



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:51 PM BST

PDB ID : 3W7D  
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-5-170  
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Deposited on : 2013-02-28  
Resolution : 1.52 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 : 2.13.1  
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) : 2.13.1

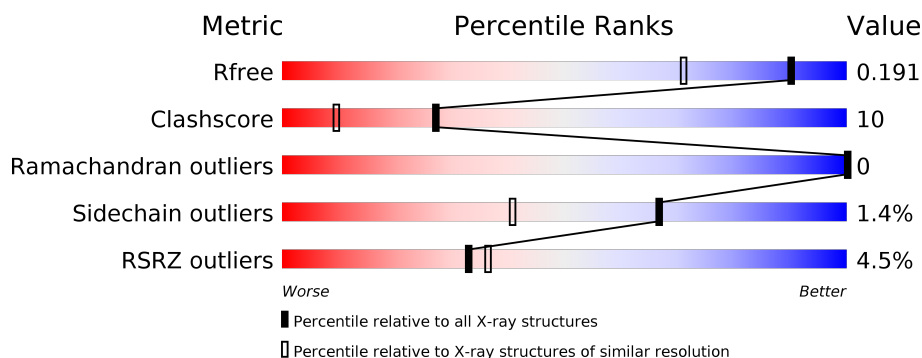
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	
1	B	313	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	402	-	X	-	-
3	GOL	A	410	-	-	X	-
3	GOL	B	402	-	X	X	-
3	GOL	B	406	-	X	-	-
3	GOL	B	408	-	-	X	-

## 2 Entry composition [i](#)

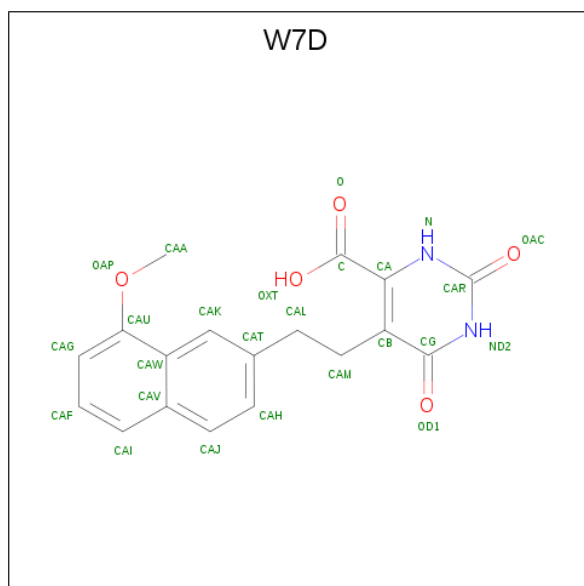
There are 6 unique types of molecules in this entry. The entry contains 5705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3	0
			2404	1540	400	446	18			
1	B	313	Total	C	N	O	S	0	3	0
			2406	1542	400	445	19			

- Molecule 2 is 5-[2-(8-methoxynaphthalen-2-yl)ethyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: W7D) (formula: C<sub>18</sub>H<sub>16</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	18	2	5		
2	B	1	Total	C	N	O	0	0
			25	18	2	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



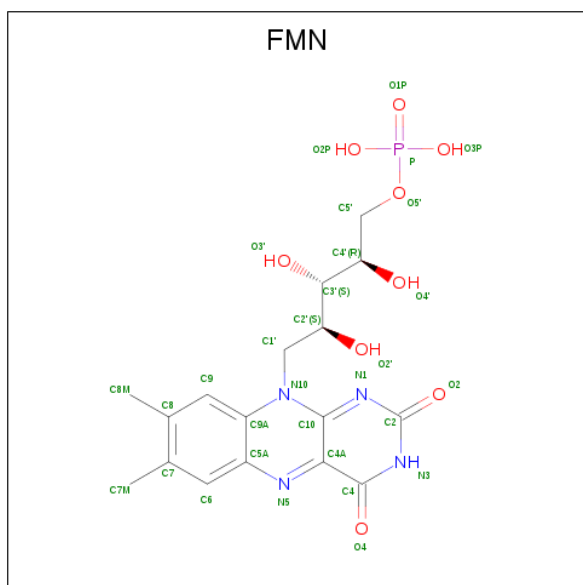
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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

- Molecule 5 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula:  $CoH_{18}N_6$ ).



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

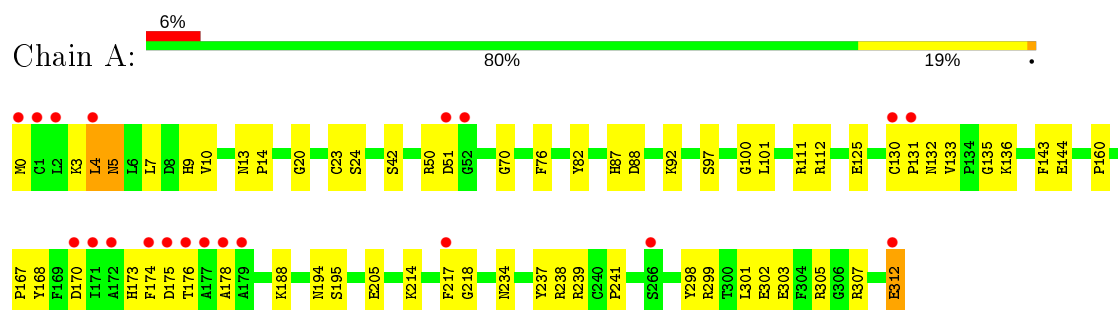
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	362	Total	O	0	0
			362	362		
6	B	312	Total	O	0	0
			312	312		

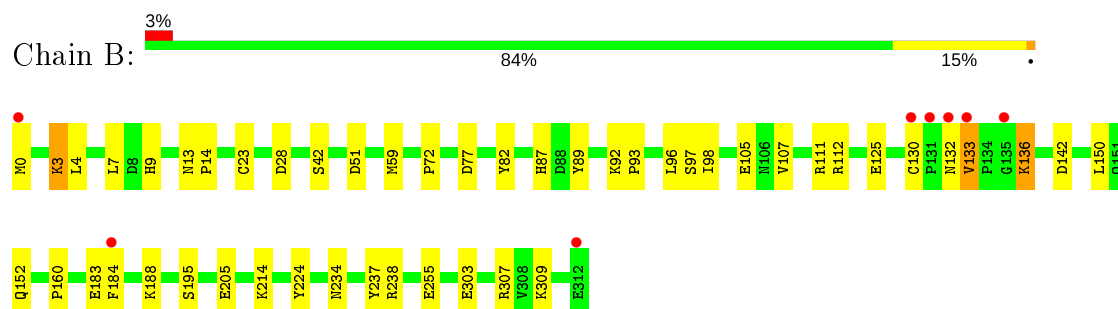
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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, $\alpha$ , $\beta$ , $\gamma$	67.99Å 71.57Å 129.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.52 49.29 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.34-1.52) 99.1 (49.29-1.52)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.145 , 0.173 0.167 , 0.191	Depositor DCC
$R_{free}$ test set	4820 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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 29.27 % 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 1.5955e-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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, GOL, W7D, 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	1.14	5/2465 (0.2%)	1.04	4/3338 (0.1%)
1	B	1.18	4/2467 (0.2%)	1.10	7/3340 (0.2%)
All	All	1.16	9/4932 (0.2%)	1.07	11/6678 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	GLY	C-N	5.86	1.47	1.34
1	B	303	GLU	CD-OE2	-5.72	1.19	1.25
1	B	183	GLU	CD-OE2	-5.50	1.19	1.25
1	B	224	TYR	CE1-CZ	-5.46	1.31	1.38
1	B	255	GLU	CD-OE1	-5.29	1.19	1.25
1	A	218	GLY	C-O	-5.18	1.15	1.23
1	A	24	SER	C-O	-5.17	1.13	1.23
1	A	144	GLU	CD-OE2	5.17	1.31	1.25
1	A	135	GLY	C-O	-5.11	1.15	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	112	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	88	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	3	LYS	CA-CB-CG	5.53	125.57	113.40
1	B	142	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	105	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	B	309	LYS	CD-CE-NZ	-5.34	99.41	111.70
1	A	76	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	A	88	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	112	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	LEU	CB-CG-CD1	5.03	119.56	111.00

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	2404	0	2415	54	0
1	B	2406	0	2419	39	0
2	A	25	0	15	0	0
2	B	25	0	15	2	0
3	A	60	0	80	5	0
3	B	42	0	53	16	0
4	A	31	0	19	1	0
4	B	31	0	19	0	0
5	A	7	0	0	0	0
6	A	362	0	0	9	0
6	B	312	0	0	15	0
All	All	5705	0	5035	102	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 10.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:HD3	6:A:844:HOH:O	1.51	1.09
1:B:214:LYS:HD3	6:B:801:HOH:O	1.53	1.06
1:A:168:TYR:HB2	1:A:174:PHE:CE1	1.93	1.03
1:B:133:VAL:HG13	1:B:136:LYS:HD3	1.48	0.94
1:B:152:GLN:HG3	6:B:807:HOH:O	1.69	0.93
1:B:195:SER:HB3	6:B:752:HOH:O	1.73	0.89
1:B:150:LEU:HB2	1:B:184:PHE:CZ	2.08	0.89
1:A:101:LEU:CD2	1:A:131:PRO:HG2	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:HIS:CE1	3:B:408:GOL:H32	2.13	0.84
1:A:195:SER:HB3	6:A:770:HOH:O	1.80	0.80
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.35	0.75
1:B:150:LEU:HB2	1:B:184:PHE:CE2	2.21	0.74
1:A:101:LEU:HD22	1:A:131:PRO:HG2	1.68	0.74
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.35	0.73
1:B:9:HIS:ND1	3:B:408:GOL:H32	2.03	0.73
1:A:217:PHE:CE1	3:A:409:GOL:H12	2.25	0.72
1:A:298:TYR:HA	1:A:303:GLU:OE1	1.88	0.72
1:A:168:TYR:HB2	1:A:174:PHE:CD1	2.27	0.69
1:B:150:LEU:CB	1:B:184:PHE:CZ	2.75	0.69
1:A:175:ASP:OD1	1:A:239:ARG:NE	2.22	0.69
1:A:4:LEU:HD12	1:A:4:LEU:N	2.08	0.69
1:A:312:GLU:C	1:A:312:GLU:OE1	2.31	0.69
1:B:133:VAL:CG1	1:B:136:LYS:HD3	2.24	0.66
1:A:51:ASP:HB2	6:A:566:HOH:O	1.95	0.66
1:B:59[A]:MET:HE3	6:B:611:HOH:O	1.96	0.66
1:A:7:LEU:O	1:A:9:HIS:HD2	1.81	0.64
1:B:214:LYS:CE	6:B:801:HOH:O	2.47	0.63
1:B:93:PRO:HA	3:B:408:GOL:H12	1.81	0.63
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.82	0.62
1:A:214:LYS:CE	6:A:844:HOH:O	2.47	0.62
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.81	0.62
1:B:96:LEU:CD2	1:B:98:ILE:HD11	2.30	0.61
1:B:150:LEU:CB	1:B:184:PHE:CE2	2.83	0.60
1:B:130:CYS:SG	6:B:558:HOH:O	2.53	0.59
1:B:96:LEU:HD22	1:B:98:ILE:HD11	1.84	0.58
1:A:0:MET:HA	1:A:299:ARG:O	2.03	0.58
1:A:214:LYS:CD	6:A:844:HOH:O	2.26	0.58
1:B:214:LYS:CD	6:B:801:HOH:O	2.28	0.58
1:B:307:ARG:NH1	1:B:307:ARG:HG3	2.18	0.57
1:A:168:TYR:HB2	1:A:174:PHE:HE1	1.61	0.57
1:A:303:GLU:O	1:A:307:ARG:HD3	2.05	0.57
3:B:408:GOL:C3	6:B:511:HOH:O	2.53	0.56
1:A:175:ASP:OD1	1:A:239:ARG:NH2	2.37	0.56
3:B:402:GOL:H12	6:B:586:HOH:O	2.05	0.56
1:A:241:PRO:HA	3:A:410:GOL:H31	1.89	0.55
1:B:237:TYR:CE2	3:B:407:GOL:H31	2.41	0.55
1:A:4:LEU:HD23	1:A:305:ARG:NH2	2.21	0.55
1:A:178:ALA:HB3	6:A:601:HOH:O	2.06	0.54
1:B:7:LEU:O	1:B:9:HIS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TYR:O	1:A:174:PHE:CZ	2.61	0.53
1:B:9:HIS:CE1	3:B:408:GOL:C3	2.89	0.53
1:B:0:MET:HE2	6:B:803:HOH:O	2.09	0.52
1:A:241:PRO:HA	3:A:410:GOL:C3	2.40	0.51
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.04	0.51
1:B:87:HIS:HE1	1:B:92:LYS:O	1.94	0.50
1:A:101:LEU:HD23	1:A:131:PRO:HG2	1.92	0.50
1:A:132:ASN:ND2	1:A:133:VAL:H	2.10	0.50
1:A:298:TYR:CA	1:A:303:GLU:OE1	2.58	0.49
1:A:50:ARG:HD2	6:A:552:HOH:O	2.13	0.49
1:B:89:TYR:HD2	3:B:408:GOL:H31	1.77	0.49
1:A:132:ASN:ND2	1:A:136:LYS:HD3	2.27	0.49
1:A:167:PRO:HD3	1:A:194:ASN:O	2.13	0.49
1:A:87:HIS:HE1	1:A:92:LYS:O	1.96	0.48
1:A:160:PRO:HB3	1:A:188:LYS:HG3	1.94	0.48
1:A:170:ASP:HB3	1:A:173:HIS:HB2	1.96	0.48
1:B:96:LEU:CD2	1:B:98:ILE:CD1	2.92	0.48
3:B:408:GOL:H31	6:B:511:HOH:O	2.12	0.48
1:A:178:ALA:HB1	1:A:239:ARG:HB3	1.97	0.47
3:B:402:GOL:H32	6:B:543:HOH:O	2.14	0.47
1:A:302:GLU:HG3	1:A:305:ARG:HH12	1.81	0.46
1:B:93:PRO:CA	3:B:408:GOL:H12	2.45	0.45
1:A:178:ALA:CB	1:A:239:ARG:HB3	2.47	0.45
1:B:13:ASN:HB2	1:B:14:PRO:HD2	1.99	0.45
3:B:402:GOL:C3	6:B:543:HOH:O	2.65	0.44
1:B:205:GLU:CD	1:B:205:GLU:C	2.76	0.44
1:A:5[B]:ASN:OD1	1:A:10:VAL:HG13	2.17	0.44
1:B:28:ASP:OD1	3:B:402:GOL:H12	2.17	0.44
2:B:401:W7D:H9	3:B:406:GOL:H32	1.99	0.44
1:A:237:TYR:O	3:A:410:GOL:H11	2.17	0.43
2:B:401:W7D:H9	3:B:406:GOL:C3	2.48	0.43
1:A:100:GLY:O	1:A:130:CYS:HB2	2.19	0.43
1:B:107:VAL:O	1:B:111:ARG:HG3	2.18	0.43
1:B:51:ASP:O	1:B:72:PRO:HB3	2.18	0.43
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.08	0.42
1:A:132:ASN:CG	1:A:133:VAL:H	2.23	0.42
1:A:23:CYS:HB2	1:A:42:SER:HA	2.01	0.42
1:A:4:LEU:HD21	1:A:301:LEU:CD1	2.49	0.42
1:B:97:SER:HA	1:B:125:GLU:O	2.20	0.42
1:A:111:ARG:NH1	6:A:545:HOH:O	2.53	0.42
1:A:13:ASN:HB2	1:A:14:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TYR:CB	1:A:174:PHE:CE1	2.85	0.42
1:B:160:PRO:HB3	1:B:188:LYS:HG3	2.01	0.41
1:A:175:ASP:OD1	1:A:239:ARG:CZ	2.68	0.41
1:A:205:GLU:CD	1:A:205:GLU:C	2.79	0.41
1:A:3:LYS:HE3	1:A:10:VAL:CG1	2.50	0.41
1:A:143:PHE:CD2	1:A:176:THR:HG21	2.55	0.41
1:B:0:MET:HG2	6:B:764:HOH:O	2.20	0.41
3:A:410:GOL:H31	6:A:569:HOH:O	2.21	0.40
1:A:20:GLY:HA3	4:A:411:FMN:N5	2.35	0.40
3:B:408:GOL:H2	6:B:740:HOH:O	2.20	0.40
1:A:97:SER:HA	1:A:125:GLU:O	2.22	0.40
1:B:23:CYS:HB2	1:B:42:SER:HA	2.03	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	314/313 (100%)	306 (98%)	8 (2%)	0	100	100
1	B	314/313 (100%)	305 (97%)	9 (3%)	0	100	100
All	All	628/626 (100%)	611 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	261/258 (101%)	257 (98%)	4 (2%)	65	38
1	B	261/258 (101%)	257 (98%)	4 (2%)	65	38
All	All	522/516 (101%)	514 (98%)	8 (2%)	67	38

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5[A]	ASN
1	A	5[B]	ASN
1	A	312	GLU
1	B	3	LYS
1	B	132	ASN
1	B	133	VAL
1	B	136	LYS

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	132	ASN
1	A	152	GLN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS
1	B	132	ASN
1	B	215	GLN
1	B	234	ASN
1	B	275	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

22 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	GOL	B	402	-	5,5,5	5.32	1 (20%)	5,5,5	4.24	4 (80%)
3	GOL	B	407	-	5,5,5	0.36	0	5,5,5	0.74	0
3	GOL	A	403	-	5,5,5	0.77	0	5,5,5	0.84	0
3	GOL	A	408	-	5,5,5	0.46	0	5,5,5	0.72	0
3	GOL	B	405	-	5,5,5	0.45	0	5,5,5	0.36	0
3	GOL	B	406	-	5,5,5	1.22	1 (20%)	5,5,5	1.78	3 (60%)
4	FMN	B	409	-	31,33,33	1.97	8 (25%)	40,50,50	2.60	12 (30%)
3	GOL	A	404	-	5,5,5	0.69	0	5,5,5	0.39	0
2	W7D	A	401	-	23,27,27	2.34	8 (34%)	25,38,38	3.34	7 (28%)
3	GOL	B	408	-	5,5,5	0.94	0	5,5,5	2.59	3 (60%)
3	GOL	B	403	-	5,5,5	0.45	0	5,5,5	0.69	0
3	GOL	A	407[A]	-	5,5,5	0.54	0	5,5,5	0.54	0
3	GOL	A	406	-	5,5,5	0.29	0	5,5,5	0.33	0
3	GOL	A	407[B]	-	5,5,5	0.91	0	5,5,5	0.87	0
5	NCO	A	412	-	6,6,6	2.68	6 (100%)	-		
4	FMN	A	411	-	31,33,33	1.79	4 (12%)	40,50,50	2.38	10 (25%)
3	GOL	A	410	-	5,5,5	0.53	0	5,5,5	0.58	0
3	GOL	B	404	-	5,5,5	0.85	0	5,5,5	1.39	1 (20%)
3	GOL	A	409	-	5,5,5	0.39	0	5,5,5	0.68	0
2	W7D	B	401	-	23,27,27	2.03	6 (26%)	25,38,38	2.90	6 (24%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	405	-	5,5,5	0.23	0	5,5,5	0.60	0
3	GOL	A	402	-	5,5,5	3.33	4 (80%)	5,5,5	3.60	3 (60%)

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	GOL	A	406	-	-	2/4/4/4	-
3	GOL	B	405	-	-	2/4/4/4	-
4	FMN	B	409	-	-	1/18/18/18	0/3/3/3
3	GOL	B	406	-	-	2/4/4/4	-
3	GOL	B	403	-	-	2/4/4/4	-
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	B	402	-	-	3/4/4/4	-
3	GOL	A	407[A]	-	-	1/4/4/4	-
3	GOL	B	408	-	-	2/4/4/4	-
3	GOL	B	407	-	-	2/4/4/4	-
2	W7D	A	401	-	-	1/7/11/11	0/3/3/3
3	GOL	A	410	-	-	4/4/4/4	-
3	GOL	A	408	-	-	0/4/4/4	-
2	W7D	B	401	-	-	2/7/11/11	0/3/3/3
3	GOL	B	404	-	-	0/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-
4	FMN	A	411	-	-	2/18/18/18	0/3/3/3
3	GOL	A	407[B]	-	-	0/4/4/4	-
3	GOL	A	409	-	-	0/4/4/4	-
3	GOL	A	405	-	-	0/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	GOL	O2-C2	-11.66	1.08	1.43
4	B	409	FMN	C4A-C10	6.27	1.45	1.38
2	A	401	W7D	CA-N	5.54	1.43	1.34
4	A	411	FMN	C4A-C10	5.49	1.44	1.38
2	A	401	W7D	CG-ND2	4.87	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	GOL	O3-C3	4.76	1.62	1.42
4	A	411	FMN	C5'-C4'	4.59	1.58	1.51
2	B	401	W7D	CAL-CAT	-4.54	1.38	1.51
2	B	401	W7D	CA-N	4.44	1.41	1.34
2	A	401	W7D	CAL-CAT	-3.97	1.40	1.51
3	A	402	GOL	O1-C1	3.61	1.57	1.42
3	A	402	GOL	C1-C2	3.58	1.66	1.51
4	B	409	FMN	C6-C5A	-3.45	1.36	1.41
4	B	409	FMN	C1'-N10	-3.40	1.44	1.48
2	B	401	W7D	CG-ND2	3.39	1.38	1.33
4	B	409	FMN	C4-C4A	3.36	1.47	1.41
4	A	411	FMN	C9A-N10	3.31	1.43	1.38
5	A	412	NCO	CO-N4	3.31	2.08	1.96
5	A	412	NCO	CO-N3	3.18	2.08	1.96
2	A	401	W7D	CAJ-CAH	2.99	1.42	1.36
4	B	409	FMN	C10-N1	2.96	1.37	1.33
2	A	401	W7D	CAK-CAT	2.90	1.44	1.37
2	B	401	W7D	CAJ-CAH	2.77	1.42	1.36
2	B	401	W7D	CAW-CAV	-2.70	1.38	1.43
2	A	401	W7D	CAG-CAU	2.68	1.44	1.38
4	B	409	FMN	C9-C9A	-2.66	1.35	1.40
5	A	412	NCO	CO-N6	2.59	2.06	1.96
3	A	402	GOL	C3-C2	2.58	1.62	1.51
2	A	401	W7D	CAK-CAW	2.57	1.47	1.42
5	A	412	NCO	CO-N5	2.47	2.05	1.96
2	A	401	W7D	OAP-CAU	-2.33	1.32	1.36
2	B	401	W7D	CA-CB	2.28	1.45	1.40
5	A	412	NCO	CO-N2	2.26	2.04	1.96
4	B	409	FMN	O2'-C2'	2.24	1.48	1.43
4	B	409	FMN	C8M-C8	2.16	1.55	1.51
4	A	411	FMN	C1'-N10	-2.07	1.46	1.48
5	A	412	NCO	CO-N1	2.02	2.04	1.96
3	B	406	GOL	O3-C3	2.00	1.50	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	W7D	CG-ND2-CAR	13.35	126.41	115.14
2	B	401	W7D	CG-ND2-CAR	12.46	125.66	115.14
4	A	411	FMN	C4-N3-C2	9.78	123.40	115.14
4	B	409	FMN	C4-N3-C2	9.17	122.88	115.14
4	B	409	FMN	C1'-N10-C9A	6.84	123.68	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	409	FMN	C4-C4A-C10	-6.61	115.58	119.95
3	B	402	GOL	O2-C2-C3	-5.61	84.39	109.12
3	A	402	GOL	C3-C2-C1	4.91	130.80	111.70
3	B	402	GOL	O1-C1-C2	-4.90	86.68	110.20
4	A	411	FMN	C1'-N10-C10	4.80	122.70	118.41
3	B	402	GOL	C3-C2-C1	4.46	129.05	111.70
3	A	402	GOL	O3-C3-C2	4.42	131.41	110.20
4	A	411	FMN	C4A-C4-N3	-4.30	117.55	123.43
2	A	401	W7D	CAR-N-CA	4.26	120.80	115.24
4	A	411	FMN	C9A-N10-C10	-4.16	116.45	121.91
2	A	401	W7D	CAF-CAI-CAV	-4.16	113.94	120.44
3	A	402	GOL	O1-C1-C2	4.16	130.14	110.20
4	A	411	FMN	C5A-C9A-N10	4.09	120.68	117.72
2	A	401	W7D	CAU-CAW-CAV	3.70	122.65	118.01
3	B	402	GOL	O2-C2-C1	-3.56	93.44	109.12
2	A	401	W7D	CAI-CAF-CAG	3.55	126.64	120.99
3	B	408	GOL	O3-C3-C2	3.43	126.65	110.20
3	B	408	GOL	C3-C2-C1	-3.32	98.79	111.70
4	A	411	FMN	C1'-N10-C9A	3.20	120.81	118.29
4	B	409	FMN	C4A-N5-C5A	3.20	119.97	116.77
2	B	401	W7D	CAR-N-CA	3.20	119.42	115.24
4	A	411	FMN	C4-C4A-C10	-3.12	117.88	119.95
4	B	409	FMN	C6-C5A-N5	3.12	122.49	119.05
4	B	409	FMN	C1'-N10-C10	-3.09	115.64	118.41
4	B	409	FMN	C4-C4A-N5	3.02	122.05	118.60
4	B	409	FMN	C4A-C10-N10	-2.98	117.24	120.30
3	B	408	GOL	O1-C1-C2	2.81	123.67	110.20
2	B	401	W7D	CB-CA-N	-2.65	118.40	122.75
4	B	409	FMN	C4A-C4-N3	-2.63	119.83	123.43
2	A	401	W7D	CAG-CAU-CAW	-2.56	116.66	121.15
3	B	406	GOL	O1-C1-C2	2.50	122.20	110.20
2	B	401	W7D	CAU-CAW-CAV	2.44	121.07	118.01
4	B	409	FMN	C7M-C7-C8	-2.43	115.76	120.74
3	B	404	GOL	C3-C2-C1	-2.43	102.27	111.70
2	B	401	W7D	CAK-CAW-CAU	-2.34	117.62	121.87
4	B	409	FMN	C9-C8-C7	-2.32	116.01	119.91
3	B	406	GOL	O2-C2-C3	-2.28	99.10	109.12
2	B	401	W7D	CAK-CAW-CAV	2.26	121.30	118.79
4	B	409	FMN	C8M-C8-C7	2.17	125.18	120.74
4	A	411	FMN	C4A-N5-C5A	2.11	118.88	116.77
3	B	406	GOL	C3-C2-C1	2.10	119.85	111.70
4	A	411	FMN	O5'-C5'-C4'	2.07	114.89	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	411	FMN	C5'-C4'-C3'	-2.07	108.21	112.20
2	A	401	W7D	CAL-CAT-CAK	2.01	125.21	121.04

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
3	B	408	GOL	C1-C2-C3-O3
3	B	403	GOL	C1-C2-C3-O3
3	A	406	GOL	C1-C2-C3-O3
3	A	410	GOL	C1-C2-C3-O3
3	B	402	GOL	O1-C1-C2-C3
3	B	406	GOL	C1-C2-C3-O3
3	A	410	GOL	O1-C1-C2-C3
3	B	402	GOL	O2-C2-C3-O3
3	B	403	GOL	O2-C2-C3-O3
3	A	410	GOL	O2-C2-C3-O3
3	B	407	GOL	O1-C1-C2-O2
3	B	408	GOL	O2-C2-C3-O3
2	B	401	W7D	CAL-CAM-CB-CG
3	B	406	GOL	O2-C2-C3-O3
3	A	406	GOL	O2-C2-C3-O3
3	A	402	GOL	O1-C1-C2-O2
4	B	409	FMN	C4'-C5'-O5'-P
4	A	411	FMN	C4'-C5'-O5'-P
3	B	405	GOL	O1-C1-C2-O2
3	A	410	GOL	O1-C1-C2-O2
3	A	402	GOL	O1-C1-C2-C3
2	A	401	W7D	CAL-CAM-CB-CG
3	B	405	GOL	O1-C1-C2-C3
4	A	411	FMN	O3'-C3'-C4'-C5'
3	A	407[A]	GOL	C1-C2-C3-O3
2	B	401	W7D	CAT-CAL-CAM-CB

There are no ring outliers.

8 monomers are involved in 22 short contacts:

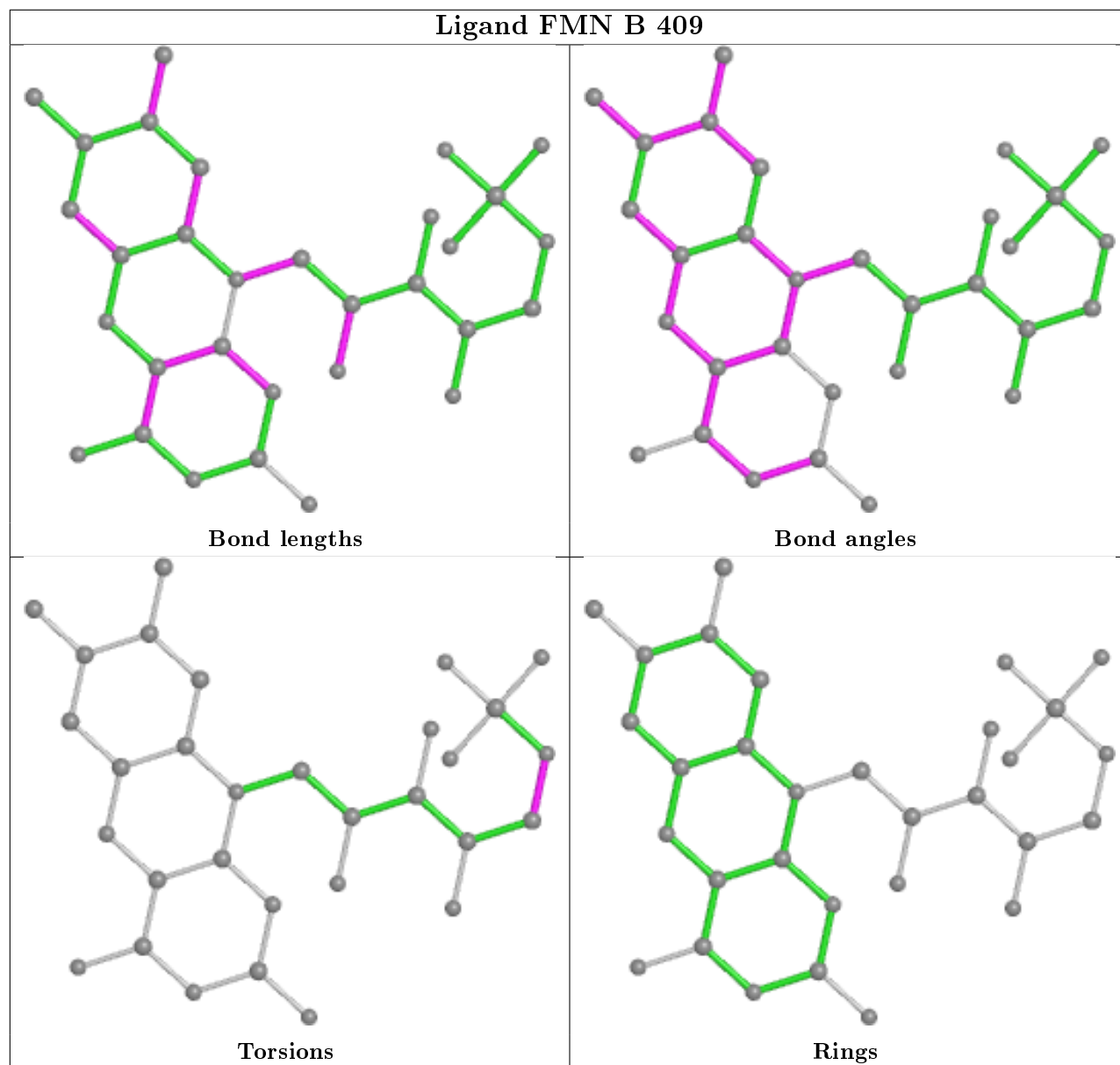
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	4	0

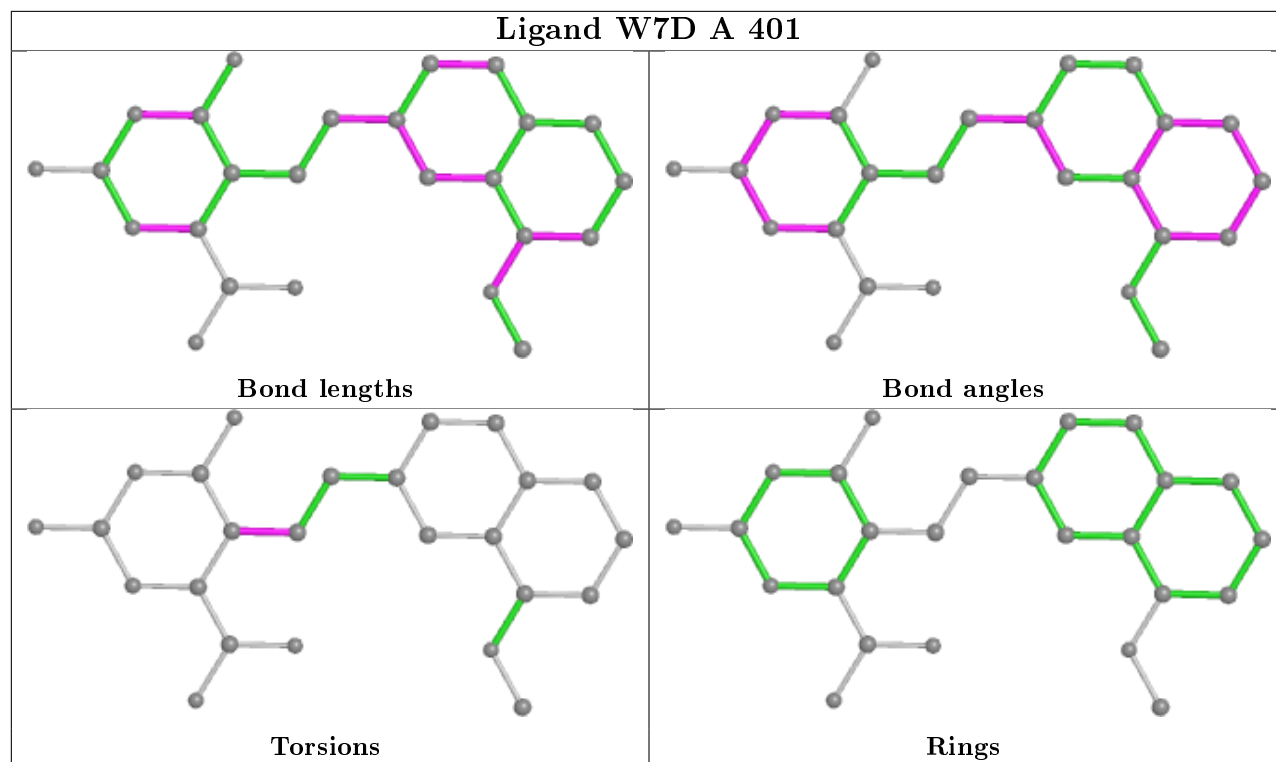
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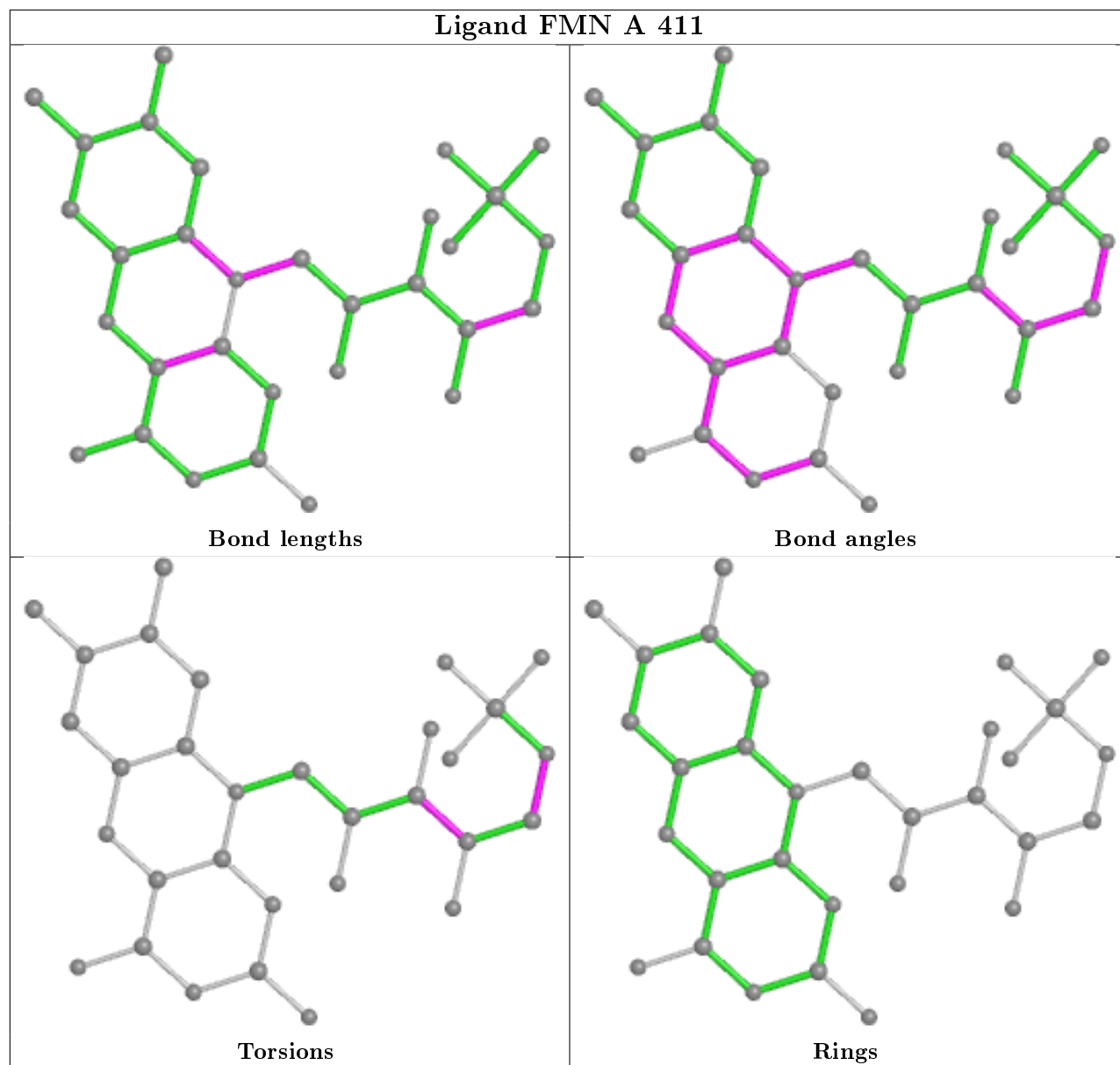
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	407	GOL	1	0
3	B	406	GOL	2	0
3	B	408	GOL	9	0
4	A	411	FMN	1	0
3	A	410	GOL	4	0
3	A	409	GOL	1	0
2	B	401	W7D	2	0

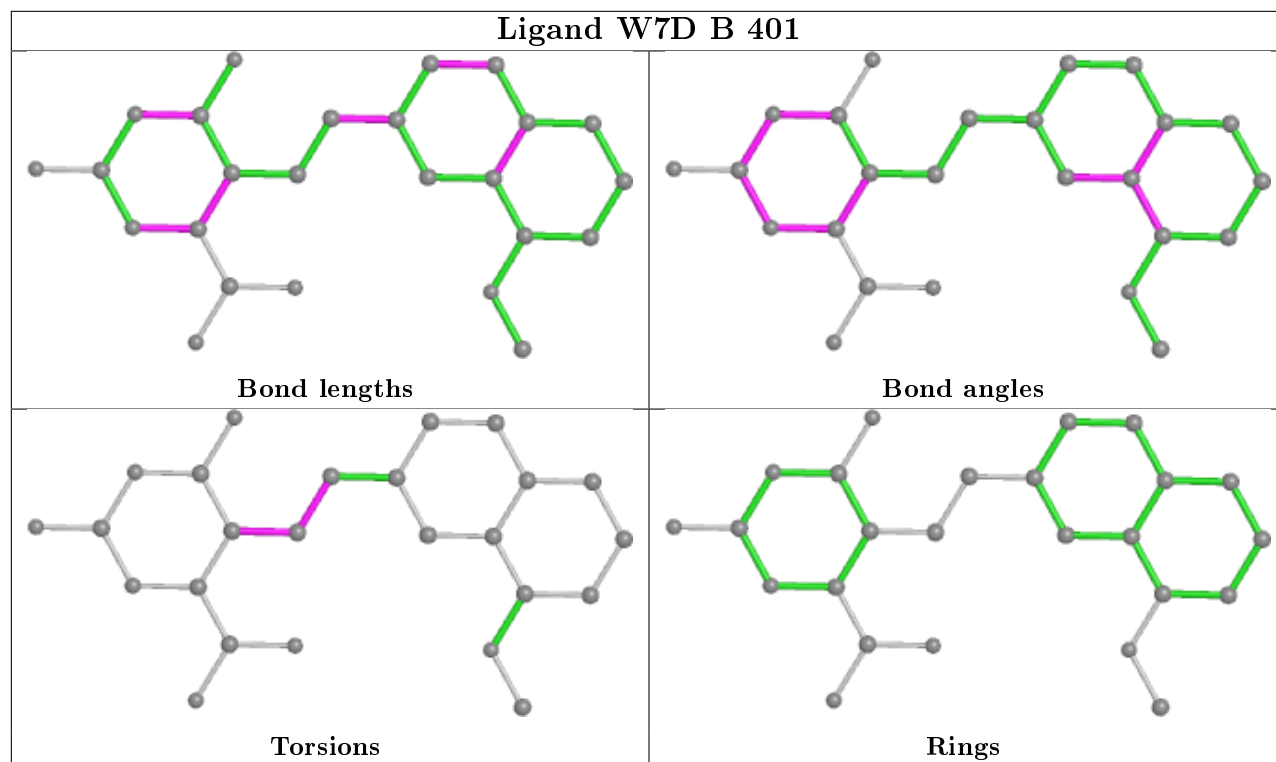
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	313/313 (100%)	0.18	20 (6%) 19 20	7, 11, 22, 48	0
1	B	313/313 (100%)	0.05	8 (2%) 56 61	7, 12, 28, 54	0
All	All	626/626 (100%)	0.12	28 (4%) 33 36	7, 12, 26, 54	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	PHE	7.7
1	B	184	PHE	7.5
1	A	1	CYS	7.1
1	A	171	ILE	6.5
1	A	177	ALA	6.5
1	B	133	VAL	6.0
1	A	172	ALA	4.8
1	A	178	ALA	4.7
1	A	176	THR	4.5
1	A	130	CYS	4.0
1	A	52	GLY	4.0
1	A	4	LEU	4.0
1	B	131	PRO	3.7
1	A	51	ASP	3.5
1	A	0	MET	3.2
1	B	135	GLY	3.0
1	B	312	GLU	3.0
1	B	130	CYS	3.0
1	A	312	GLU	2.9
1	A	217	PHE	2.9
1	A	175	ASP	2.9
1	A	179	ALA	2.8
1	A	2	LEU	2.5
1	A	131	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	170	ASP	2.2
1	A	266	SER	2.1
1	B	132	ASN	2.1
1	B	0	MET	2.0

## 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, 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.

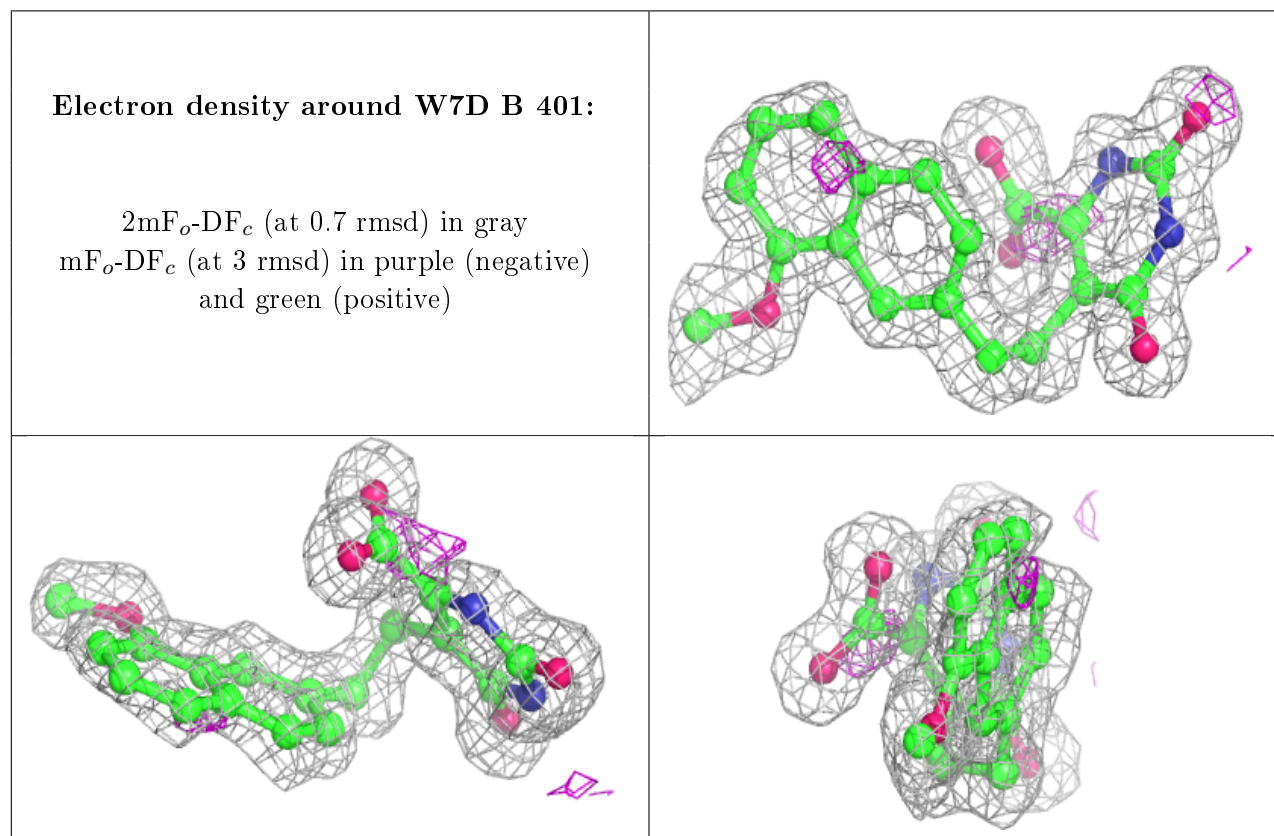
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	403	6/6	0.72	0.17	29,33,35,39	0
3	GOL	A	410	6/6	0.78	0.14	40,46,47,50	0
3	GOL	B	407	6/6	0.79	0.21	39,44,47,56	0
3	GOL	B	405	6/6	0.81	0.19	31,36,43,49	0
3	GOL	A	406	6/6	0.82	0.40	55,59,61,67	0
3	GOL	B	406	6/6	0.83	0.24	18,24,27,31	0
3	GOL	B	404	6/6	0.84	0.16	28,32,36,40	0
3	GOL	B	403	6/6	0.85	0.14	34,45,48,53	0
3	GOL	A	409	6/6	0.86	0.09	23,25,29,33	0
3	GOL	A	402	6/6	0.86	0.21	17,29,31,42	0
3	GOL	B	408	6/6	0.88	0.28	24,29,34,39	0
3	GOL	A	405	6/6	0.89	0.13	34,41,45,47	0
3	GOL	A	404	6/6	0.89	0.20	26,32,33,33	0
3	GOL	B	402	6/6	0.93	0.27	8,20,26,27	0
3	GOL	A	407[B]	6/6	0.94	0.12	11,13,14,14	6
3	GOL	A	407[A]	6/6	0.94	0.12	15,16,17,17	6
3	GOL	A	408	6/6	0.94	0.08	21,22,23,24	0
2	W7D	B	401	25/25	0.95	0.11	9,12,25,28	0
2	W7D	A	401	25/25	0.96	0.09	8,10,20,22	0

*Continued on next page...*

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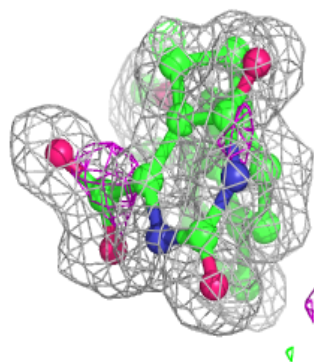
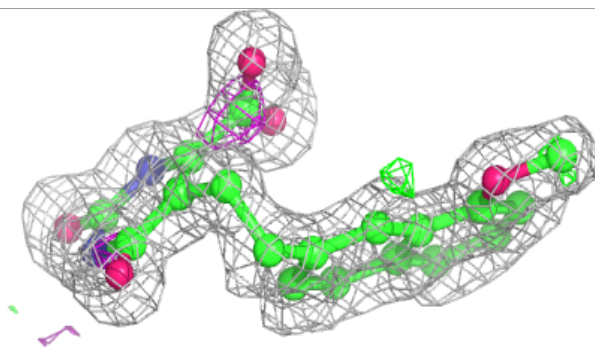
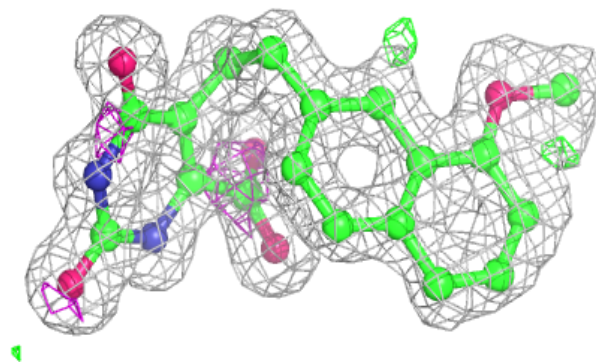
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FMN	A	411	31/31	0.97	0.08	6,7,8,9	0
4	FMN	B	409	31/31	0.98	0.07	7,8,10,10	0
5	NCO	A	412	7/7	0.99	0.12	9,10,10,11	0

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.



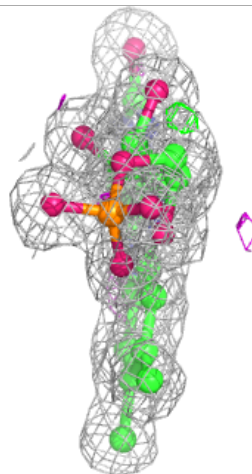
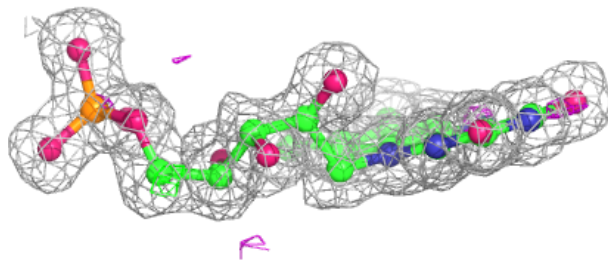
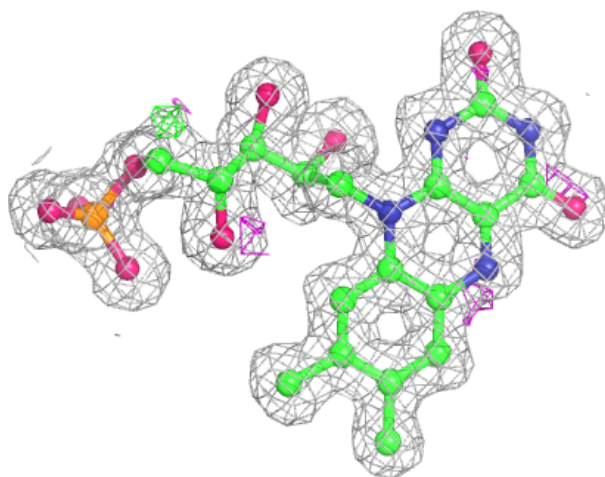
**Electron density around W7D A 401:**

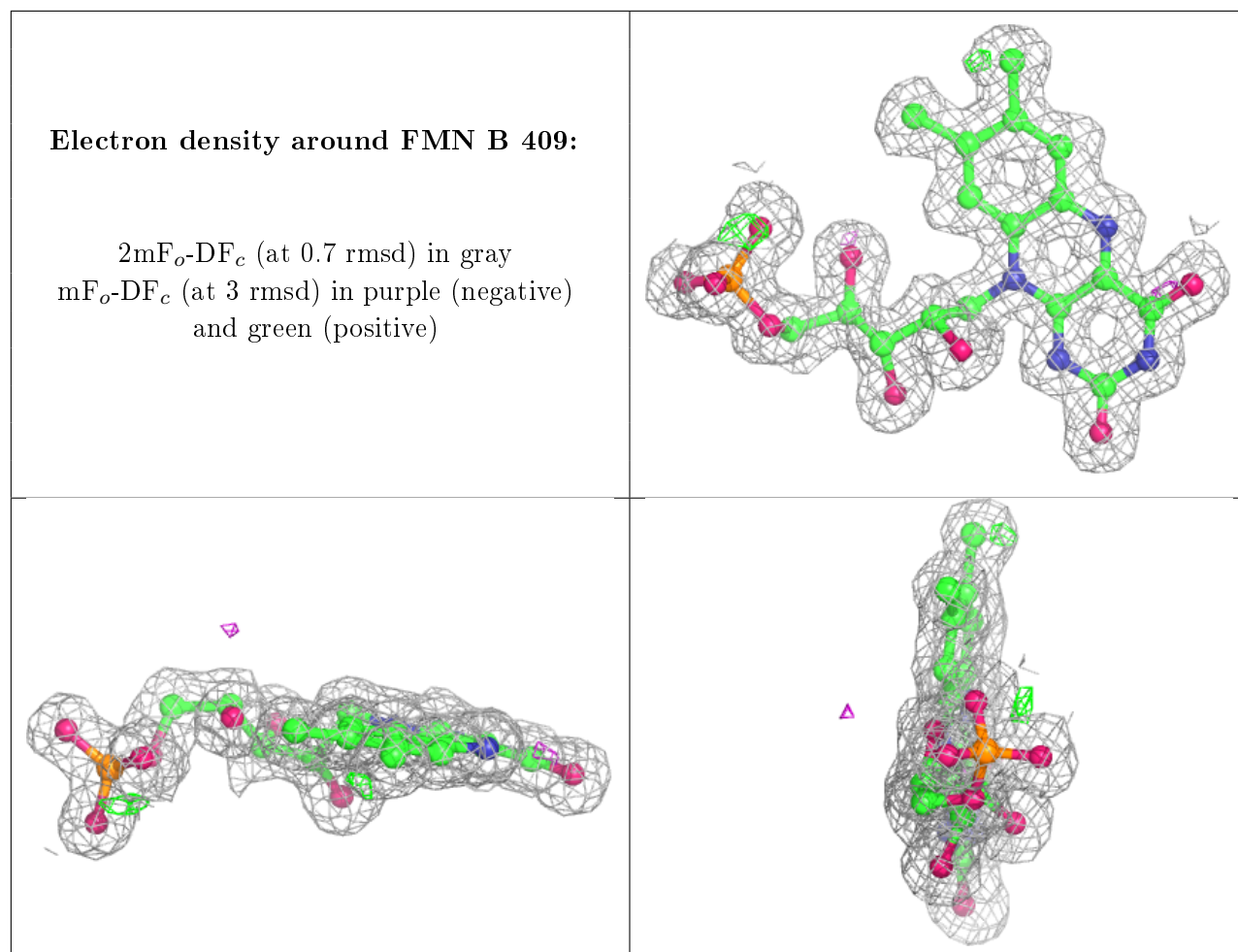
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN A 411:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.