



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:41 am BST

PDB ID : 3W7P  
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with TT2-4-031  
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Deposited on : 2013-03-02  
Resolution : 1.70 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

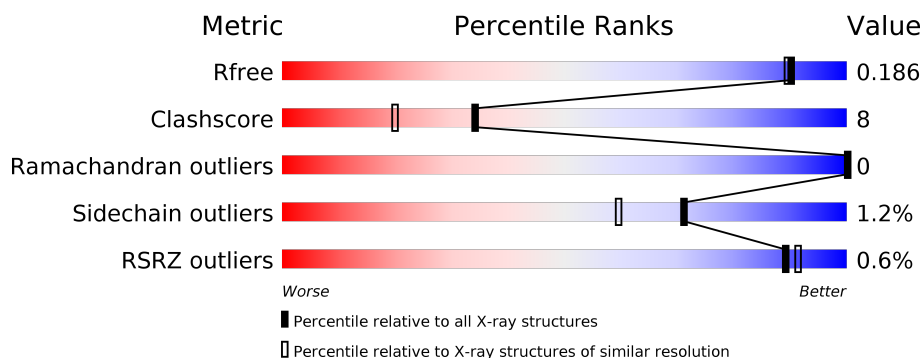
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 86%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>12%</span> <span>•</span> </div> </div>
1	B	313	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 84%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>84%</span> <span>14%</span> <span>•</span> </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
3	GOL	B	405	-	-	X	-
3	GOL	B	409	-	-	X	-
3	GOL	B	410	-	-	X	-

## 2 Entry composition [i](#)

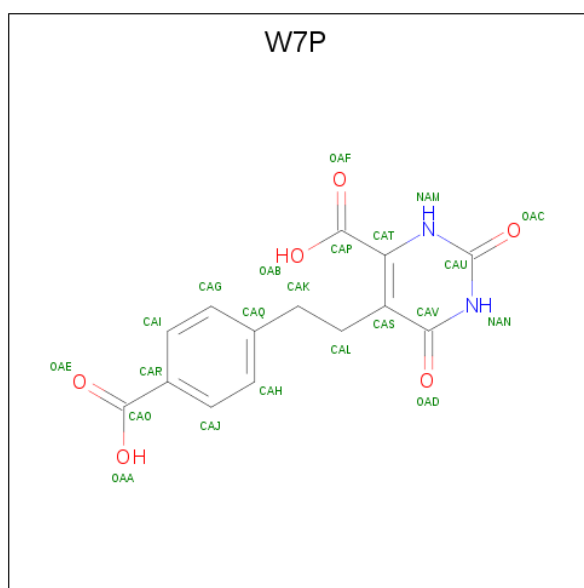
There are 6 unique types of molecules in this entry. The entry contains 6057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	15	0
			2515	1599	424	474	18			
1	B	313	Total	C	N	O	S	0	15	0
			2502	1595	416	472	19			

- Molecule 2 is 5-[2-(4-carboxyphenyl)ethyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: W7P) (formula: C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	14	2	6		
2	B	1	Total	C	N	O	0	0
			22	14	2	6		

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



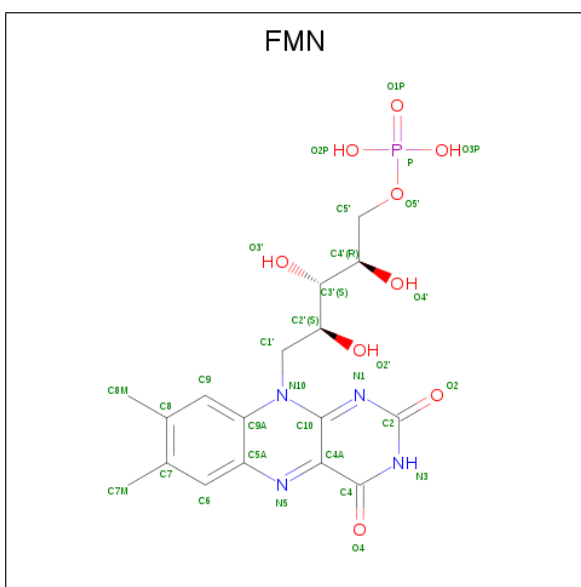
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

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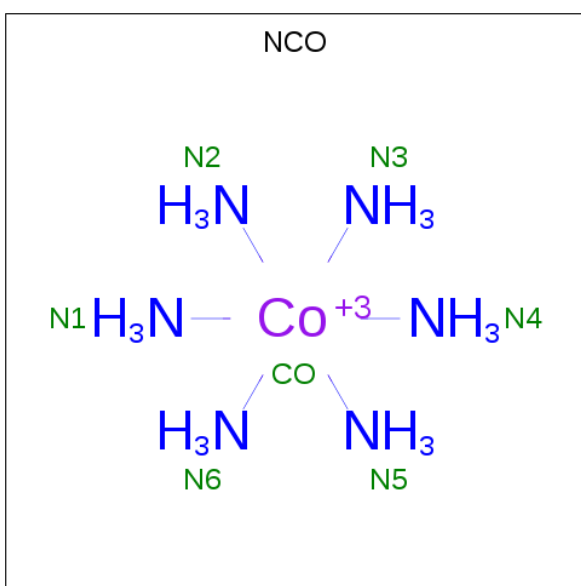
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total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

- Molecule 4 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
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:  $\text{CoH}_{18}\text{N}_6$ ).



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

- Molecule 6 is water.

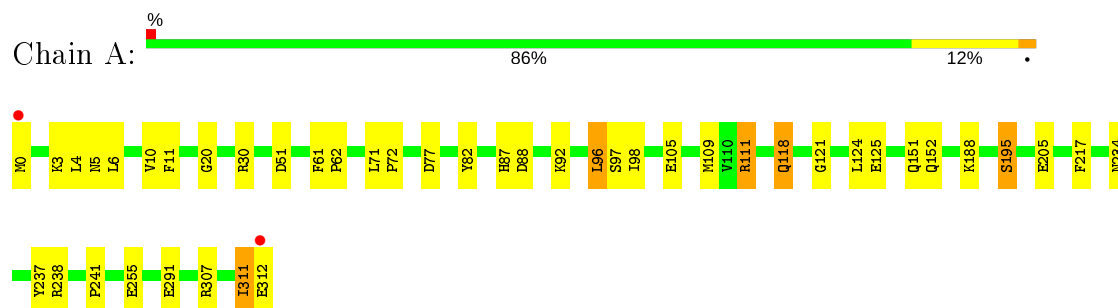
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	390	Total 394	O 394	0	4
6	B	364	Total 365	O 365	0	1



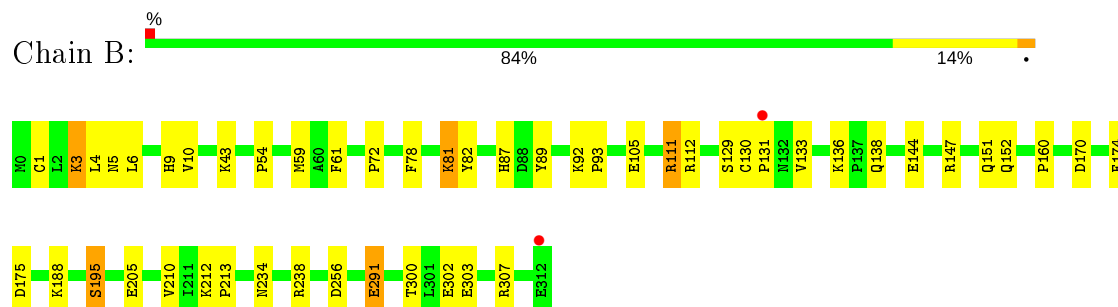
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	67.91Å 71.78Å 129.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.67 – 1.70 24.67 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.67-1.70) 99.7 (24.67-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.21 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.141 , 0.175 0.155 , 0.186	Depositor DCC
$R_{free}$ test set	3557 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6057	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 27.72 % 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 2.0901e-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, W7P, 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	1.10	5/2566 (0.2%)	1.06	11/3469 (0.3%)
1	B	1.17	10/2553 (0.4%)	1.10	13/3456 (0.4%)
All	All	1.14	15/5119 (0.3%)	1.08	24/6925 (0.3%)

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	A	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	302	GLU	CD-OE2	9.76	1.36	1.25
1	A	205	GLU	CD-OE2	-9.43	1.15	1.25
1	B	105	GLU	CD-OE1	-9.28	1.15	1.25
1	B	302	GLU	CD-OE1	-8.88	1.15	1.25
1	B	3	LYS	CE-NZ	8.08	1.69	1.49
1	B	144	GLU	CD-OE1	7.80	1.34	1.25
1	A	255	GLU	CD-OE1	-6.82	1.18	1.25
1	B	1	CYS	CB-SG	-6.71	1.70	1.82
1	A	195	SER	CB-OG	-6.13	1.34	1.42
1	A	291	GLU	CG-CD	5.88	1.60	1.51
1	B	205	GLU	CD-OE1	5.57	1.31	1.25
1	B	291	GLU	CG-CD	5.48	1.60	1.51
1	A	105	GLU	CD-OE2	-5.44	1.19	1.25
1	B	195	SER	CB-OG	-5.35	1.35	1.42
1	B	291	GLU	CD-OE2	5.06	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LYS	CD-CE-NZ	12.79	141.13	111.70
1	B	112	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	302	GLU	CG-CD-OE2	6.82	131.94	118.30
1	A	51	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	302	GLU	CG-CD-OE1	-6.34	105.61	118.30
1	B	307	ARG	CG-CD-NE	-6.25	98.68	111.80
1	A	88	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	B	111	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	4	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	4	LEU	CB-CG-CD1	5.78	120.83	111.00
1	A	30[A]	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	30[B]	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	175	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	11	PHE	CB-CG-CD1	5.58	124.71	120.80
1	B	147	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	77	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	174	PHE	CB-CG-CD1	5.50	124.65	120.80
1	B	291	GLU	CG-CD-OE2	5.34	128.99	118.30
1	A	111[A]	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	111[B]	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	96	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	B	170	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	256	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	1	CYS	N-CA-CB	-5.21	101.23	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	ILE	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	2515	0	2494	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2502	0	2487	48	0
2	A	22	0	10	0	0
2	B	22	0	10	0	0
3	A	90	0	120	10	0
3	B	78	0	104	32	0
4	A	31	0	19	1	0
4	B	31	0	19	0	0
5	A	7	0	0	0	0
6	A	394	0	0	13	0
6	B	365	0	0	9	0
All	All	6057	0	5263	89	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 8.

All (89) 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:3:LYS:NZ	1:B:3:LYS:CE	1.69	1.53
1:B:93:PRO:HD3	3:B:409:GOL:H31	1.35	1.05
3:B:405:GOL:O3	3:B:409:GOL:H12	1.67	0.93
1:A:151[A]:GLN:NE2	1:A:152[A]:GLN:OE1	2.03	0.90
1:B:89:TYR:HD2	3:B:405:GOL:H12	1.40	0.86
1:A:241:PRO:HA	3:A:405:GOL:H31	1.58	0.84
1:B:54:PRO:HG2	3:B:410:GOL:H12	1.65	0.76
1:B:59:MET:HE3	6:B:607:HOH:O	1.86	0.75
1:B:61:PHE:CE1	3:B:406:GOL:H11	2.20	0.75
1:A:188:LYS:HE3	6:A:565:HOH:O	1.86	0.74
1:B:129[B]:SER:HA	1:B:138:GLN:NE2	2.03	0.74
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.36	0.73
1:B:89:TYR:CD2	3:B:405:GOL:H12	2.23	0.73
1:B:111:ARG:NH1	6:B:613:HOH:O	2.22	0.72
1:B:129[A]:SER:HA	1:B:138:GLN:NE2	2.04	0.72
1:B:9:HIS:CD2	3:B:405:GOL:H11	2.26	0.71
1:B:129[A]:SER:OG	3:B:402:GOL:H11	1.89	0.70
1:B:93:PRO:HA	3:B:405:GOL:H31	1.74	0.69
3:B:405:GOL:H11	6:B:510:HOH:O	1.93	0.68
1:A:98:ILE:HD12	1:A:124:LEU:HD13	1.78	0.66
1:B:81:LYS:HE2	3:B:412:GOL:C1	2.26	0.66
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.42	0.65
1:A:111[A]:ARG:NH2	6:A:835:HOH:O	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:410:GOL:H31	6:B:794:HOH:O	1.98	0.64
3:B:405:GOL:C1	6:B:510:HOH:O	2.47	0.63
1:A:98:ILE:HD12	1:A:124:LEU:CD1	2.30	0.62
3:A:410:GOL:H32	6:A:576:HOH:O	2.01	0.60
3:B:405:GOL:C3	3:B:409:GOL:H12	2.32	0.59
1:A:307[A]:ARG:HD3	6:A:746:HOH:O	2.02	0.59
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.86	0.57
3:A:414:GOL:H12	6:A:580:HOH:O	2.05	0.57
1:B:93:PRO:HG3	3:B:409:GOL:H11	1.87	0.55
1:A:195:SER:HB3	6:A:758:HOH:O	2.05	0.55
1:B:151[B]:GLN:NE2	1:B:152:GLN:OE1	2.35	0.55
1:A:87:HIS:HE1	1:A:92:LYS:O	1.90	0.55
1:B:10:VAL:O	3:B:409:GOL:H11	2.06	0.55
1:B:59:MET:CE	6:B:607:HOH:O	2.50	0.54
1:B:87:HIS:HE1	1:B:92:LYS:O	1.89	0.54
1:B:129[A]:SER:HA	1:B:138:GLN:HE21	1.73	0.54
1:A:121:GLY:HA2	3:A:414:GOL:H2	1.90	0.54
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.91	0.54
1:A:96:LEU:HG	6:A:742:HOH:O	2.07	0.53
1:B:5[B]:ASN:ND2	1:B:10:VAL:HG22	2.24	0.53
1:A:118:GLN:HG2	6:A:776:HOH:O	2.09	0.53
1:B:6[B]:LEU:HD23	3:B:411:GOL:C3	2.40	0.52
1:B:78:PHE:HA	3:B:412:GOL:C1	2.40	0.52
1:B:78:PHE:HA	3:B:412:GOL:H11	1.91	0.52
1:A:96:LEU:CG	6:A:742:HOH:O	2.57	0.51
1:B:93:PRO:HG3	3:B:409:GOL:C1	2.40	0.51
1:B:93:PRO:CA	3:B:405:GOL:H31	2.39	0.51
1:B:9:HIS:NE2	3:B:405:GOL:H11	2.25	0.51
1:B:6[B]:LEU:HD23	3:B:411:GOL:H31	1.92	0.51
1:A:311:ILE:HG22	1:A:312[A]:GLU:HG3	1.93	0.50
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.04	0.50
3:A:410:GOL:C3	6:A:576:HOH:O	2.57	0.50
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.10	0.50
1:A:5[A]:ASN:OD1	1:A:10:VAL:HG22	2.12	0.49
1:A:20:GLY:HA3	4:A:416:FMN:N5	2.28	0.49
1:B:210:VAL:HA	3:B:407:GOL:H31	1.95	0.49
1:B:195:SER:HB3	6:B:743:HOH:O	2.13	0.48
1:A:312[B]:GLU:HB2	1:B:212:LYS:HE3	1.96	0.48
1:A:61:PHE:CE1	3:A:408:GOL:H11	2.50	0.46
1:B:300:THR:OG1	1:B:303[A]:GLU:HG3	2.16	0.46
1:A:96:LEU:HD12	6:A:742:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:NE2	6:A:772:HOH:O	2.50	0.45
1:B:129[A]:SER:OG	3:B:402:GOL:C1	2.62	0.45
1:B:129[B]:SER:HA	1:B:138:GLN:HE22	1.80	0.45
1:B:291:GLU:CD	6:B:602:HOH:O	2.54	0.45
1:A:241:PRO:CA	3:A:405:GOL:H31	2.39	0.45
1:A:61:PHE:HB3	1:A:62:PRO:HD2	1.99	0.45
1:B:213:PRO:HA	3:B:410:GOL:H32	1.99	0.45
1:B:9:HIS:CD2	3:B:405:GOL:C1	2.97	0.44
3:A:414:GOL:C1	6:A:580:HOH:O	2.63	0.43
1:B:89:TYR:HB3	3:B:405:GOL:H32	2.00	0.43
1:A:97:SER:HA	1:A:125:GLU:O	2.19	0.43
1:B:43:LYS:HE2	1:B:72:PRO:O	2.19	0.42
1:B:130[A]:CYS:HB2	1:B:131:PRO:HD2	2.01	0.42
3:B:410:GOL:C3	6:B:794:HOH:O	2.64	0.42
1:B:160:PRO:HB3	1:B:188:LYS:HG3	2.01	0.42
1:B:9:HIS:HD2	3:B:405:GOL:H2	1.83	0.42
1:A:217:PHE:CE1	3:A:404:GOL:H12	2.54	0.42
1:A:61:PHE:HB3	1:A:62:PRO:CD	2.50	0.42
1:A:71:LEU:N	1:A:72:PRO:CD	2.83	0.41
1:A:98:ILE:HG23	1:A:109:MET:HE1	2.02	0.41
1:B:129[A]:SER:HG	3:B:402:GOL:H11	1.85	0.41
1:A:311:ILE:O	1:A:312[B]:GLU:HB3	2.21	0.40
1:B:133:VAL:HB	1:B:136:LYS:HG3	2.03	0.40
1:B:213:PRO:HA	3:B:410:GOL:H11	2.02	0.40
1:A:237:TYR:O	3:A:405:GOL:H11	2.22	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	325/313 (104%)	315 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	325/313 (104%)	316 (97%)	9 (3%)	0	100	100
All	All	650/626 (104%)	631 (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	273/258 (106%)	269 (98%)	4 (2%)	65	51
1	B	273/258 (106%)	270 (99%)	3 (1%)	73	63
All	All	546/516 (106%)	539 (99%)	7 (1%)	71	56

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	3	LYS
1	A	6	LEU
1	A	118	GLN
1	B	4[A]	LEU
1	B	4[B]	LEU
1	B	81	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

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

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

33 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	406	-	5,5,5	0.85	0	5,5,5	1.28	1 (20%)
3	GOL	A	404	-	5,5,5	0.58	0	5,5,5	0.61	0
3	GOL	B	403	-	5,5,5	0.48	0	5,5,5	0.72	0
3	GOL	B	414	-	5,5,5	0.50	0	5,5,5	0.88	0
3	GOL	B	408	-	5,5,5	0.74	0	5,5,5	0.98	0
3	GOL	A	408	-	5,5,5	0.96	0	5,5,5	1.26	0
3	GOL	A	405	-	5,5,5	0.62	0	5,5,5	0.92	0
3	GOL	B	411	-	5,5,5	0.76	0	5,5,5	1.15	1 (20%)
3	GOL	A	413	-	5,5,5	0.91	0	5,5,5	1.05	0
3	GOL	A	403	-	5,5,5	0.72	0	5,5,5	0.59	0
3	GOL	A	407	-	5,5,5	0.81	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	409	-	5,5,5	0.84	0	5,5,5	1.19	0
3	GOL	B	413	-	5,5,5	0.48	0	5,5,5	0.65	0
3	GOL	A	411	-	5,5,5	0.84	0	5,5,5	1.21	1 (20%)
3	GOL	A	415	-	5,5,5	0.43	0	5,5,5	0.45	0
3	GOL	A	402[B]	-	5,5,5	0.88	0	5,5,5	0.55	0
3	GOL	B	410	-	5,5,5	0.62	0	5,5,5	0.76	0
2	W7P	B	401	-	17,23,23	2.81	7 (41%)	16,32,32	3.71	6 (37%)
3	GOL	B	407	-	5,5,5	0.62	0	5,5,5	1.06	0
3	GOL	A	412	-	5,5,5	1.09	1 (20%)	5,5,5	1.63	2 (40%)
2	W7P	A	401	-	17,23,23	2.31	6 (35%)	16,32,32	3.32	8 (50%)
3	GOL	B	412	-	5,5,5	0.93	0	5,5,5	0.99	1 (20%)
3	GOL	B	402	-	5,5,5	0.87	0	5,5,5	1.01	0
3	GOL	B	405	-	5,5,5	0.52	0	5,5,5	1.96	1 (20%)
3	GOL	B	409	-	5,5,5	0.78	0	5,5,5	1.79	1 (20%)
3	GOL	A	410	-	5,5,5	0.71	0	5,5,5	0.91	0
3	GOL	A	402[A]	-	5,5,5	0.43	0	5,5,5	0.71	0
3	GOL	A	414	-	5,5,5	0.39	0	5,5,5	0.78	0
4	FMN	A	416	-	31,33,33	2.06	5 (16%)	40,50,50	2.39	10 (25%)
3	GOL	B	404	-	5,5,5	0.72	0	5,5,5	0.62	0
5	NCO	A	417	-	6,6,6	2.77	4 (66%)	-	-	-
3	GOL	A	406	-	5,5,5	0.52	0	5,5,5	0.54	0
4	FMN	B	415	-	31,33,33	2.28	5 (16%)	40,50,50	2.06	8 (20%)

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	B	406	-	-	2/4/4/4	-
3	GOL	A	404	-	-	0/4/4/4	-
3	GOL	B	403	-	-	4/4/4/4	-
3	GOL	B	414	-	-	0/4/4/4	-
3	GOL	B	408	-	-	0/4/4/4	-
3	GOL	A	408	-	-	2/4/4/4	-
3	GOL	A	405	-	-	2/4/4/4	-
3	GOL	B	411	-	-	1/4/4/4	-
3	GOL	A	413	-	-	2/4/4/4	-
3	GOL	A	403	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	407	-	-	2/4/4/4	-
3	GOL	A	409	-	-	2/4/4/4	-
3	GOL	B	413	-	-	2/4/4/4	-
3	GOL	A	411	-	-	2/4/4/4	-
3	GOL	A	415	-	-	4/4/4/4	-
3	GOL	A	402[B]	-	-	0/4/4/4	-
3	GOL	B	410	-	-	4/4/4/4	-
2	W7P	B	401	-	-	0/5/13/13	0/2/2/2
3	GOL	B	407	-	-	2/4/4/4	-
3	GOL	A	412	-	-	0/4/4/4	-
2	W7P	A	401	-	-	0/5/13/13	0/2/2/2
3	GOL	B	412	-	-	4/4/4/4	-
3	GOL	B	402	-	-	3/4/4/4	-
3	GOL	B	405	-	-	2/4/4/4	-
3	GOL	B	409	-	-	2/4/4/4	-
3	GOL	A	410	-	-	1/4/4/4	-
3	GOL	A	402[A]	-	-	0/4/4/4	-
3	GOL	A	414	-	-	4/4/4/4	-
4	FMN	A	416	-	-	1/18/18/18	0/3/3/3
3	GOL	B	404	-	-	2/4/4/4	-
3	GOL	A	406	-	-	0/4/4/4	-
4	FMN	B	415	-	-	1/18/18/18	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	415	FMN	C4A-C10	9.75	1.48	1.38
4	A	416	FMN	C4A-C10	8.85	1.47	1.38
2	B	401	W7P	CAT-NAM	6.01	1.44	1.34
2	A	401	W7P	CAT-NAM	5.73	1.43	1.34
2	B	401	W7P	CAL-CAS	-5.42	1.42	1.52
2	B	401	W7P	CAV-NAN	4.60	1.41	1.33
5	A	417	NCO	CO-N6	4.32	2.12	1.96
4	B	415	FMN	C5'-C4'	4.22	1.57	1.51
2	A	401	W7P	CAH-CAJ	4.17	1.46	1.38
5	A	417	NCO	CO-N2	3.91	2.10	1.96
2	B	401	W7P	CAH-CAJ	3.62	1.45	1.38
2	A	401	W7P	CAI-CAR	-3.53	1.31	1.39
2	A	401	W7P	CAV-NAN	3.31	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	415	FMN	C2'-C3'	-3.07	1.47	1.53
2	B	401	W7P	CAK-CAQ	-2.93	1.43	1.51
4	A	416	FMN	C6-C5A	-2.92	1.37	1.41
2	B	401	W7P	CAR-CAO	-2.68	1.44	1.47
4	A	416	FMN	C4-N3	-2.65	1.28	1.33
4	A	416	FMN	C4-C4A	2.62	1.45	1.41
5	A	417	NCO	CO-N4	2.60	2.06	1.96
2	B	401	W7P	CAT-CAS	-2.59	1.35	1.40
4	B	415	FMN	C5A-N5	2.47	1.39	1.35
3	A	412	GOL	O2-C2	2.26	1.50	1.43
2	A	401	W7P	CAK-CAQ	-2.23	1.45	1.51
5	A	417	NCO	CO-N1	2.21	2.04	1.96
4	A	416	FMN	C2'-C3'	-2.17	1.49	1.53
4	B	415	FMN	C9A-N10	2.11	1.41	1.38
2	A	401	W7P	CAR-CAO	-2.06	1.45	1.47

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	W7P	CAV-NAN-CAU	12.28	125.51	115.14
2	A	401	W7P	CAV-NAN-CAU	10.24	123.78	115.14
4	A	416	FMN	C4-N3-C2	9.57	123.22	115.14
4	B	415	FMN	C4-N3-C2	7.61	121.57	115.14
4	B	415	FMN	C4-C4A-C10	-5.80	116.11	119.95
4	A	416	FMN	C1'-N10-C9A	5.72	122.79	118.29
4	A	416	FMN	C4-C4A-C10	-4.50	116.97	119.95
2	B	401	W7P	CAJ-CAR-CAO	4.46	126.36	120.37
2	B	401	W7P	CAI-CAR-CAO	-4.15	114.80	120.37
2	A	401	W7P	CAI-CAR-CAO	-4.10	114.86	120.37
4	A	416	FMN	C4A-C4-N3	-3.97	118.00	123.43
2	A	401	W7P	CAH-CAJ-CAR	-3.90	115.52	121.13
2	B	401	W7P	CAU-NAM-CAT	3.75	120.14	115.24
4	B	415	FMN	C4A-C4-N3	-3.52	118.62	123.43
3	B	405	GOL	C3-C2-C1	-3.48	98.16	111.70
4	B	415	FMN	C1'-N10-C9A	3.26	120.86	118.29
3	B	409	GOL	O1-C1-C2	3.19	125.52	110.20
4	A	416	FMN	C4-C4A-N5	3.11	122.15	118.60
4	A	416	FMN	C4A-N5-C5A	2.98	119.75	116.77
2	A	401	W7P	CAJ-CAR-CAO	2.91	124.28	120.37
4	B	415	FMN	C4A-N5-C5A	2.78	119.55	116.77
4	A	416	FMN	C1'-N10-C10	-2.68	116.01	118.41
2	A	401	W7P	CAK-CAL-CAS	-2.66	107.58	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	412	GOL	C3-C2-C1	-2.64	101.43	111.70
4	B	415	FMN	C5A-C9A-N10	2.64	119.62	117.72
2	A	401	W7P	CAK-CAQ-CAG	-2.60	114.66	121.23
4	A	416	FMN	C6-C5A-N5	2.53	121.83	119.05
2	A	401	W7P	CAU-NAM-CAT	2.51	118.51	115.24
3	B	411	GOL	O1-C1-C2	2.47	122.05	110.20
3	A	412	GOL	O2-C2-C1	2.40	119.70	109.12
4	B	415	FMN	C4-C4A-N5	2.35	121.29	118.60
2	B	401	W7P	CAK-CAQ-CAG	-2.27	115.48	121.23
2	B	401	W7P	CAK-CAQ-CAH	2.26	126.95	121.23
3	A	411	GOL	O1-C1-C2	2.16	120.54	110.20
4	A	416	FMN	C7-C6-C5A	2.11	124.20	121.22
2	A	401	W7P	CAK-CAQ-CAH	2.10	126.53	121.23
3	B	412	GOL	O1-C1-C2	2.06	120.08	110.20
3	B	406	GOL	O1-C1-C2	2.06	120.07	110.20
4	B	415	FMN	C6-C5A-C9A	2.04	121.72	119.05
4	A	416	FMN	C9-C9A-C5A	-2.02	116.43	119.88

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	406	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	A	408	GOL	O1-C1-C2-C3
3	A	407	GOL	O1-C1-C2-C3
3	B	413	GOL	O1-C1-C2-C3
3	A	411	GOL	O1-C1-C2-C3
3	A	415	GOL	O1-C1-C2-O2
3	A	415	GOL	O1-C1-C2-C3
3	A	415	GOL	C1-C2-C3-O3
3	B	410	GOL	O1-C1-C2-C3
3	B	410	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-C3
3	B	412	GOL	O1-C1-C2-C3
3	B	412	GOL	C1-C2-C3-O3
3	B	402	GOL	C1-C2-C3-O3
3	B	402	GOL	O2-C2-C3-O3
3	B	405	GOL	O1-C1-C2-C3
3	B	409	GOL	C1-C2-C3-O3
3	B	409	GOL	O2-C2-C3-O3
3	A	414	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	414	GOL	C1-C2-C3-O3
3	A	408	GOL	O1-C1-C2-O2
3	A	407	GOL	O1-C1-C2-O2
3	B	413	GOL	O1-C1-C2-O2
3	B	407	GOL	O1-C1-C2-O2
3	A	405	GOL	C1-C2-C3-O3
3	A	413	GOL	C1-C2-C3-O3
3	A	409	GOL	O1-C1-C2-C3
3	B	402	GOL	O1-C1-C2-C3
3	A	410	GOL	O1-C1-C2-C3
3	B	406	GOL	O1-C1-C2-O2
3	B	403	GOL	O2-C2-C3-O3
3	A	405	GOL	O2-C2-C3-O3
3	A	409	GOL	O1-C1-C2-O2
3	A	411	GOL	O1-C1-C2-O2
3	A	415	GOL	O2-C2-C3-O3
3	B	410	GOL	O2-C2-C3-O3
3	B	412	GOL	O1-C1-C2-O2
3	B	412	GOL	O2-C2-C3-O3
3	B	405	GOL	O1-C1-C2-O2
3	A	414	GOL	O1-C1-C2-O2
3	B	410	GOL	O1-C1-C2-O2
3	A	414	GOL	O2-C2-C3-O3
3	B	404	GOL	O2-C2-C3-O3
4	A	416	FMN	C4'-C5'-O5'-P
4	B	415	FMN	C4'-C5'-O5'-P
3	B	411	GOL	O1-C1-C2-C3
3	B	404	GOL	C1-C2-C3-O3
3	A	413	GOL	O2-C2-C3-O3
3	B	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-C3

There are no ring outliers.

14 monomers are involved in 43 short contacts:

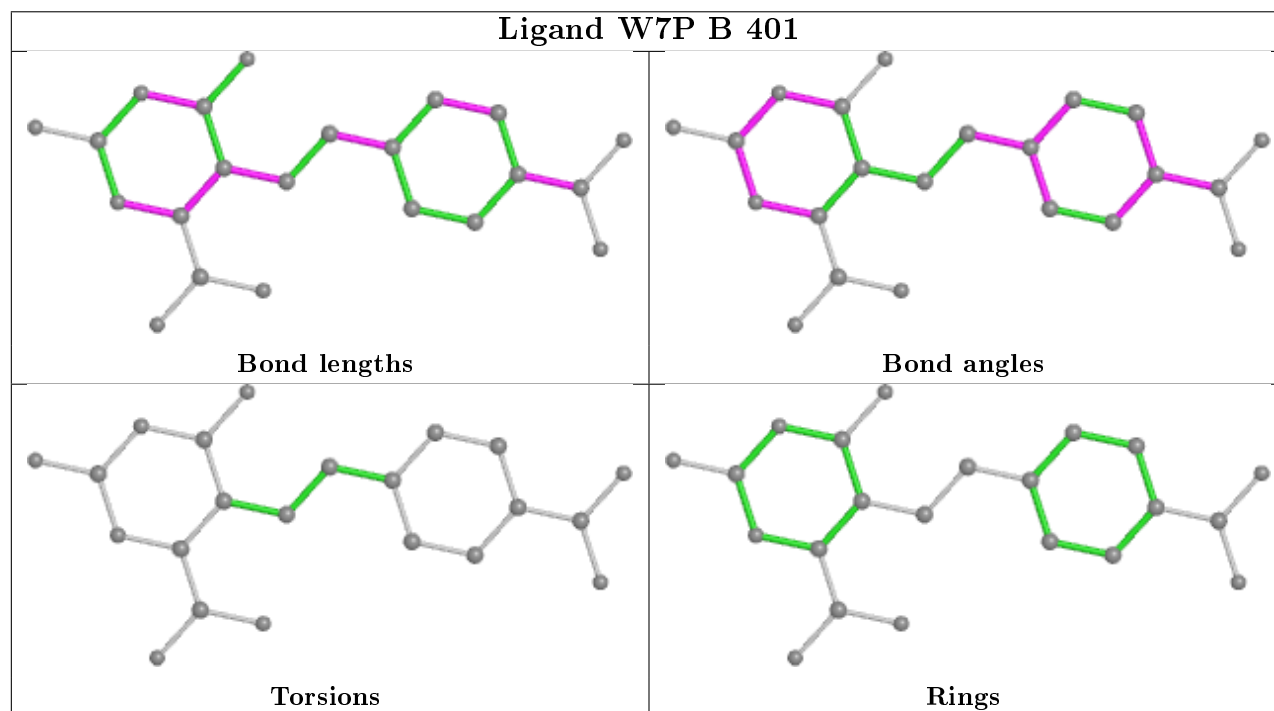
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	GOL	1	0
3	A	404	GOL	1	0
3	A	408	GOL	1	0
3	A	405	GOL	3	0
3	B	411	GOL	2	0
3	B	410	GOL	5	0

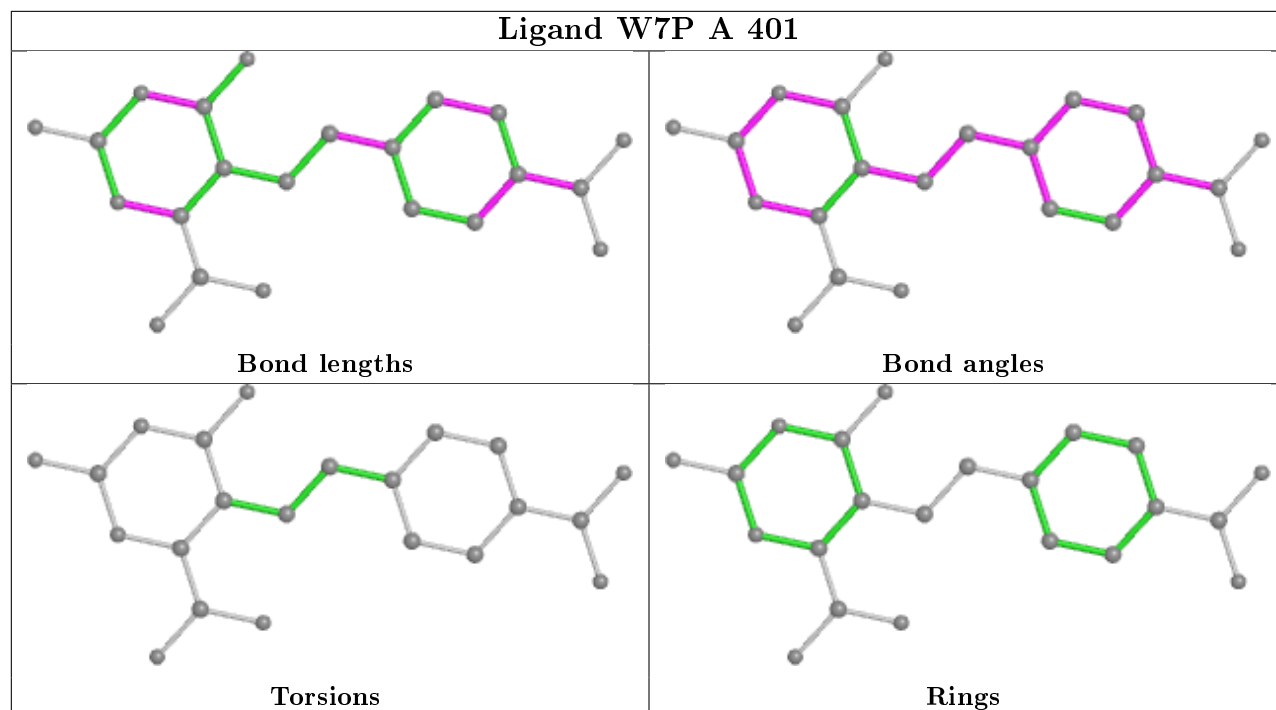
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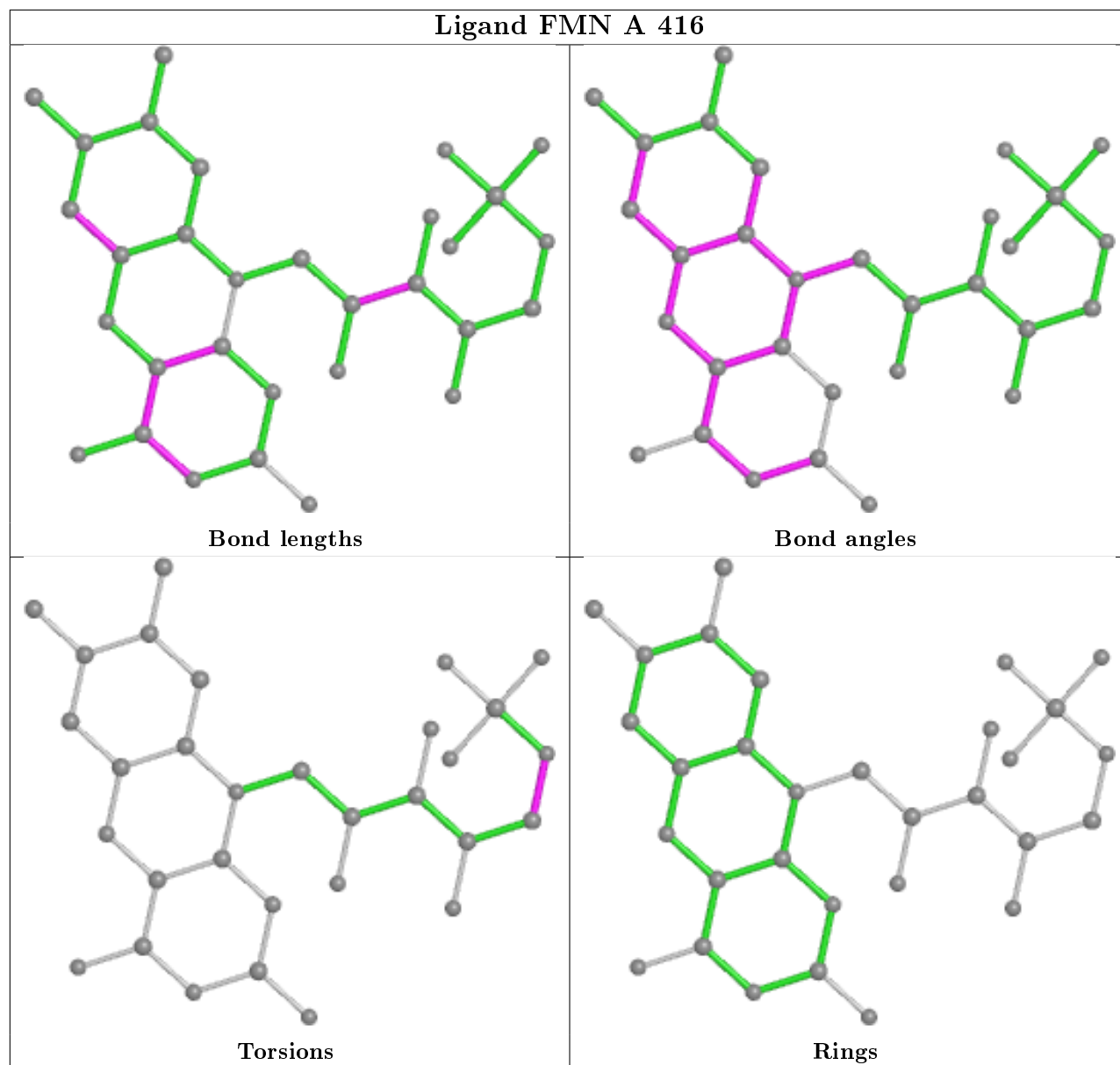
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	407	GOL	1	0
3	B	412	GOL	3	0
3	B	402	GOL	3	0
3	B	405	GOL	13	0
3	B	409	GOL	6	0
3	A	410	GOL	2	0
3	A	414	GOL	3	0
4	A	416	FMN	1	0

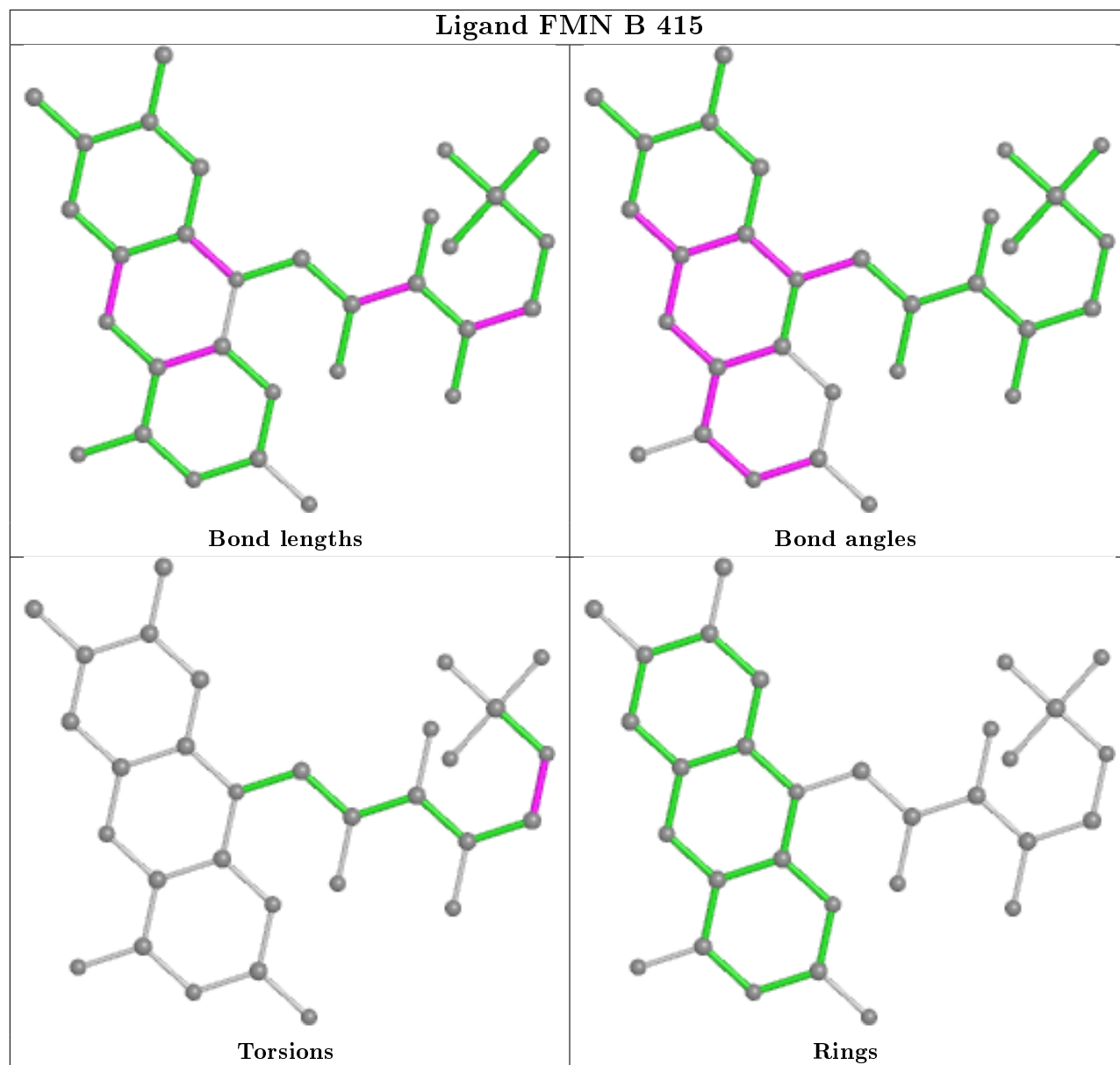
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	-0.27	2 (0%) 89 91	7, 11, 22, 40	0
1	B	313/313 (100%)	-0.33	2 (0%) 89 91	6, 11, 22, 32	0
All	All	626/626 (100%)	-0.30	4 (0%) 89 91	6, 11, 22, 40	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312[A]	GLU	4.1
1	A	312[A]	GLU	3.4
1	A	0	MET	3.3
1	B	131	PRO	2.8

### 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(Å <sup>2</sup> )	Q<0.9
3	GOL	B	404	6/6	0.53	0.37	48,49,56,57	0

*Continued on next page...*

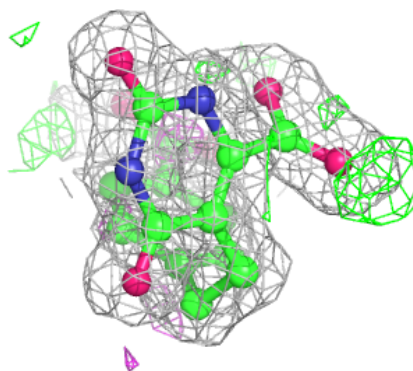
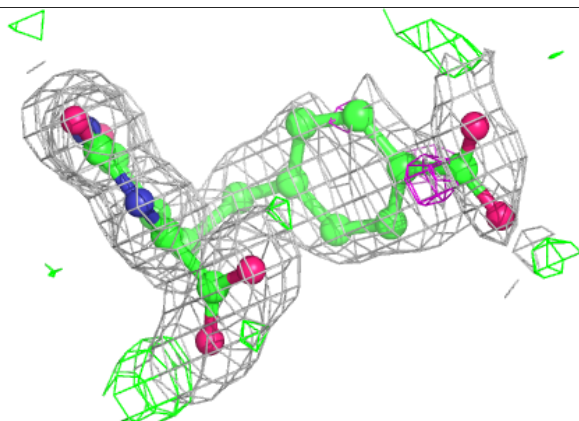
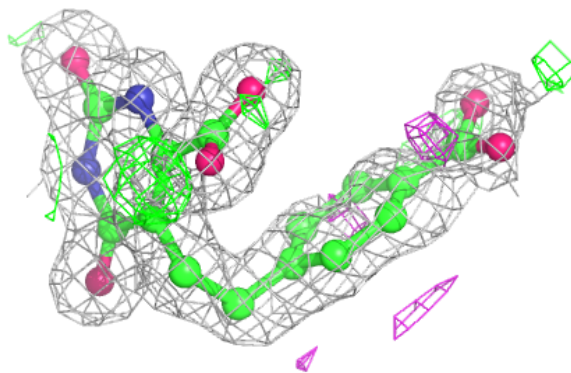
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	413	6/6	0.54	0.23	43,48,49,51	0
3	GOL	B	413	6/6	0.59	0.33	44,48,59,62	0
3	GOL	B	412	6/6	0.69	0.39	39,47,51,53	0
3	GOL	A	415	6/6	0.73	0.24	52,55,58,59	0
3	GOL	A	406	6/6	0.76	0.22	36,39,40,46	0
3	GOL	B	407	6/6	0.77	0.30	31,42,44,45	0
3	GOL	A	405	6/6	0.79	0.24	37,40,41,42	0
3	GOL	B	402	6/6	0.79	0.30	21,32,43,46	0
3	GOL	A	407	6/6	0.80	0.37	28,35,40,41	0
3	GOL	A	410	6/6	0.80	0.24	33,37,40,50	0
3	GOL	B	410	6/6	0.81	0.27	20,33,34,36	0
3	GOL	B	409	6/6	0.82	0.21	30,38,41,50	0
3	GOL	A	412	6/6	0.82	0.17	26,34,40,46	0
3	GOL	B	408	6/6	0.83	0.21	40,44,50,54	0
3	GOL	A	411	6/6	0.83	0.17	32,43,44,44	0
3	GOL	A	414	6/6	0.85	0.37	46,47,48,49	0
3	GOL	B	405	6/6	0.86	0.35	23,35,36,37	0
3	GOL	B	414	6/6	0.86	0.12	26,31,33,35	0
3	GOL	A	408	6/6	0.87	0.16	27,32,35,37	0
3	GOL	B	403	6/6	0.87	0.16	36,42,43,56	0
3	GOL	B	411	6/6	0.88	0.17	22,28,28,32	0
3	GOL	A	409	6/6	0.90	0.18	18,30,34,37	0
3	GOL	A	403	6/6	0.92	0.09	19,19,20,24	0
3	GOL	B	406	6/6	0.94	0.10	26,30,33,34	0
2	W7P	B	401	22/22	0.94	0.10	8,13,38,46	0
2	W7P	A	401	22/22	0.95	0.09	8,11,25,32	0
3	GOL	A	402[B]	6/6	0.95	0.11	9,11,12,12	6
3	GOL	A	402[A]	6/6	0.95	0.11	11,12,13,14	6
3	GOL	A	404	6/6	0.96	0.07	16,19,20,20	0
4	FMN	B	415	31/31	0.97	0.07	6,7,9,10	0
4	FMN	A	416	31/31	0.98	0.06	6,7,9,9	0
5	NCO	A	417	7/7	0.99	0.10	10,10,11,11	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.

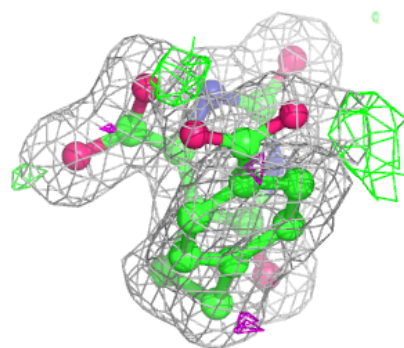
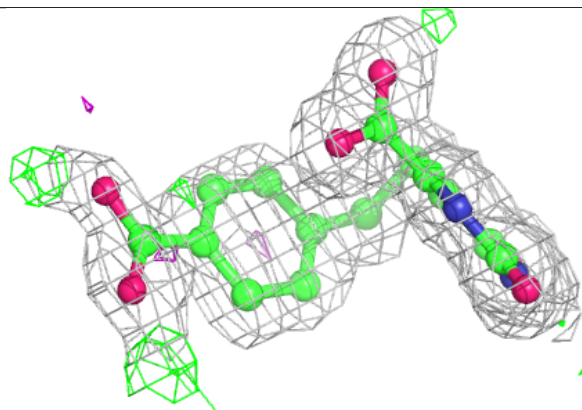
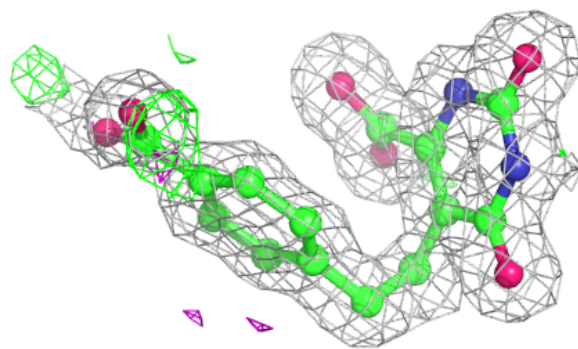
**Electron density around W7P B 401:**

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



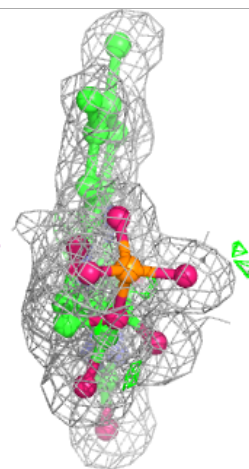
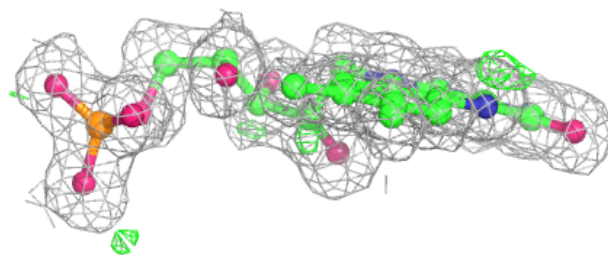
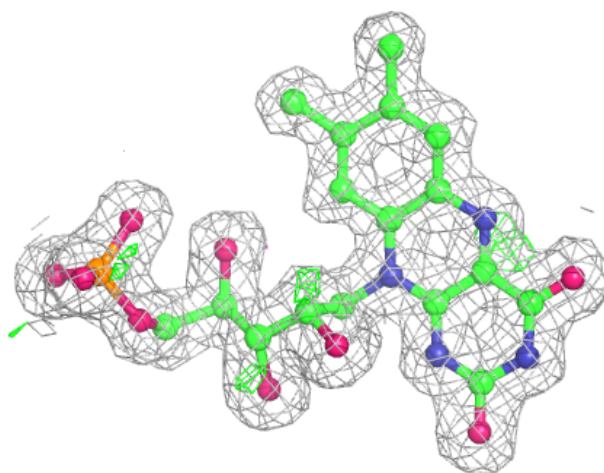
**Electron density around W7P A 401:**

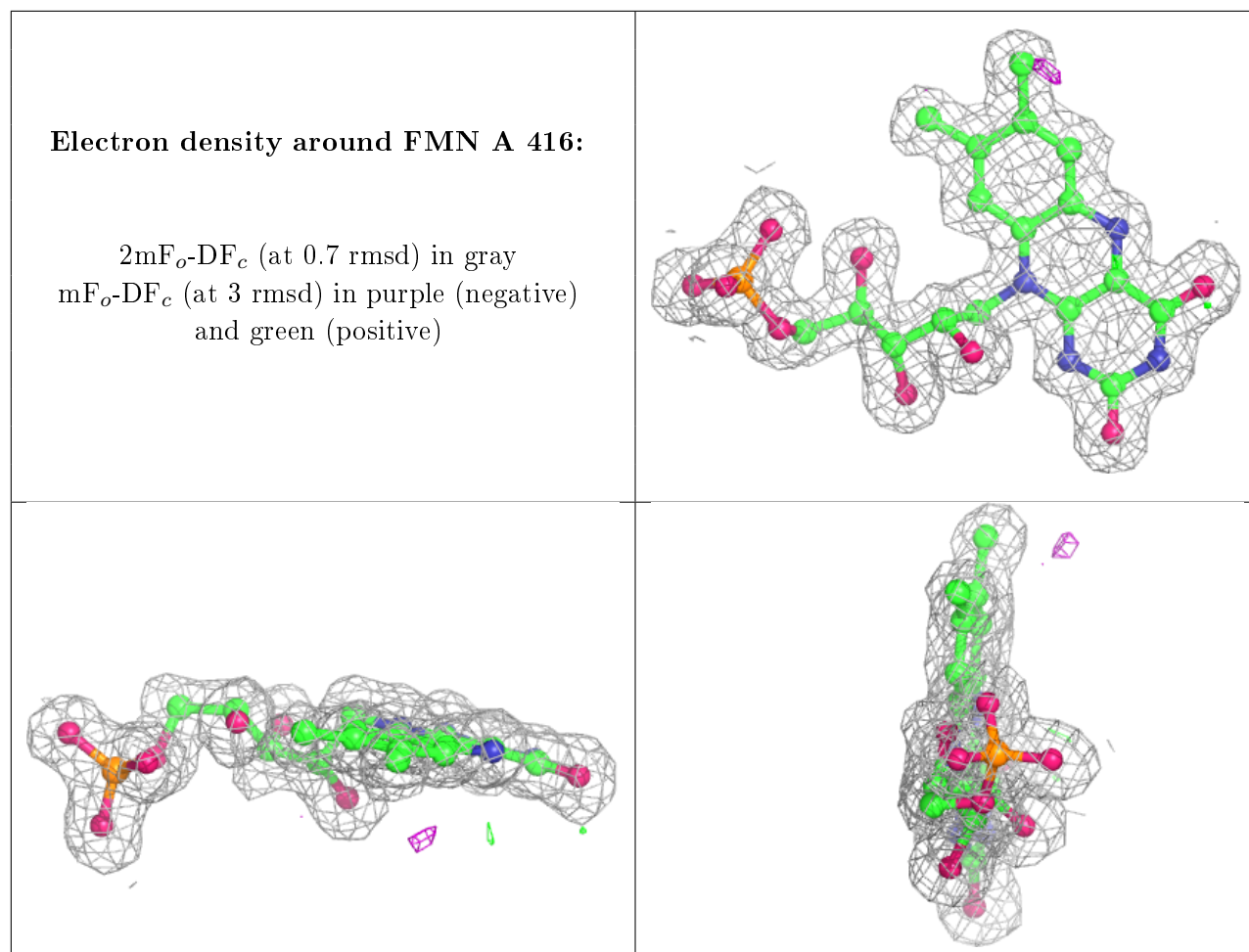
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN B 415:**

$2mF_o-DF_c$  (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.