



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:14 am BST

PDB ID : 3W1R  
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-3-045a  
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Deposited on : 2012-11-20  
Resolution : 1.58 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

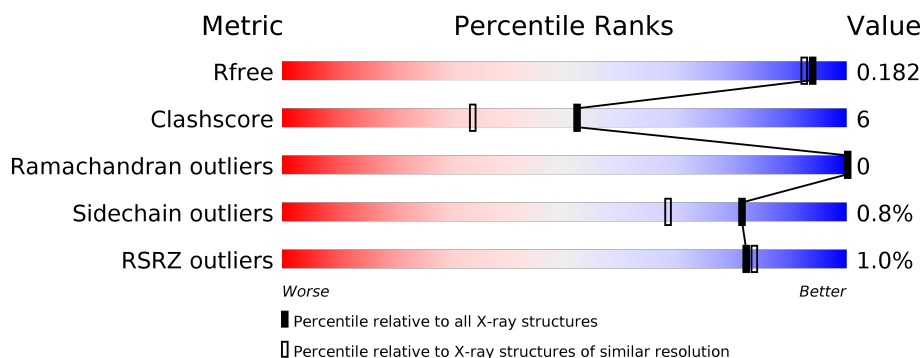
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	313	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>
1	B	313	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	406	-	-	X	-

## 2 Entry composition [i](#)

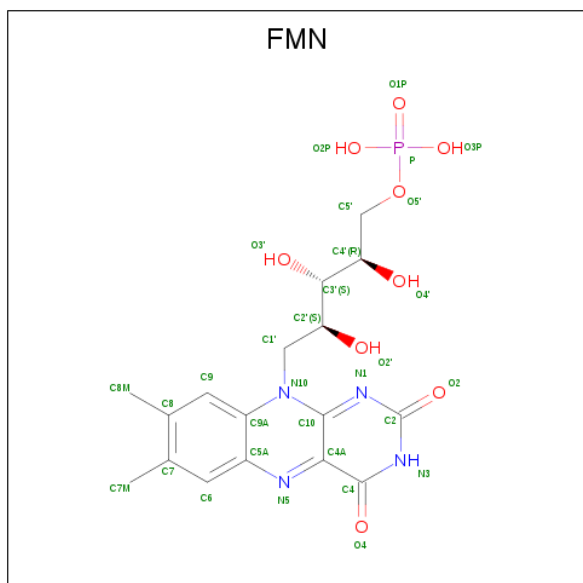
There are 6 unique types of molecules in this entry. The entry contains 5594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydroorotate dehydrogenase (fumarate).

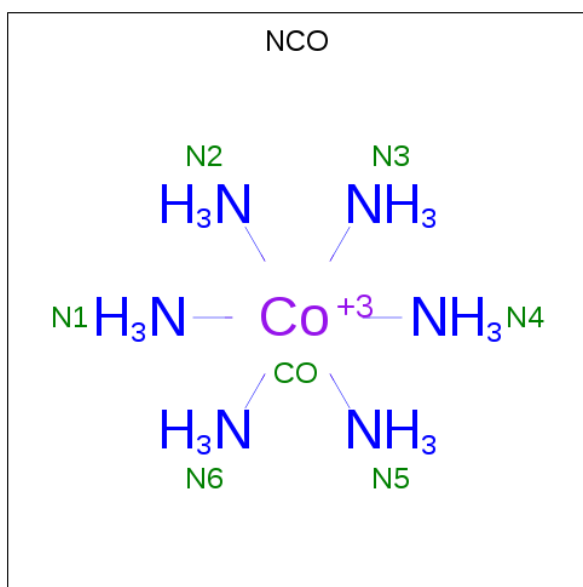
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			
1	B	313	Total	C	N	O	S	0	0	0
			2388	1530	396	444	18			

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



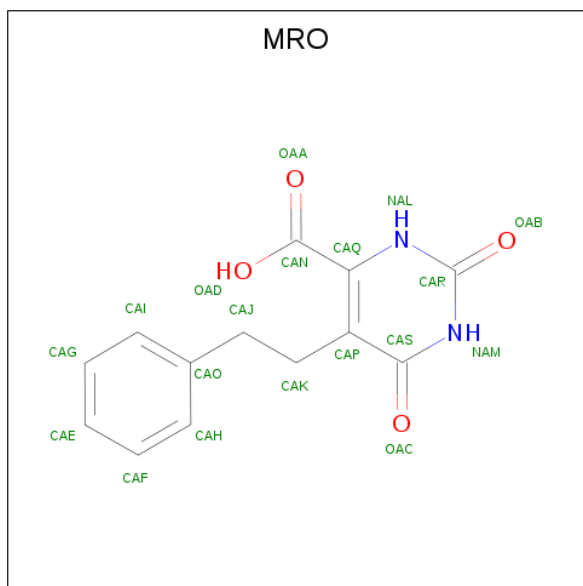
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula:  $CoH_{18}N_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Co	N	0	0
			7	1	6		

- Molecule 4 is 2,6-dioxo-5-(2-phenylethyl)-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: MRO) (formula:  $C_{13}H_{12}N_2O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	13	2	4		
4	B	1	Total	C	N	O	0	0
			19	13	2	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

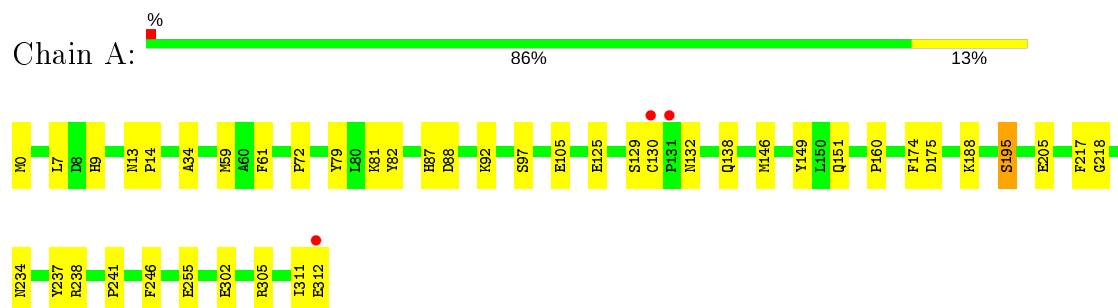
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	336	Total	O	0	0
			336	336		
6	B	339	Total	O	0	0
			339	339		

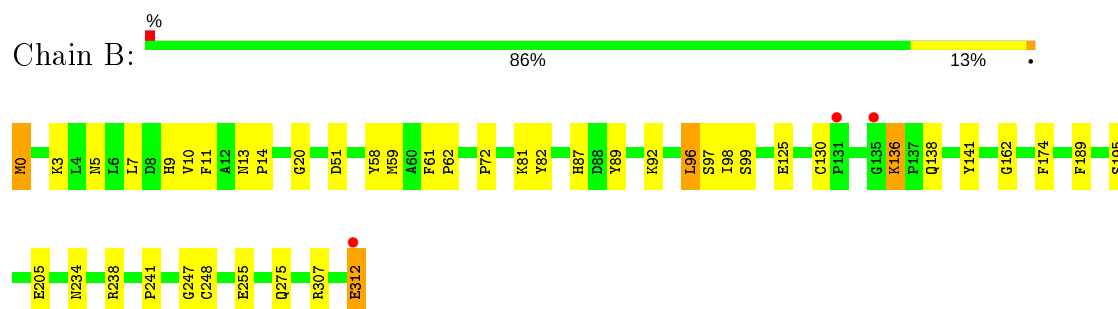
### 3 Residue-property plots [i](#)

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: Dihydroorotate dehydrogenase (fumarate)



- Molecule 1: Dihydroorotate dehydrogenase (fumarate)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.95Å 71.81Å 129.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 – 1.58 46.10 – 1.58	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.10-1.58) 98.6 (46.10-1.58)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.156 , 0.181 0.156 , 0.182	Depositor DCC
$R_{free}$ test set	4286 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	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 26.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6341e-03. 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, GOL, MRO, NCO

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	1.32	10/2440 (0.4%)	1.21	8/3305 (0.2%)
1	B	1.33	10/2440 (0.4%)	1.21	4/3305 (0.1%)
All	All	1.33	20/4880 (0.4%)	1.21	12/6610 (0.2%)

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

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLY	C-O	-6.15	1.13	1.23
1	A	218	GLY	C-O	-6.07	1.14	1.23
1	A	72	PRO	N-CD	5.92	1.56	1.47
1	B	205	GLU	CD-OE1	5.80	1.32	1.25
1	A	195	SER	CB-OG	-5.79	1.34	1.42
1	A	205	GLU	CD-OE2	5.79	1.32	1.25
1	A	105	GLU	CD-OE2	-5.69	1.19	1.25
1	A	61	PHE	CG-CD1	5.69	1.47	1.38
1	B	99	SER	CB-OG	-5.64	1.34	1.42
1	A	149	TYR	CE1-CZ	-5.60	1.31	1.38
1	B	141	TYR	CE1-CZ	-5.50	1.31	1.38
1	B	72	PRO	N-CD	5.49	1.55	1.47
1	A	79	TYR	CG-CD1	5.43	1.46	1.39
1	B	255	GLU	CD-OE1	-5.24	1.19	1.25
1	B	11	PHE	CG-CD1	5.22	1.46	1.38
1	B	58	TYR	CG-CD1	5.11	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLU	CD-OE1	-5.08	1.20	1.25
1	B	248	CYS	C-O	-5.08	1.13	1.23
1	B	89	TYR	CE1-CZ	5.03	1.45	1.38
1	A	255	GLU	CD-OE1	-5.01	1.20	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	51	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	88	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	0	MET	CG-SD-CE	5.69	109.31	100.20
1	A	146	MET	CG-SD-CE	-5.64	91.17	100.20
1	A	237	TYR	CG-CD1-CE1	-5.55	116.86	121.30
1	A	246	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	A	174	PHE	CB-CG-CD1	5.35	124.55	120.80
1	A	130	CYS	N-CA-CB	-5.35	100.97	110.60
1	B	3	LYS	CA-CB-CG	5.12	124.67	113.40
1	B	174	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	B	96	LEU	CB-CG-CD2	-5.02	102.46	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	0	MET	Peptide

## 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	2388	0	2391	24	0
1	B	2388	0	2391	26	0
2	A	31	0	19	0	0
2	B	31	0	19	1	0
3	A	7	0	0	0	0
4	A	19	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	11	3	0
5	A	18	0	24	5	0
5	B	18	0	24	6	0
6	A	336	0	0	8	0
6	B	339	0	0	6	0
All	All	5594	0	4890	54	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 6.

All (54) 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:234:ASN:HD21	1:B:238:ARG:HE	1.21	0.87
1:B:195:SER:HB3	6:B:791:HOH:O	1.76	0.82
1:B:96:LEU:CD2	1:B:98:ILE:HD11	2.16	0.76
1:A:59:MET:CE	6:A:624:HOH:O	2.35	0.74
4:B:402:MRO:CAF	5:B:404:GOL:H31	2.21	0.71
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.40	0.70
5:A:406:GOL:H31	6:A:568:HOH:O	1.91	0.69
4:B:402:MRO:H9	5:B:404:GOL:H31	1.74	0.69
1:B:59:MET:HE3	6:B:623:HOH:O	1.91	0.69
1:A:241:PRO:HA	5:A:406:GOL:H32	1.76	0.67
1:B:234:ASN:ND2	1:B:238:ARG:HE	1.94	0.66
1:A:59:MET:HE3	6:A:624:HOH:O	1.93	0.65
1:B:130:CYS:H	1:B:138:GLN:HE22	1.43	0.64
1:B:96:LEU:CD2	1:B:98:ILE:CD1	2.75	0.64
1:A:129:SER:HA	1:A:138:GLN:OE1	1.97	0.64
1:A:195:SER:HB3	6:A:793:HOH:O	1.98	0.63
1:A:7:LEU:O	1:A:9:HIS:HD2	1.83	0.62
1:B:241:PRO:HA	5:B:405:GOL:H11	1.81	0.62
1:B:136:LYS:HD2	6:B:839:HOH:O	2.00	0.61
1:A:59:MET:HE2	6:A:624:HOH:O	2.00	0.60
1:A:87:HIS:HE1	1:A:92:LYS:O	1.86	0.59
1:B:96:LEU:HD22	1:B:98:ILE:HD11	1.87	0.56
1:B:87:HIS:HE1	1:B:92:LYS:O	1.87	0.56
1:B:59:MET:CE	6:B:623:HOH:O	2.50	0.56
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.89	0.55
1:A:132:ASN:HB3	6:A:808:HOH:O	2.06	0.54
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.90	0.54
1:A:241:PRO:HA	5:A:406:GOL:C3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:402:MRO:CAH	5:B:404:GOL:H31	2.40	0.52
1:A:151:GLN:HB3	6:A:718:HOH:O	2.10	0.50
1:A:160:PRO:HB3	1:A:188:LYS:HG3	1.94	0.50
1:A:9:HIS:HE1	6:A:524:HOH:O	1.96	0.48
1:A:241:PRO:CA	5:A:406:GOL:H32	2.43	0.48
1:B:7:LEU:O	1:B:9:HIS:HD2	1.95	0.48
1:A:302:GLU:HG3	1:A:305:ARG:HH12	1.78	0.47
1:B:307:ARG:NH1	1:B:307:ARG:HG3	2.29	0.47
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.10	0.45
1:B:312:GLU:OE2	1:B:312:GLU:N	2.50	0.45
1:B:97:SER:HA	1:B:125:GLU:O	2.17	0.45
1:A:311:ILE:HG22	1:A:312:GLU:HG3	1.99	0.45
1:A:34:ALA:HB3	5:A:404:GOL:H12	2.00	0.44
1:B:162:GLY:HA3	1:B:189:PHE:CZ	2.53	0.44
1:A:81:LYS:NZ	1:A:81:LYS:HB2	2.34	0.43
1:B:136:LYS:NZ	6:B:805:HOH:O	2.51	0.43
1:B:275:GLN:NE2	6:B:613:HOH:O	2.51	0.43
1:B:13:ASN:HB2	1:B:14:PRO:HD2	2.01	0.43
1:A:217:PHE:CE1	5:B:403:GOL:H12	2.53	0.42
1:A:97:SER:HA	1:A:125:GLU:O	2.20	0.42
1:B:61:PHE:HB3	1:B:62:PRO:HD2	2.01	0.42
1:B:5:ASN:OD1	1:B:10:VAL:HG22	2.20	0.42
1:B:59:MET:HB3	1:B:59:MET:HE3	1.88	0.40
1:B:20:GLY:HA3	2:B:401:FMN:N5	2.36	0.40
1:A:13:ASN:HB2	1:A:14:PRO:HD2	2.04	0.40
1:B:241:PRO:CA	5:B:405:GOL:H11	2.49	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/313 (99%)	301 (97%)	10 (3%)	0	100	100
1	B	311/313 (99%)	302 (97%)	9 (3%)	0	100	100
All	All	622/626 (99%)	603 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/258 (100%)	258 (100%)	0	100	100
1	B	258/258 (100%)	254 (98%)	4 (2%)	62	39
All	All	516/516 (100%)	512 (99%)	4 (1%)	81	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	MET
1	B	81	LYS
1	B	136	LYS
1	B	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	87	HIS
1	A	118	GLN
1	A	151	GLN
1	A	152	GLN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS

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Mol	Chain	Res	Type
1	B	138	GLN
1	B	152	GLN
1	B	234	ASN
1	B	275	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

11 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	$\# Z  > 2$
4	MRO	A	403	-	16,20,20	3.31	8 (50%)	14,27,27	4.07	9 (64%)
2	FMN	A	401	-	31,33,33	2.12	9 (29%)	40,50,50	2.01	7 (17%)
5	GOL	B	403	-	5,5,5	0.69	0	5,5,5	0.63	0
5	GOL	B	404	-	5,5,5	1.20	0	5,5,5	2.22	2 (40%)
5	GOL	A	406	-	5,5,5	0.53	0	5,5,5	0.78	0
5	GOL	A	405	-	5,5,5	0.61	0	5,5,5	0.76	0
5	GOL	B	405	-	5,5,5	0.54	0	5,5,5	1.08	0
3	NCO	A	402	-	6,6,6	2.65	5 (83%)	-		
5	GOL	A	404	-	5,5,5	0.76	0	5,5,5	2.49	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MRO	B	402	-	16,20,20	2.39	7 (43%)	14,27,27	2.39	5 (35%)
2	FMN	B	401	-	31,33,33	1.90	6 (19%)	40,50,50	2.69	10 (25%)

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
4	MRO	A	403	-	-	0/5/9/9	0/2/2/2
2	FMN	A	401	-	-	2/18/18/18	0/3/3/3
5	GOL	B	403	-	-	0/4/4/4	-
5	GOL	B	404	-	-	2/4/4/4	-
5	GOL	A	406	-	-	4/4/4/4	-
5	GOL	A	405	-	-	0/4/4/4	-
5	GOL	B	405	-	-	2/4/4/4	-
5	GOL	A	404	-	-	2/4/4/4	-
4	MRO	B	402	-	-	0/5/9/9	0/2/2/2
2	FMN	B	401	-	-	1/18/18/18	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C4A-C10	8.12	1.46	1.38
2	B	401	FMN	C4A-C10	6.74	1.45	1.38
4	A	403	MRO	CAQ-NAL	6.22	1.44	1.34
4	B	402	MRO	CAQ-NAL	5.79	1.43	1.34
4	A	403	MRO	CAS-NAM	5.73	1.43	1.33
4	A	403	MRO	CAK-CAP	-5.67	1.42	1.52
4	A	403	MRO	CAJ-CAO	-5.41	1.36	1.51
4	B	402	MRO	CAS-NAM	4.22	1.40	1.33
2	B	401	FMN	C4-C4A	3.86	1.48	1.41
4	B	402	MRO	CAJ-CAO	-3.59	1.41	1.51
4	A	403	MRO	CAI-CAO	3.57	1.46	1.38
2	B	401	FMN	C5'-C4'	3.46	1.56	1.51
3	A	402	NCO	CO-N6	3.28	2.08	1.96
3	A	402	NCO	CO-N1	3.17	2.08	1.96
3	A	402	NCO	CO-N3	3.11	2.07	1.96
4	A	403	MRO	CAG-CAI	3.03	1.45	1.38
2	A	401	FMN	C5'-C4'	2.86	1.55	1.51
2	A	401	FMN	C4-C4A	2.71	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C9A-N10	2.67	1.42	1.38
2	A	401	FMN	C1'-N10	-2.59	1.45	1.48
2	A	401	FMN	C8-C7	2.42	1.46	1.40
4	B	402	MRO	CAF-CAH	2.41	1.44	1.38
2	B	401	FMN	C4A-N5	2.41	1.36	1.33
4	A	403	MRO	CAQ-CAP	-2.40	1.36	1.40
2	A	401	FMN	C4-N3	2.31	1.37	1.33
4	B	402	MRO	CAH-CAO	2.26	1.43	1.38
2	B	401	FMN	C6-C7	2.22	1.43	1.37
4	A	403	MRO	CAG-CAE	2.20	1.43	1.38
2	A	401	FMN	C4'-C3'	2.14	1.57	1.53
3	A	402	NCO	CO-N4	2.13	2.04	1.96
4	B	402	MRO	CAK-CAP	2.12	1.55	1.52
2	A	401	FMN	C9-C8	2.10	1.43	1.37
3	A	402	NCO	CO-N2	2.08	2.04	1.96
2	B	401	FMN	C1'-N10	-2.05	1.46	1.48
4	B	402	MRO	CAQ-CAP	-2.04	1.36	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	MRO	CAS-NAM-CAR	10.03	123.61	115.14
2	B	401	FMN	C1'-N10-C9A	8.23	124.77	118.29
2	B	401	FMN	C4-N3-C2	8.13	122.01	115.14
2	A	401	FMN	C4-N3-C2	7.75	121.68	115.14
2	B	401	FMN	C4-C4A-C10	-7.31	115.11	119.95
4	B	402	MRO	CAS-NAM-CAR	6.68	120.79	115.14
4	A	403	MRO	CAE-CAG-CAI	-6.22	110.71	120.19
4	A	403	MRO	CAF-CAH-CAO	-6.04	111.37	120.63
2	A	401	FMN	C4-C4A-C10	-5.92	116.03	119.95
2	B	401	FMN	C1'-N10-C10	-4.36	114.50	118.41
4	A	403	MRO	CAE-CAF-CAH	4.25	126.66	120.19
2	B	401	FMN	C7-C6-C5A	-4.15	115.34	121.22
5	A	404	GOL	O2-C2-C1	-3.67	92.95	109.12
2	A	401	FMN	C4A-C4-N3	-3.56	118.56	123.43
5	B	404	GOL	O2-C2-C3	-3.36	94.31	109.12
2	B	401	FMN	C4-C4A-N5	3.34	122.42	118.60
5	B	404	GOL	O1-C1-C2	3.32	126.12	110.20
4	B	402	MRO	CAE-CAG-CAI	3.20	125.06	120.19
2	B	401	FMN	C4A-C4-N3	-3.19	119.07	123.43
4	B	402	MRO	CAR-NAL-CAQ	3.07	119.25	115.24
5	A	404	GOL	O2-C2-C3	-3.00	95.90	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	MRO	CAI-CAO-CAH	2.93	122.77	118.17
2	B	401	FMN	C4A-C10-N10	-2.89	117.33	120.30
4	A	403	MRO	CAJ-CAO-CAH	-2.81	114.11	121.23
5	A	404	GOL	C3-C2-C1	2.73	122.33	111.70
2	A	401	FMN	C4A-C10-N10	-2.70	117.53	120.30
2	A	401	FMN	C10-C4A-N5	2.66	123.10	121.26
4	A	403	MRO	CAG-CAI-CAO	2.66	124.71	120.63
4	A	403	MRO	CAR-NAL-CAQ	2.53	118.55	115.24
2	A	401	FMN	C1'-N10-C9A	2.40	120.18	118.29
4	B	402	MRO	CAG-CAI-CAO	-2.32	117.07	120.63
2	B	401	FMN	C6-C5A-N5	-2.28	116.54	119.05
4	B	402	MRO	CAJ-CAK-CAP	-2.25	108.33	112.48
2	A	401	FMN	O2'-C2'-C1'	-2.18	104.36	109.59
2	B	401	FMN	C6-C7-C8	2.17	123.57	119.91
4	A	403	MRO	CAG-CAE-CAF	2.06	123.76	119.93

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406	GOL	O1-C1-C2-C3
5	A	406	GOL	C1-C2-C3-O3
5	B	404	GOL	C1-C2-C3-O3
5	B	405	GOL	O1-C1-C2-C3
5	A	404	GOL	O2-C2-C3-O3
5	A	406	GOL	O1-C1-C2-O2
5	B	405	GOL	O1-C1-C2-O2
5	A	406	GOL	O2-C2-C3-O3
5	B	404	GOL	O2-C2-C3-O3
2	A	401	FMN	C4'-C5'-O5'-P
2	B	401	FMN	C4'-C5'-O5'-P
5	A	404	GOL	C1-C2-C3-O3
2	A	401	FMN	O3'-C3'-C4'-C5'

There are no ring outliers.

7 monomers are involved in 12 short contacts:

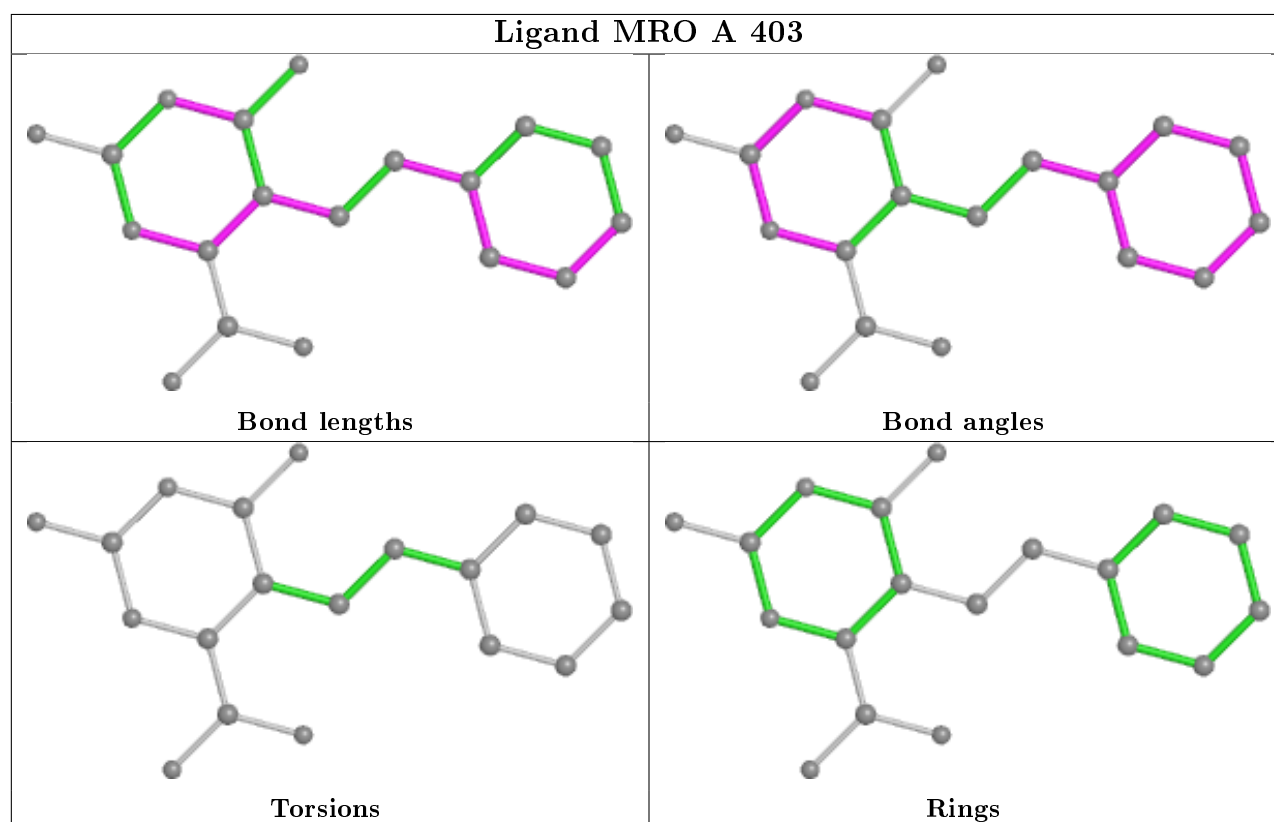
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	GOL	1	0
5	B	404	GOL	3	0
5	A	406	GOL	4	0

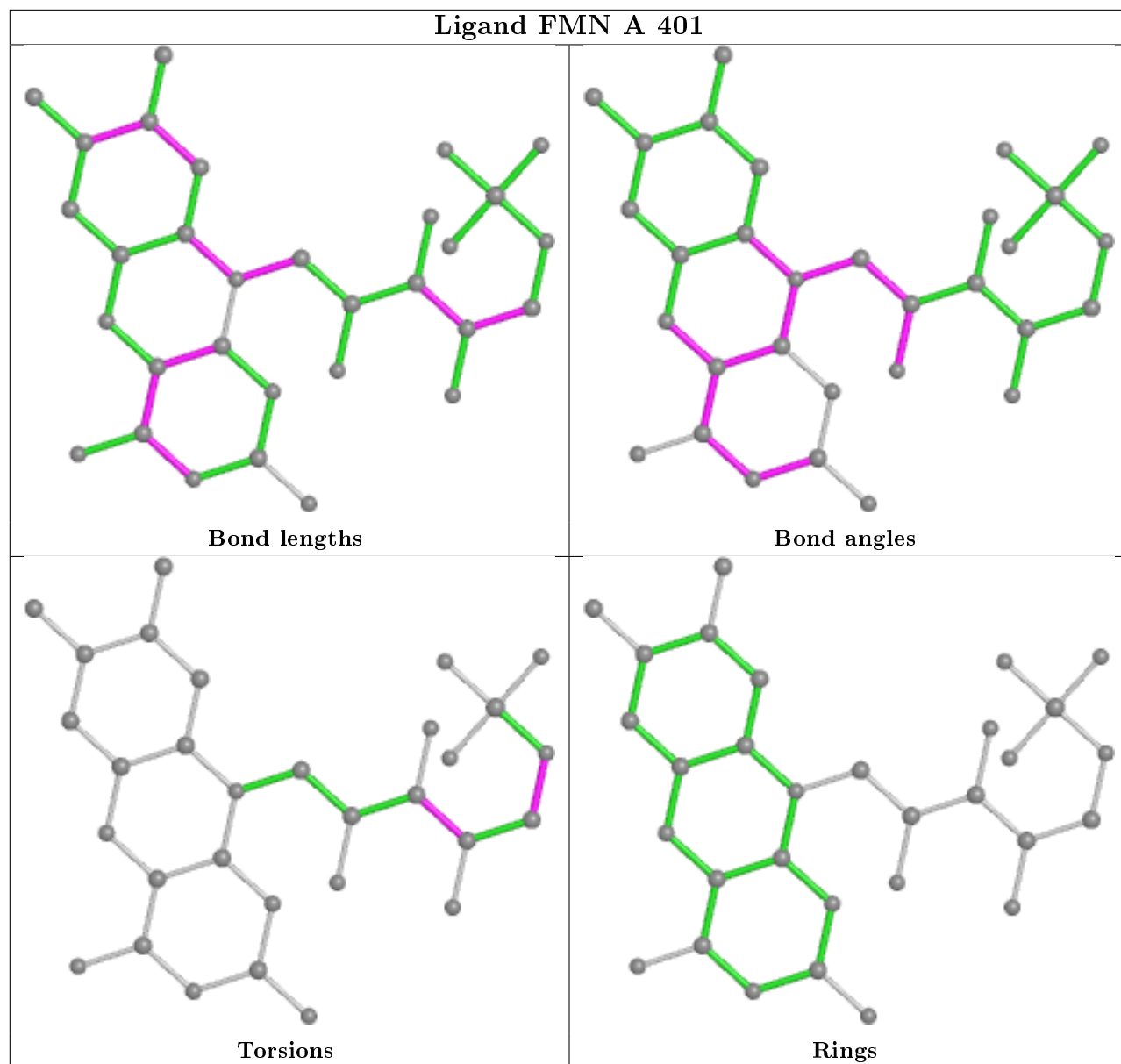
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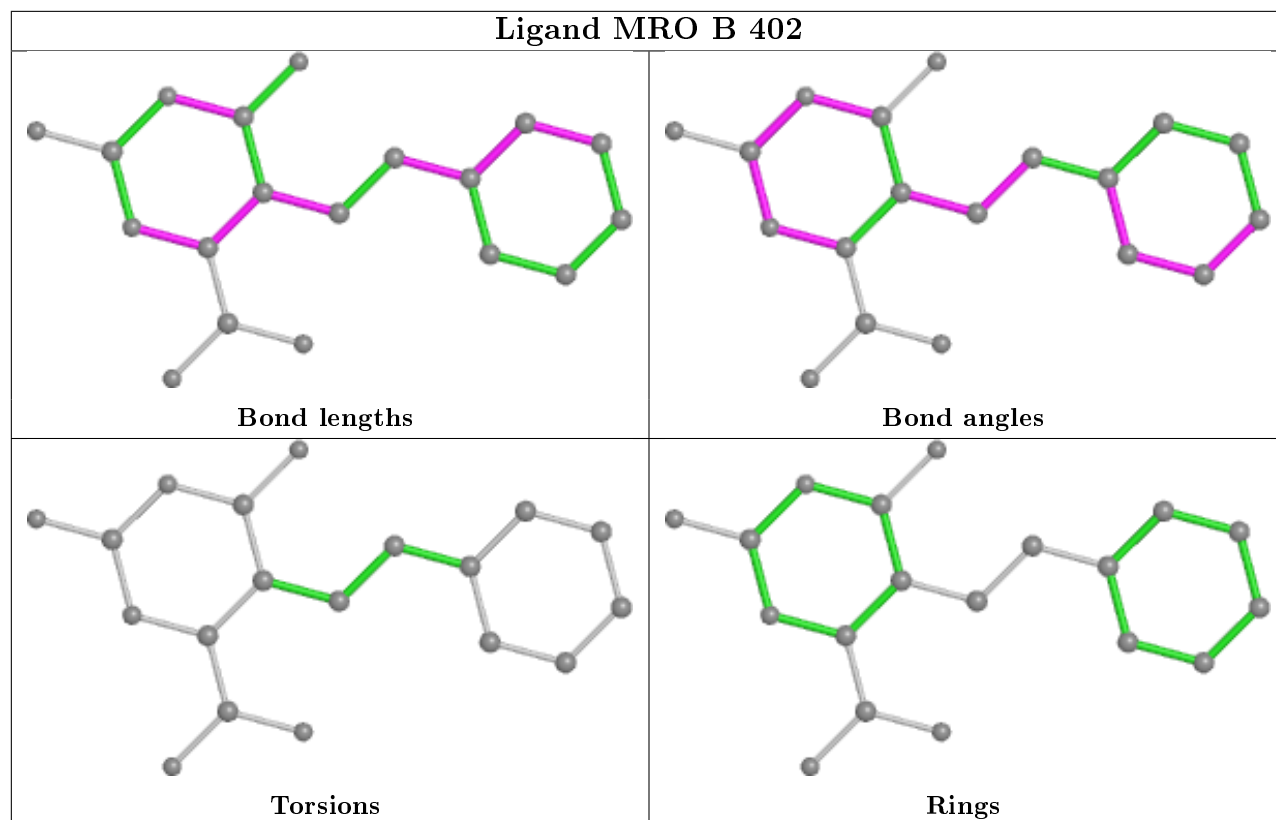
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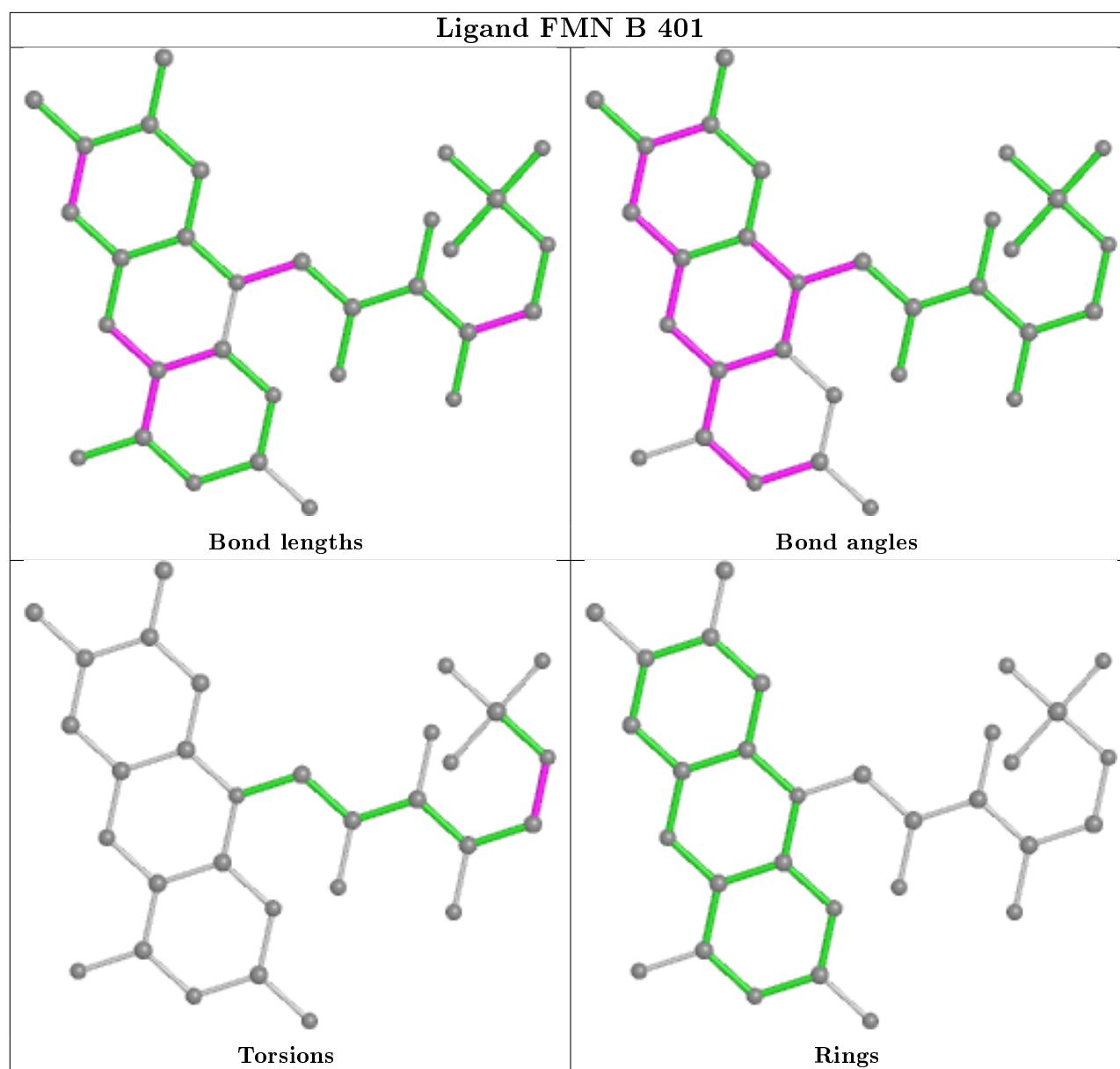
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	405	GOL	2	0
5	A	404	GOL	1	0
4	B	402	MRO	3	0
2	B	401	FMN	1	0

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, 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	313/313 (100%)	-0.41	3 (0%) 82 83	5, 9, 21, 41	0
1	B	313/313 (100%)	-0.29	3 (0%) 82 83	5, 10, 22, 47	0
All	All	626/626 (100%)	-0.35	6 (0%) 82 83	5, 10, 21, 47	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	CYS	3.3
1	B	312	GLU	3.2
1	A	312	GLU	2.9
1	A	131	PRO	2.7
1	B	135	GLY	2.4
1	B	131	PRO	2.2

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

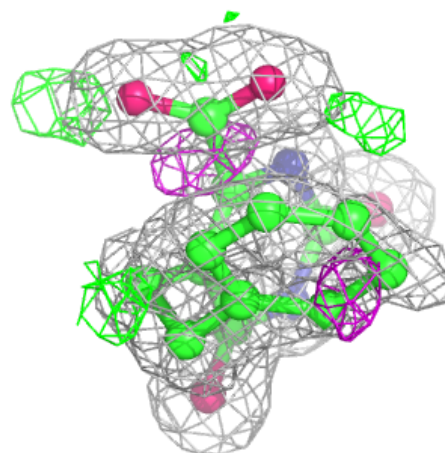
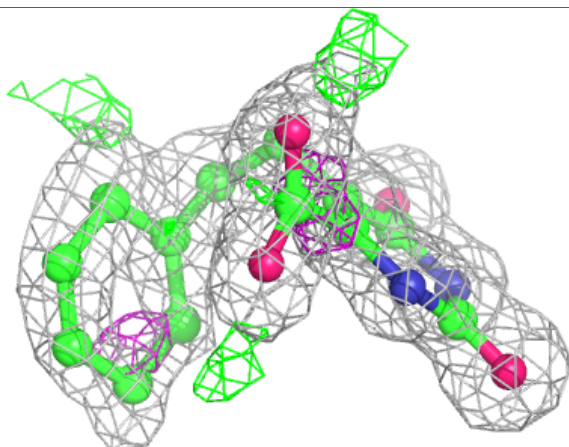
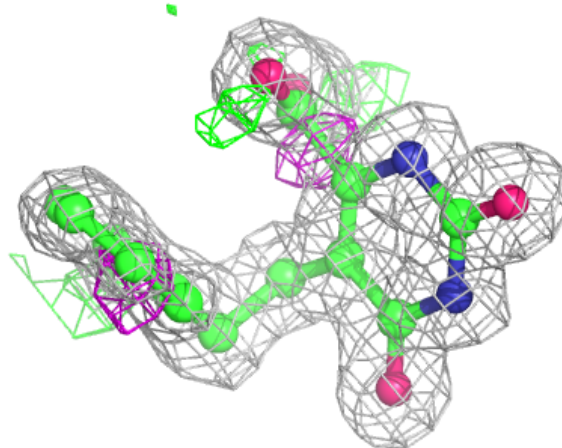
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
5	GOL	A	406	6/6	0.80	0.15	30,38,41,42	0
5	GOL	B	405	6/6	0.84	0.14	32,37,37,42	0
5	GOL	B	404	6/6	0.85	0.19	17,24,30,32	0
5	GOL	A	404	6/6	0.92	0.10	13,17,19,20	0
5	GOL	B	403	6/6	0.94	0.07	17,20,21,24	0
4	MRO	A	403	19/19	0.95	0.09	7,10,23,23	0
5	GOL	A	405	6/6	0.96	0.06	14,15,17,18	0
4	MRO	B	402	19/19	0.97	0.07	7,9,19,20	0
2	FMN	A	401	31/31	0.98	0.07	5,5,8,10	0
3	NCO	A	402	7/7	0.99	0.08	8,8,10,10	0
2	FMN	B	401	31/31	0.99	0.06	5,6,7,8	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.

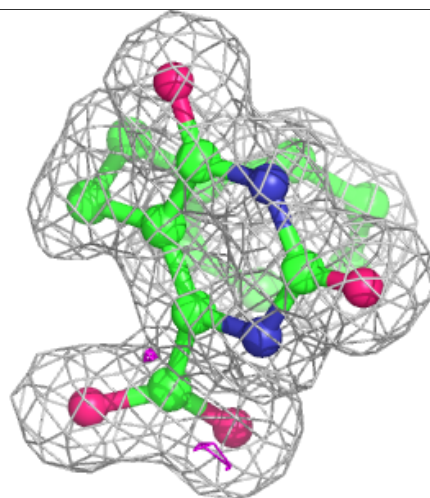
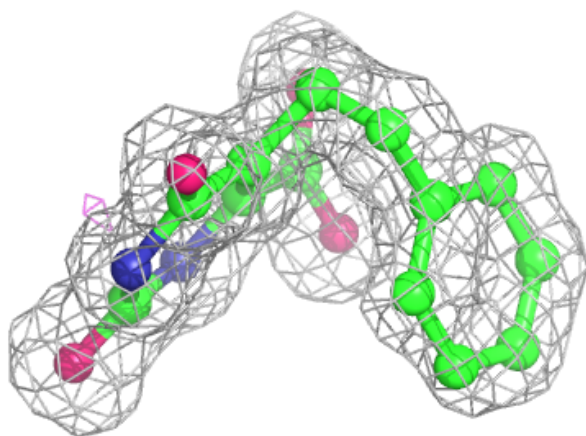
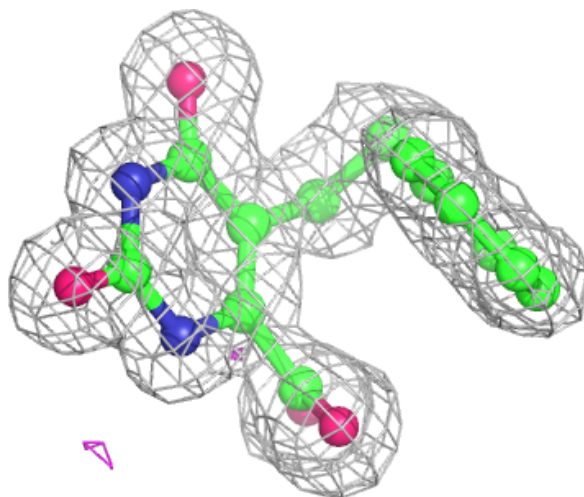
**Electron density around MRO A 403:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MRO B 402:**

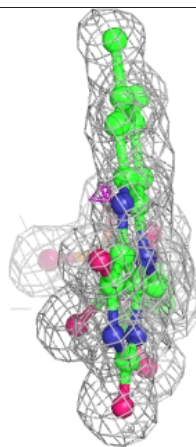
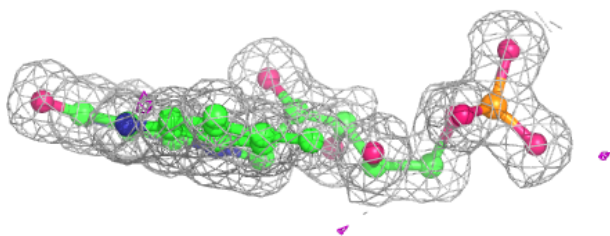
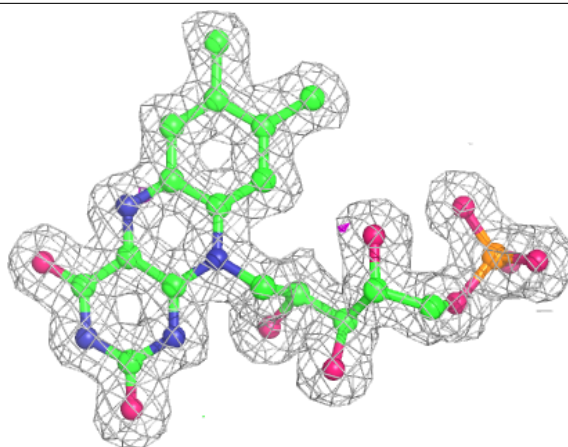
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





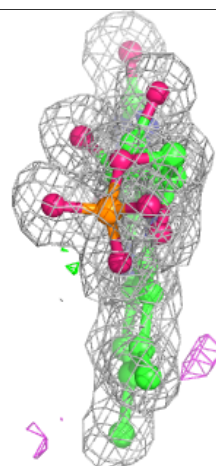
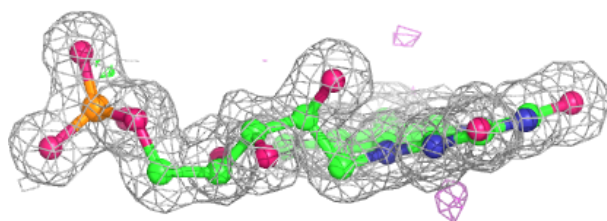
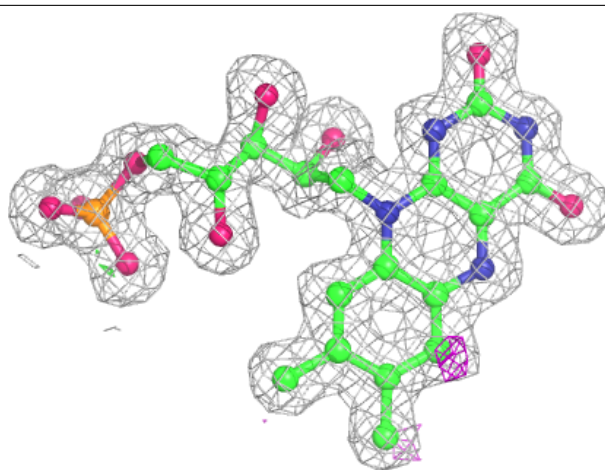
**Electron density around FMN A 401:**

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



**Electron density around FMN B 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.