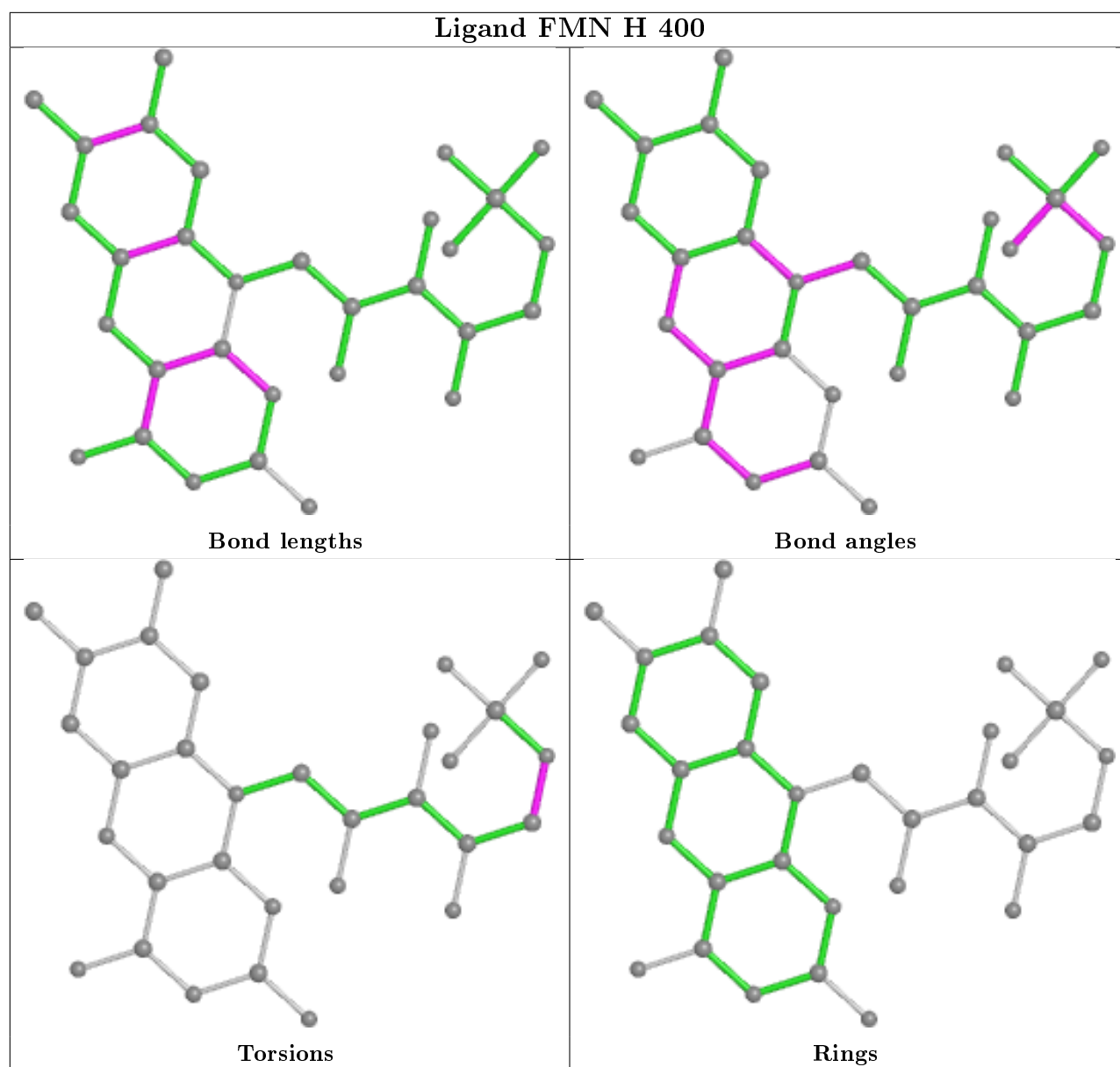












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	367/374 (98%)	-0.73	0 100 100	11, 22, 35, 72	0
1	B	367/374 (98%)	-0.70	0 100 100	10, 21, 35, 49	0
1	C	367/374 (98%)	-0.47	1 (0%) 94 93	14, 26, 44, 102	0
1	D	353/374 (94%)	-0.55	1 (0%) 94 93	12, 23, 40, 72	0
1	E	367/374 (98%)	-0.71	1 (0%) 94 93	10, 21, 36, 88	0
1	F	367/374 (98%)	-0.44	7 (1%) 66 62	13, 25, 56, 83	0
1	G	367/374 (98%)	-0.61	0 100 100	14, 24, 36, 54	0
1	H	350/374 (93%)	-0.56	0 100 100	12, 25, 40, 59	0
All	All	2905/2992 (97%)	-0.60	10 (0%) 94 93	10, 23, 41, 102	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	216	GLY	3.8
1	F	201	TYR	3.7
1	D	199	GLN	3.6
1	C	203	ARG	3.4
1	F	205	THR	3.1
1	F	208	GLY	2.8
1	F	202	LEU	2.6
1	F	207	GLU	2.2
1	E	203	ARG	2.2
1	F	130	GLU	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

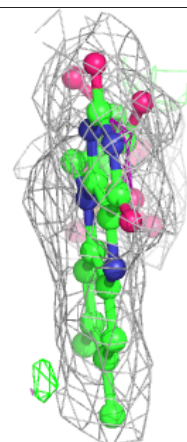
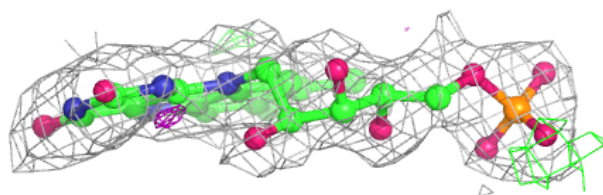
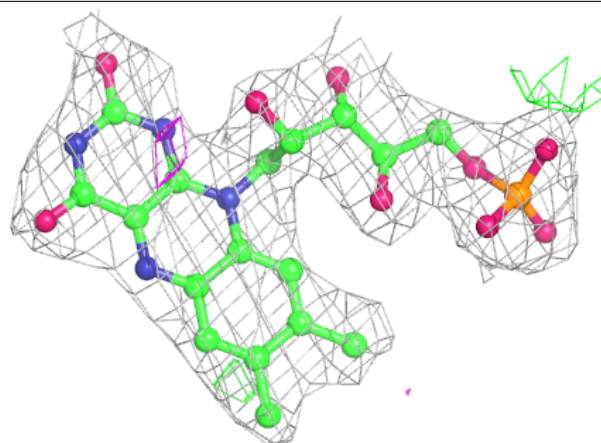
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PYR	D	401	6/6	0.88	0.25	48,55,59,60	0
3	PYR	H	401	6/6	0.92	0.18	55,59,61,62	0
3	PYR	C	401	6/6	0.96	0.16	36,38,39,43	0
3	PYR	A	401	6/6	0.96	0.16	22,23,24,25	0
3	PYR	F	401	6/6	0.96	0.17	47,51,52,54	0
3	PYR	B	401	6/6	0.96	0.20	30,32,34,38	0
2	FMN	F	400	31/31	0.97	0.18	15,22,28,30	0
2	FMN	A	400	31/31	0.97	0.14	12,16,17,17	0
2	FMN	H	400	31/31	0.97	0.16	17,22,24,25	0
3	PYR	G	401	6/6	0.97	0.12	25,29,29,32	0
2	FMN	G	400	31/31	0.97	0.15	14,21,23,24	0
2	FMN	B	400	31/31	0.97	0.15	13,21,22,23	0
2	FMN	C	400	31/31	0.97	0.16	17,23,25,26	0
2	FMN	E	400	31/31	0.98	0.12	13,16,17,18	0
3	PYR	E	401	6/6	0.98	0.14	25,26,26,28	0
2	FMN	D	400	31/31	0.98	0.15	18,23,27,29	0

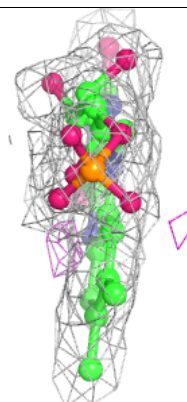
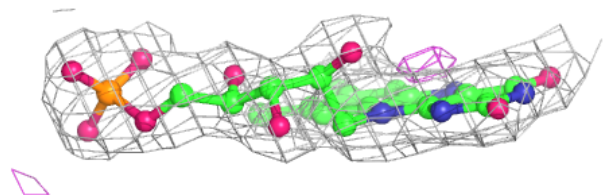
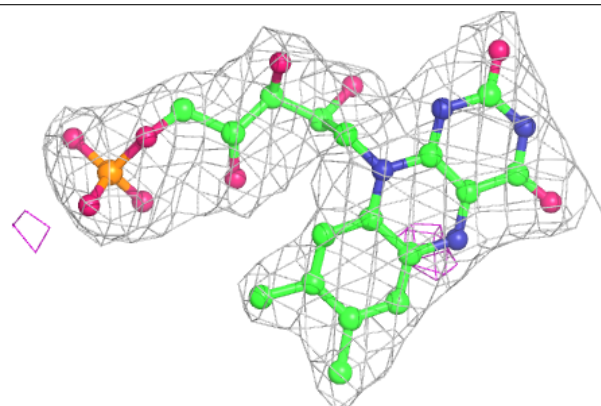
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FMN F 400:**

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

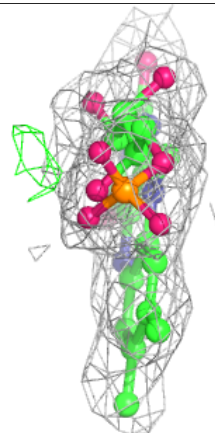
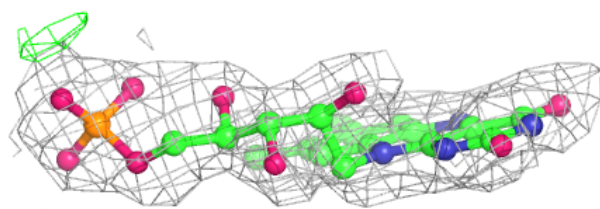
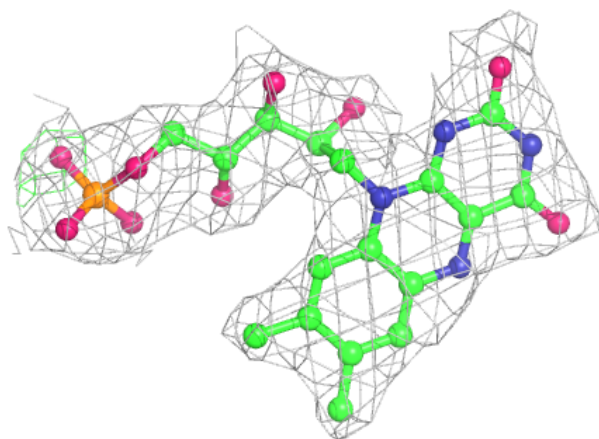
**Electron density around FMN A 400:**

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



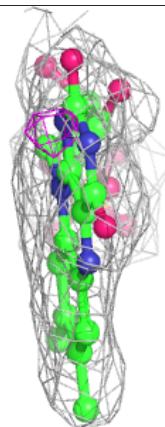
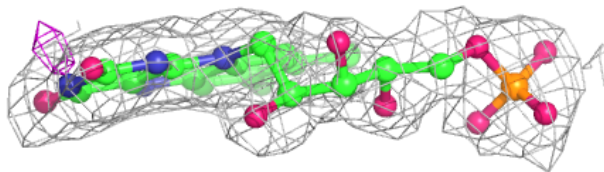
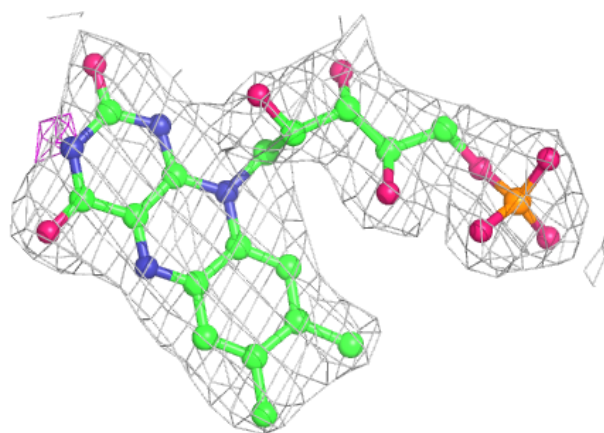
**Electron density around FMN H 400:**

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



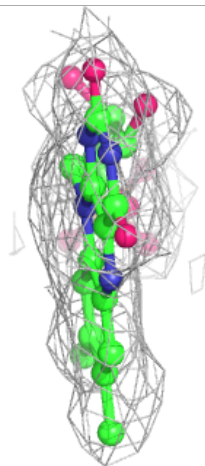
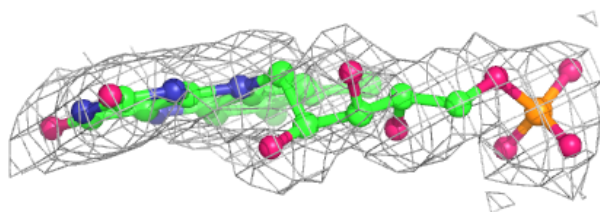
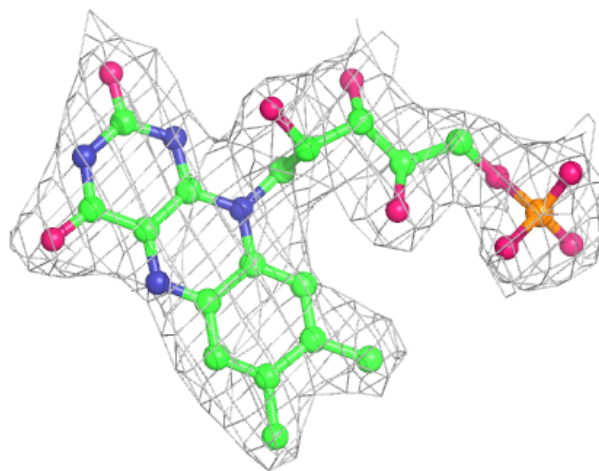
**Electron density around FMN G 400:**

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



**Electron density around FMN B 400:**

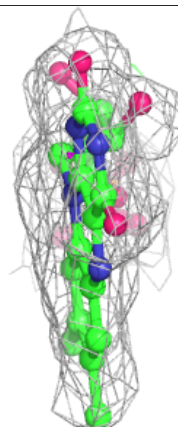
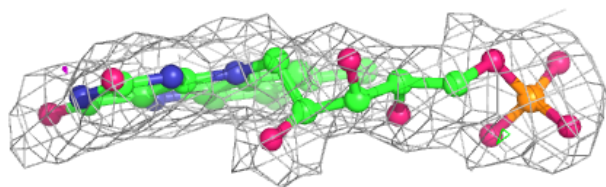
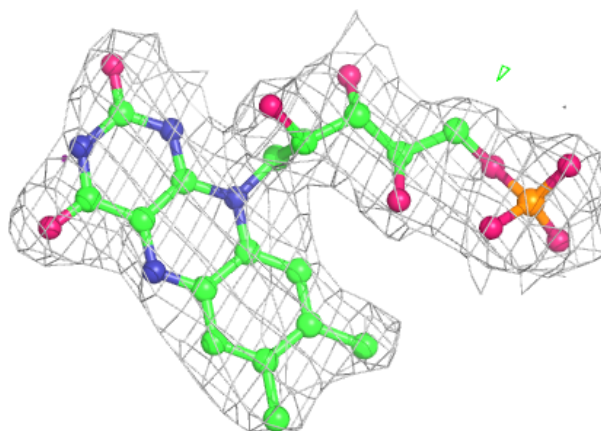
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





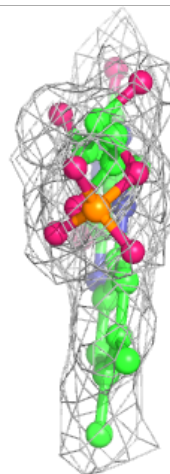
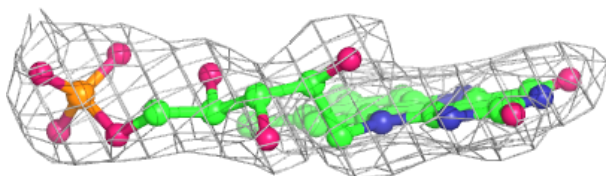
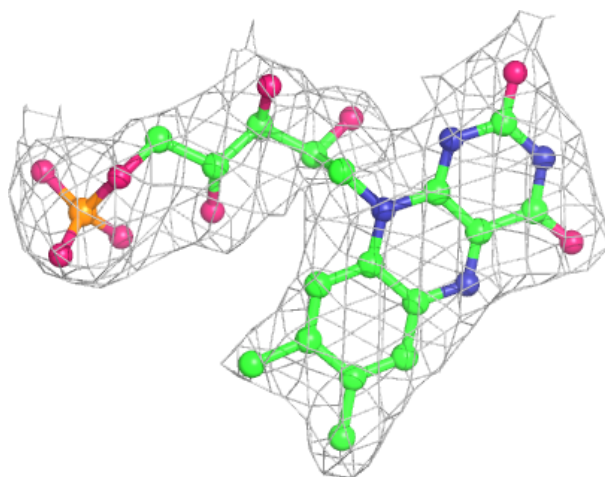
**Electron density around FMN C 400:**

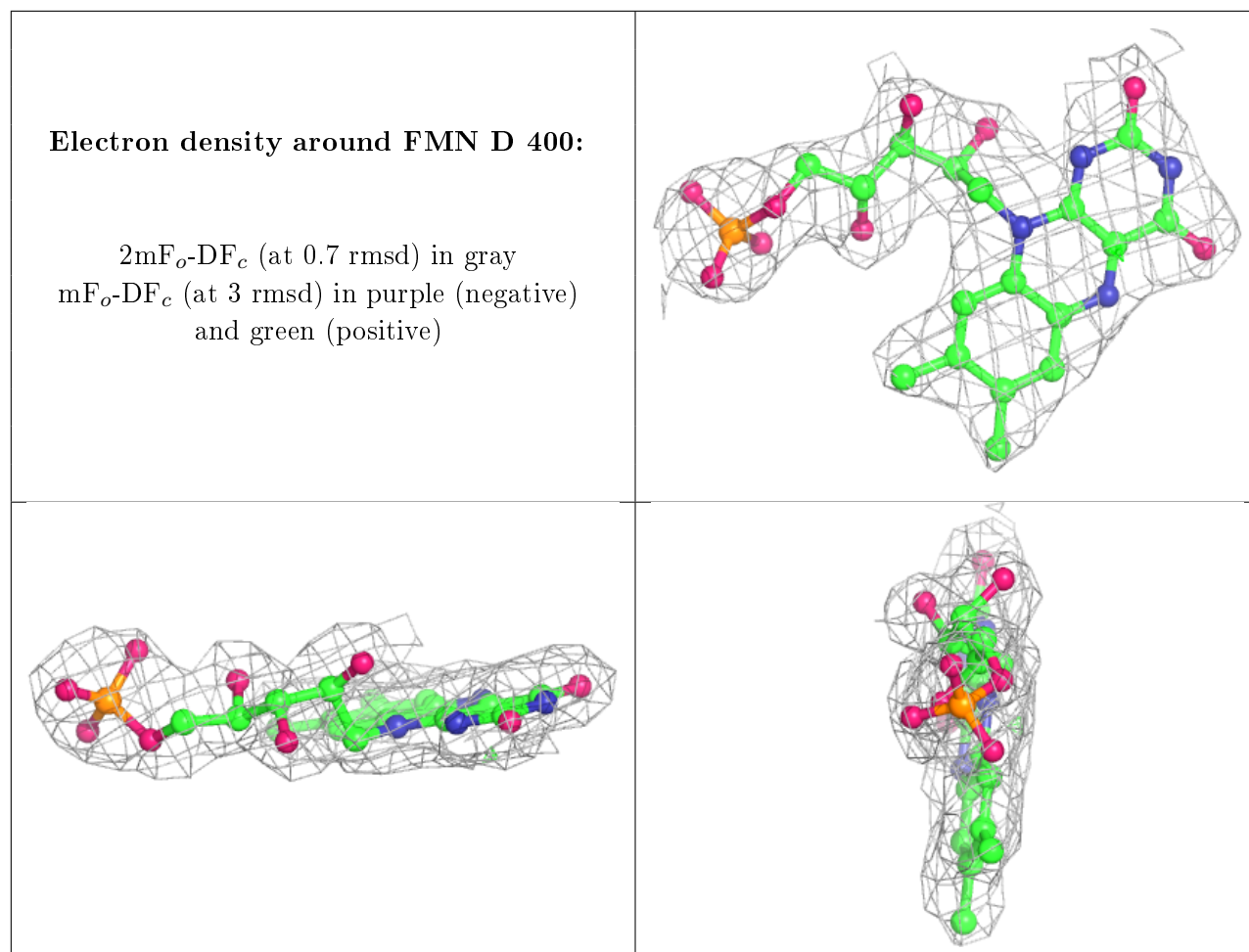
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN E 400:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.