



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 10:16 AM EDT

PDB ID : 3W73  
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with MII-4-129  
Authors : Inaoka, D.K.; Iida, M.; Tabuchi, T.; Lee, N.; Hashimoto, S.; Matsuoka, S.; Kuranaga, T.; Shiba, T.; Sakamoto, K.; Suzuki, S.; Balogun, E.O.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.  
Deposited on : 2013-02-27  
Resolution : 1.78 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

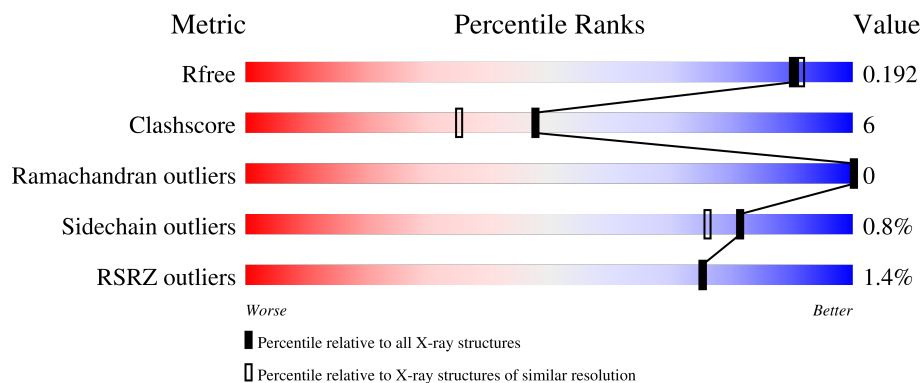
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 2% 88% 12%
1	B	313	 2% 88% 10%

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	408	-	-	X	-
3	GOL	B	408	-	X	-	-

## 2 Entry composition i

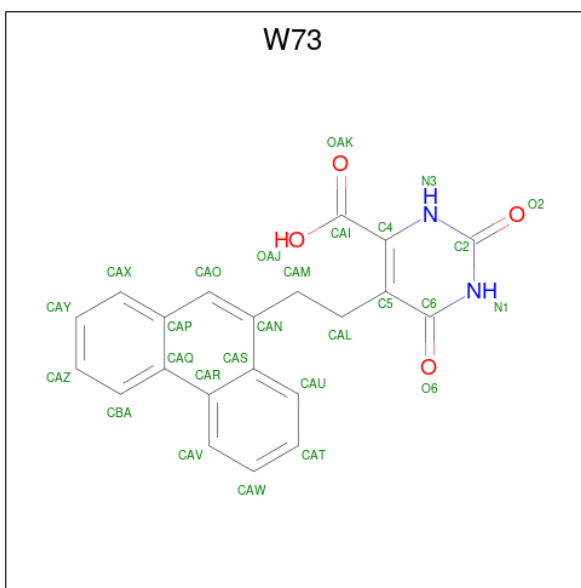
There are 6 unique types of molecules in this entry. The entry contains 5612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	313	Total 2388	C 1530	N 396	O 444	S 18	0	0	0
1	B	313	Total 2388	C 1530	N 396	O 444	S 18	0	0	0

- Molecule 2 is 2,6-dioxo-5-[2-(phenanthren-9-yl)ethyl]-1,2,3,6- tetrahydropyrimidine-4-carboxylic acid (three-letter code: W73) (formula: C<sub>21</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 27	C 21	N 2	O 4	0	0
2	B	1	Total 27	C 21	N 2	O 4	0	0

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



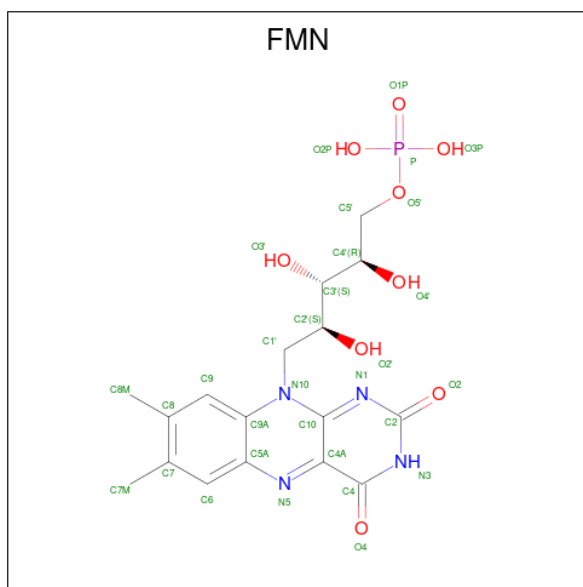
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0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

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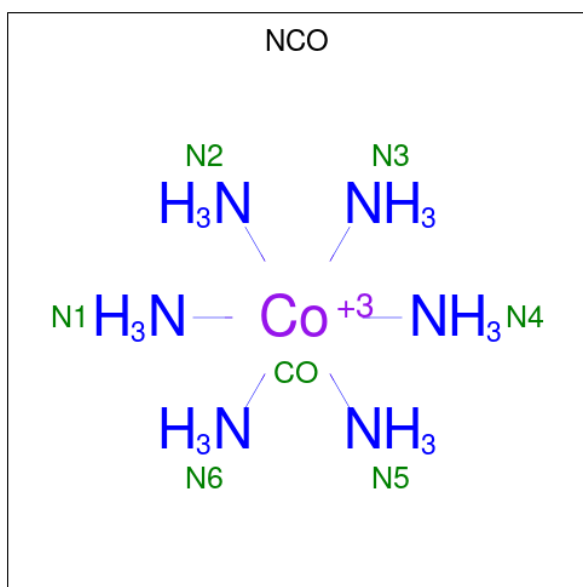
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<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: CoH<sub>18</sub>N<sub>6</sub>).



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

- Molecule 6 is water.

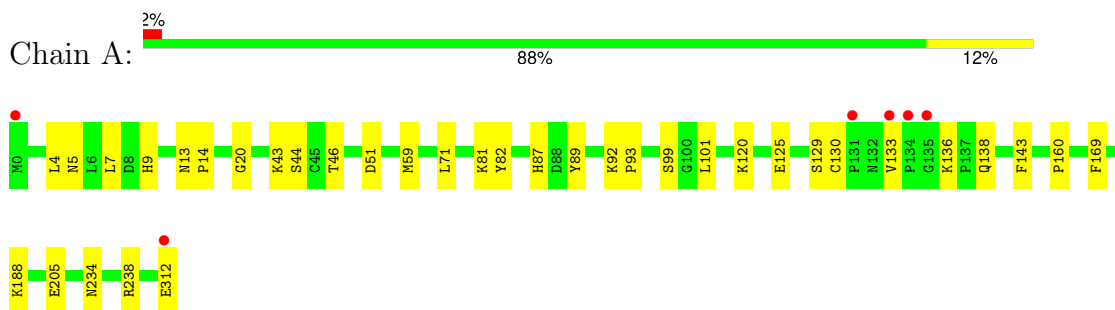
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	295	Total	O	0	0
			295	295		
6	B	322	Total	O	0	0
			322	322		



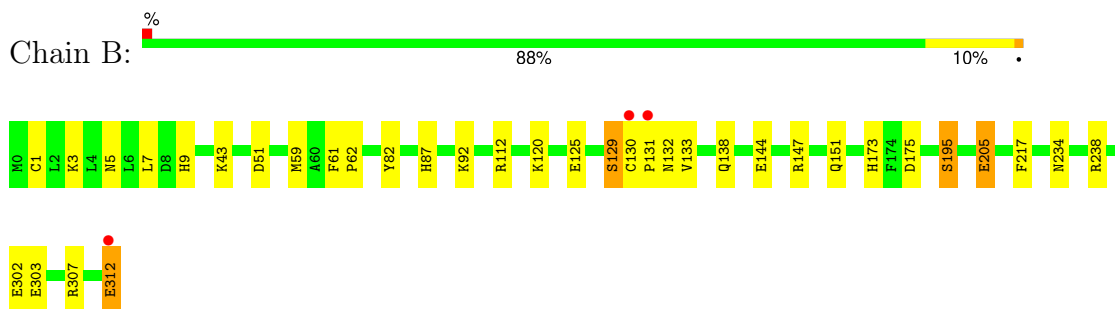
### 3 Residue-property plots [i](#)

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 i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.41Å 71.96Å 129.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.89 – 1.78 30.89 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.89-1.78) 93.5 (30.89-1.78)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.85 (at 1.78Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.144 , 0.181 0.158 , 0.192	Depositor DCC
$R_{free}$ test set	2918 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.3	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.017 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.92 % 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 2.0174e-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: NCO, W73, GOL, FMN

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	1.06	2/2440 (0.1%)	0.98	2/3305 (0.1%)
1	B	1.12	5/2440 (0.2%)	1.02	6/3305 (0.2%)
All	All	1.09	7/4880 (0.1%)	1.00	8/6610 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	GLU	CD-OE1	-5.98	1.19	1.25
1	B	125	GLU	CG-CD	5.95	1.60	1.51
1	A	125	GLU	CG-CD	5.89	1.60	1.51
1	B	195	SER	CB-OG	-5.78	1.34	1.42
1	B	303	GLU	CD-OE2	-5.43	1.19	1.25
1	B	43	LYS	CE-NZ	5.25	1.62	1.49
1	A	205	GLU	CD-OE1	5.16	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LYS	CD-CE-NZ	7.95	129.98	111.70
1	B	130	CYS	N-CA-CB	-7.36	97.36	110.60
1	B	112	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	175	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	4	LEU	CA-CB-CG	5.57	128.12	115.30
1	A	51	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	131	PRO	N-CA-C	5.45	126.28	112.10
1	B	51	ASP	CB-CG-OD2	-5.16	113.66	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2391	27	0
1	B	2388	0	2391	28	0
2	A	27	0	15	4	0
2	B	27	0	15	0	0
3	A	48	0	64	8	0
3	B	48	0	64	6	0
4	A	31	0	19	1	0
4	B	31	0	19	0	0
5	B	7	0	0	0	0
6	A	295	0	0	8	0
6	B	322	0	0	13	0
All	All	5612	0	4978	61	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 (61) 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)
2:A:401:W73:H13	6:A:503:HOH:O	1.54	1.08
3:A:409:GOL:O1	3:B:408:GOL:H2	1.78	0.83
1:A:5:ASN:HB3	6:A:791:HOH:O	1.78	0.82
1:A:59:MET:HE3	6:A:714:HOH:O	1.81	0.79
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.35	0.74
1:B:5:ASN:HB3	6:B:689:HOH:O	1.88	0.74
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.38	0.72
1:A:9:HIS:ND1	3:A:408:GOL:H11	2.13	0.63
1:B:59:MET:CE	6:B:809:HOH:O	2.47	0.61
1:A:89:TYR:HB3	3:A:408:GOL:H2	1.82	0.61
1:B:129:SER:HA	1:B:138:GLN:OE1	2.02	0.59
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.86	0.57
1:B:5:ASN:CB	6:B:689:HOH:O	2.46	0.57
1:A:101:LEU:HD11	2:A:401:W73:H10	1.86	0.57
1:A:143:PHE:CE2	3:A:409:GOL:H31	2.40	0.57
1:A:133:VAL:O	1:A:136:LYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:W73:CAZ	6:A:503:HOH:O	2.32	0.55
1:B:132:ASN:CG	6:B:602:HOH:O	2.44	0.55
1:A:89:TYR:HD2	3:A:408:GOL:H12	1.71	0.55
1:A:9:HIS:CE1	3:A:408:GOL:H11	2.42	0.54
1:A:20:GLY:HA2	1:A:43:LYS:HD2	1.89	0.54
1:A:129:SER:HA	1:A:138:GLN:NE2	2.24	0.53
1:B:59:MET:HE3	6:B:809:HOH:O	2.08	0.53
1:B:195:SER:HB3	6:B:651:HOH:O	2.08	0.53
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.91	0.53
1:A:81:LYS:CE	6:A:789:HOH:O	2.56	0.53
1:A:44:SER:HB3	1:A:99:SER:HB2	1.92	0.52
1:B:312:GLU:C	1:B:312:GLU:CD	2.68	0.51
1:B:132:ASN:ND2	1:B:133:VAL:H	2.09	0.51
1:B:59:MET:HE1	6:B:809:HOH:O	2.07	0.51
1:B:61:PHE:HB3	1:B:62:PRO:HD2	1.93	0.50
1:A:130:CYS:SG	6:A:783:HOH:O	2.55	0.50
1:B:205:GLU:OE1	6:B:723:HOH:O	2.18	0.50
1:B:151:GLN:NE2	6:B:774:HOH:O	2.38	0.49
1:A:169:PHE:HD2	3:B:408:GOL:H12	1.77	0.49
1:B:302:GLU:OE1	6:B:800:HOH:O	2.20	0.48
1:A:93:PRO:HG3	3:A:408:GOL:H32	1.96	0.48
1:B:217:PHE:CE1	3:B:403:GOL:H12	2.49	0.48
1:A:13:ASN:HB2	1:A:14:PRO:HD2	1.96	0.48
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.07	0.47
1:B:7:LEU:O	1:B:9:HIS:HD2	1.96	0.47
1:B:144:GLU:OE2	1:B:147:ARG:NH1	2.47	0.47
1:A:87:HIS:HE1	1:A:92:LYS:O	1.97	0.47
3:B:407:GOL:O3	3:B:408:GOL:C2	2.63	0.47
1:B:120:LYS:HE2	6:B:668:HOH:O	2.13	0.46
1:A:7:LEU:O	1:A:9:HIS:HD2	1.98	0.46
1:B:87:HIS:HE1	1:B:92:LYS:O	1.99	0.45
1:B:59:MET:HE3	1:B:59:MET:HB3	1.73	0.45
1:B:173:HIS:CE1	3:B:407:GOL:H2	2.52	0.45
1:A:81:LYS:HE2	6:A:789:HOH:O	2.16	0.44
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.07	0.44
1:B:61:PHE:HB3	1:B:62:PRO:CD	2.46	0.44
3:A:409:GOL:H2	3:B:407:GOL:O2	2.18	0.43
1:B:132:ASN:CG	1:B:133:VAL:H	2.22	0.43
1:A:120:LYS:HE3	6:A:794:HOH:O	2.19	0.42
1:A:160:PRO:HB3	1:A:188:LYS:HG3	2.02	0.42
1:A:20:GLY:HA3	4:A:410:FMN:N5	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ASN:ND2	6:B:602:HOH:O	2.54	0.41
1:B:307:ARG:NH2	6:B:746:HOH:O	2.54	0.41
1:A:46:THR:HG23	1:A:71:LEU:CD2	2.51	0.41
2:A:401:W73:H12	2:A:401:W73:H11	1.84	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%)	303 (97%)	8 (3%)	0	100	100
1	B	311/313 (99%)	301 (97%)	10 (3%)	0	100	100
All	All	622/626 (99%)	604 (97%)	18 (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	258/258 (100%)	257 (100%)	1 (0%)	91	88
1	B	258/258 (100%)	255 (99%)	3 (1%)	71	62
All	All	516/516 (100%)	512 (99%)	4 (1%)	81	76

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

Mol	Chain	Res	Type
1	A	312	GLU
1	B	1	CYS
1	B	129	SER
1	B	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	87	HIS
1	A	138	GLN
1	A	152	GLN
1	A	215	GLN
1	A	234	ASN
1	A	275	GLN
1	B	9	HIS
1	B	87	HIS
1	B	151	GLN
1	B	152	GLN
1	B	234	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

21 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	A	408	-	5,5,5	0.49	0	5,5,5	0.66	0
3	GOL	A	403	-	5,5,5	0.77	0	5,5,5	0.77	0
3	GOL	A	409	-	5,5,5	0.17	0	5,5,5	0.68	0
3	GOL	B	404	-	5,5,5	0.77	0	5,5,5	1.08	0
3	GOL	B	403	-	5,5,5	0.75	0	5,5,5	0.83	0
3	GOL	A	407	-	5,5,5	0.89	0	5,5,5	0.47	0
2	W73	A	401	-	30,30,30	1.42	5 (16%)	41,43,43	1.61	8 (19%)
3	GOL	A	406	-	5,5,5	0.45	0	5,5,5	0.72	0
4	FMN	B	410	-	33,33,33	1.56	7 (21%)	48,50,50	1.64	11 (22%)
3	GOL	B	409	-	5,5,5	0.99	0	5,5,5	0.37	0
3	GOL	A	402	-	5,5,5	0.56	0	5,5,5	0.65	0
3	GOL	B	405	-	5,5,5	0.62	0	5,5,5	0.98	0
3	GOL	A	404	-	5,5,5	0.42	0	5,5,5	0.45	0
3	GOL	B	406	-	5,5,5	0.31	0	5,5,5	0.38	0
2	W73	B	401	-	30,30,30	1.79	6 (20%)	41,43,43	1.73	7 (17%)
3	GOL	B	408	-	5,5,5	2.89	4 (80%)	5,5,5	3.31	3 (60%)
4	FMN	A	410	-	33,33,33	1.76	7 (21%)	48,50,50	1.66	6 (12%)
3	GOL	A	405	-	5,5,5	0.71	0	5,5,5	1.09	0
3	GOL	B	407	-	5,5,5	0.43	0	5,5,5	0.36	0
5	NCO	B	411	-	6,6,6	2.60	4 (66%)	-	-	-
3	GOL	B	402	-	5,5,5	0.54	0	5,5,5	1.53	2 (40%)

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	408	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	A	409	-	-	0/4/4/4	-
3	GOL	B	404	-	-	0/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	A	407	-	-	0/4/4/4	-
2	W73	A	401	-	-	3/9/9/9	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	406	-	-	0/4/4/4	-
4	FMN	B	410	-	-	2/18/18/18	0/3/3/3
3	GOL	B	409	-	-	2/4/4/4	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	A	404	-	-	4/4/4/4	-
3	GOL	B	406	-	-	2/4/4/4	-
2	W73	B	401	-	-	4/9/9/9	0/4/4/4
3	GOL	B	408	-	-	1/4/4/4	-
4	FMN	A	410	-	-	2/18/18/18	0/3/3/3
3	GOL	A	405	-	-	1/4/4/4	-
3	GOL	B	407	-	-	0/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	410	FMN	C4-N3	-5.87	1.27	1.38
2	B	401	W73	C4-N3	4.81	1.48	1.38
2	B	401	W73	CAL-C5	-4.22	1.40	1.51
4	B	410	FMN	C5'-C4'	3.94	1.57	1.51
5	B	411	NCO	CO-N6	3.65	2.08	1.96
3	B	408	GOL	O3-C3	3.62	1.57	1.42
3	B	408	GOL	O1-C1	3.60	1.57	1.42
5	B	411	NCO	CO-N1	3.54	2.08	1.96
4	B	410	FMN	C4'-C3'	3.50	1.59	1.53
3	B	408	GOL	C1-C2	3.33	1.64	1.51
4	A	410	FMN	C9A-C5A	3.27	1.46	1.41
2	B	401	W73	OAJ-CAI	-3.21	1.21	1.30
2	A	401	W73	C4-N3	3.21	1.45	1.38
4	A	410	FMN	C9A-N10	-3.10	1.35	1.41
4	A	410	FMN	C8-C7	3.09	1.48	1.40
4	B	410	FMN	C8-C7	2.90	1.47	1.40
5	B	411	NCO	CO-N4	2.68	2.05	1.96
4	A	410	FMN	O4-C4	2.67	1.28	1.23
2	B	401	W73	CAY-CAX	2.57	1.42	1.36
4	B	410	FMN	C9A-C5A	2.55	1.45	1.41
2	A	401	W73	CAQ-CAP	-2.51	1.37	1.42
2	B	401	W73	CAZ-CBA	2.46	1.41	1.36
4	A	410	FMN	C4A-N5	2.45	1.36	1.30
4	B	410	FMN	C4A-N5	2.44	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	410	FMN	O4-C4	2.44	1.28	1.23
5	B	411	NCO	CO-N2	2.42	2.04	1.96
4	A	410	FMN	C2-N3	-2.39	1.33	1.39
2	A	401	W73	C4-CAI	-2.34	1.44	1.48
2	A	401	W73	C4-C5	2.19	1.41	1.37
4	B	410	FMN	C8M-C8	-2.17	1.46	1.51
2	B	401	W73	CAU-CAS	-2.13	1.38	1.42
3	B	408	GOL	C3-C2	2.11	1.59	1.51
2	A	401	W73	CAM-CAN	-2.02	1.45	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	W73	C5-C6-N1	5.45	119.85	115.70
2	A	401	W73	C5-C6-N1	4.98	119.49	115.70
4	A	410	FMN	O4-C4-N3	4.90	129.34	120.11
3	B	408	GOL	O1-C1-C2	4.48	130.56	110.38
4	B	410	FMN	O4-C4-C4A	-4.40	114.92	126.53
4	A	410	FMN	O4-C4-C4A	-4.29	115.22	126.53
2	B	401	W73	CAL-C5-C6	4.23	122.31	116.64
3	B	408	GOL	O3-C3-C2	4.19	129.25	110.38
4	A	410	FMN	C9A-C5A-N5	-4.16	118.04	122.45
3	B	408	GOL	C3-C2-C1	3.74	125.51	111.80
4	B	410	FMN	O2-C2-N1	-3.58	115.85	121.80
4	A	410	FMN	C6-C5A-N5	3.46	124.19	118.44
4	B	410	FMN	O4-C4-N3	3.29	126.29	120.11
2	B	401	W73	CAM-CAN-CAS	3.27	128.25	120.99
4	A	410	FMN	O2-C2-N1	-3.27	116.37	121.80
4	B	410	FMN	C9A-C5A-N5	-2.71	119.57	122.45
4	B	410	FMN	C4-N3-C2	-2.70	120.84	125.64
4	B	410	FMN	C4A-C10-N1	-2.66	118.06	124.59
4	B	410	FMN	C5A-C9A-N10	2.62	120.33	117.97
2	A	401	W73	CAU-CAS-CAN	-2.60	118.20	122.55
2	B	401	W73	CAL-CAM-CAN	-2.57	105.53	112.64
2	A	401	W73	CAL-C5-C6	2.46	119.94	116.64
2	A	401	W73	CAL-CAM-CAN	-2.46	105.84	112.64
3	B	402	GOL	O3-C3-C2	2.43	121.30	110.38
2	B	401	W73	CAN-CAO-CAP	2.42	125.72	121.60
2	A	401	W73	CAV-CAR-CAS	2.35	120.62	117.72
2	A	401	W73	OAJ-CAI-C4	2.34	120.44	116.73
2	B	401	W73	CAU-CAS-CAN	-2.34	118.64	122.55
3	B	402	GOL	O2-C2-C1	-2.30	99.65	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	W73	CAV-CAR-CAQ	-2.24	117.84	122.35
2	B	401	W73	O2-C2-N1	2.21	125.80	121.86
4	B	410	FMN	C9-C9A-N10	-2.16	118.95	121.85
4	B	410	FMN	C4A-C4-N3	2.16	118.75	113.25
4	A	410	FMN	N3-C2-N1	2.10	123.97	119.50
2	A	401	W73	CAZ-CAY-CAX	-2.06	117.64	120.40
4	B	410	FMN	O2P-P-O1P	2.01	118.67	110.83
4	B	410	FMN	C4A-C10-N10	2.01	119.35	116.48

There are no chirality outliers.

All (25) torsion outliers are listed below:

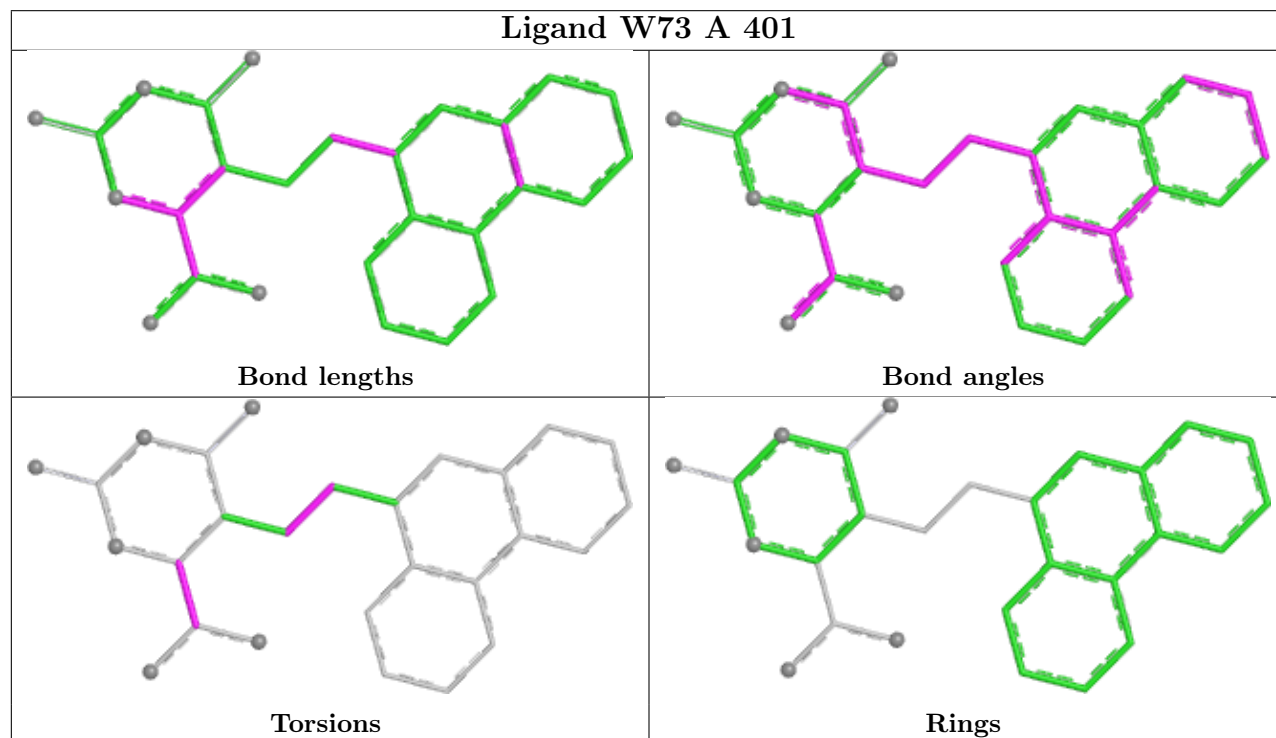
Mol	Chain	Res	Type	Atoms
2	A	401	W73	N3-C4-CAI-OAJ
2	A	401	W73	C5-CAL-CAM-CAN
2	B	401	W73	N3-C4-CAI-OAJ
2	B	401	W73	C5-CAL-CAM-CAN
3	A	403	GOL	C1-C2-C3-O3
3	A	404	GOL	O1-C1-C2-C3
3	A	404	GOL	C1-C2-C3-O3
3	A	408	GOL	O2-C2-C3-O3
3	B	406	GOL	O1-C1-C2-C3
3	A	408	GOL	C1-C2-C3-O3
3	B	409	GOL	O1-C1-C2-C3
3	A	403	GOL	O2-C2-C3-O3
3	A	404	GOL	O1-C1-C2-O2
3	A	404	GOL	O2-C2-C3-O3
3	B	409	GOL	O1-C1-C2-O2
3	B	406	GOL	O1-C1-C2-O2
4	A	410	FMN	C4'-C5'-O5'-P
4	B	410	FMN	C4'-C5'-O5'-P
3	A	405	GOL	O1-C1-C2-O2
4	B	410	FMN	C2'-C3'-C4'-O4'
3	B	408	GOL	O1-C1-C2-O2
2	B	401	W73	C5-C4-CAI-OAK
2	A	401	W73	N3-C4-CAI-OAK
2	B	401	W73	N3-C4-CAI-OAK
4	A	410	FMN	C2'-C3'-C4'-O4'

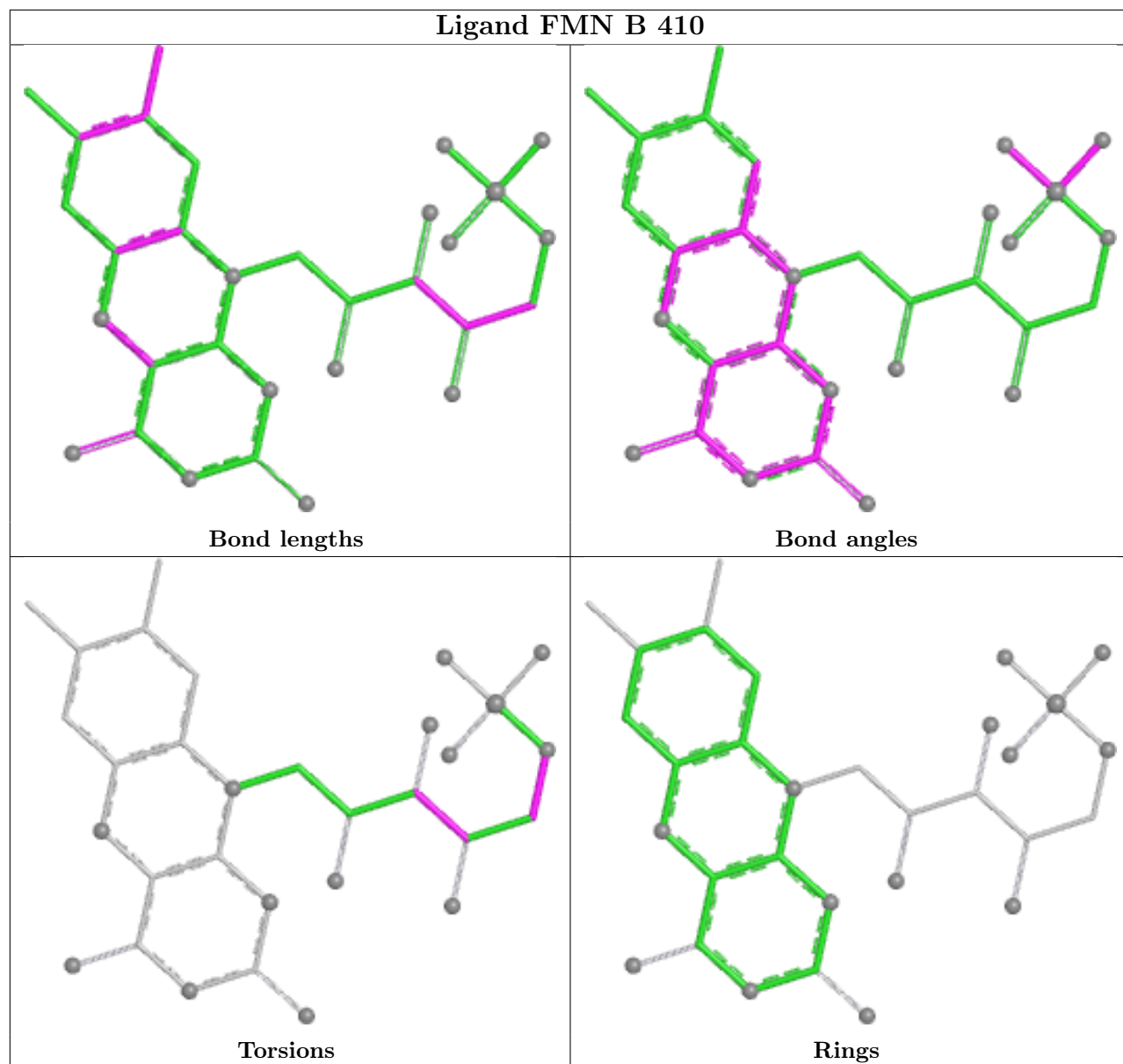
There are no ring outliers.

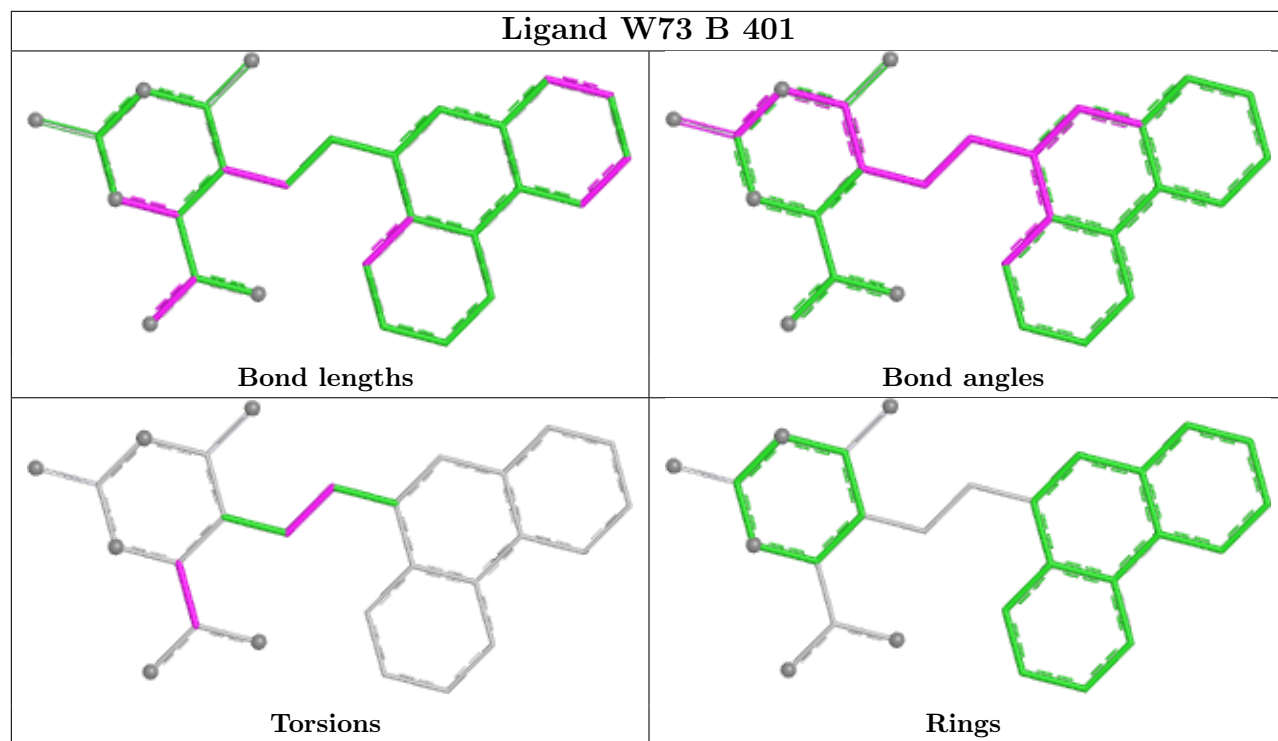
7 monomers are involved in 17 short contacts:

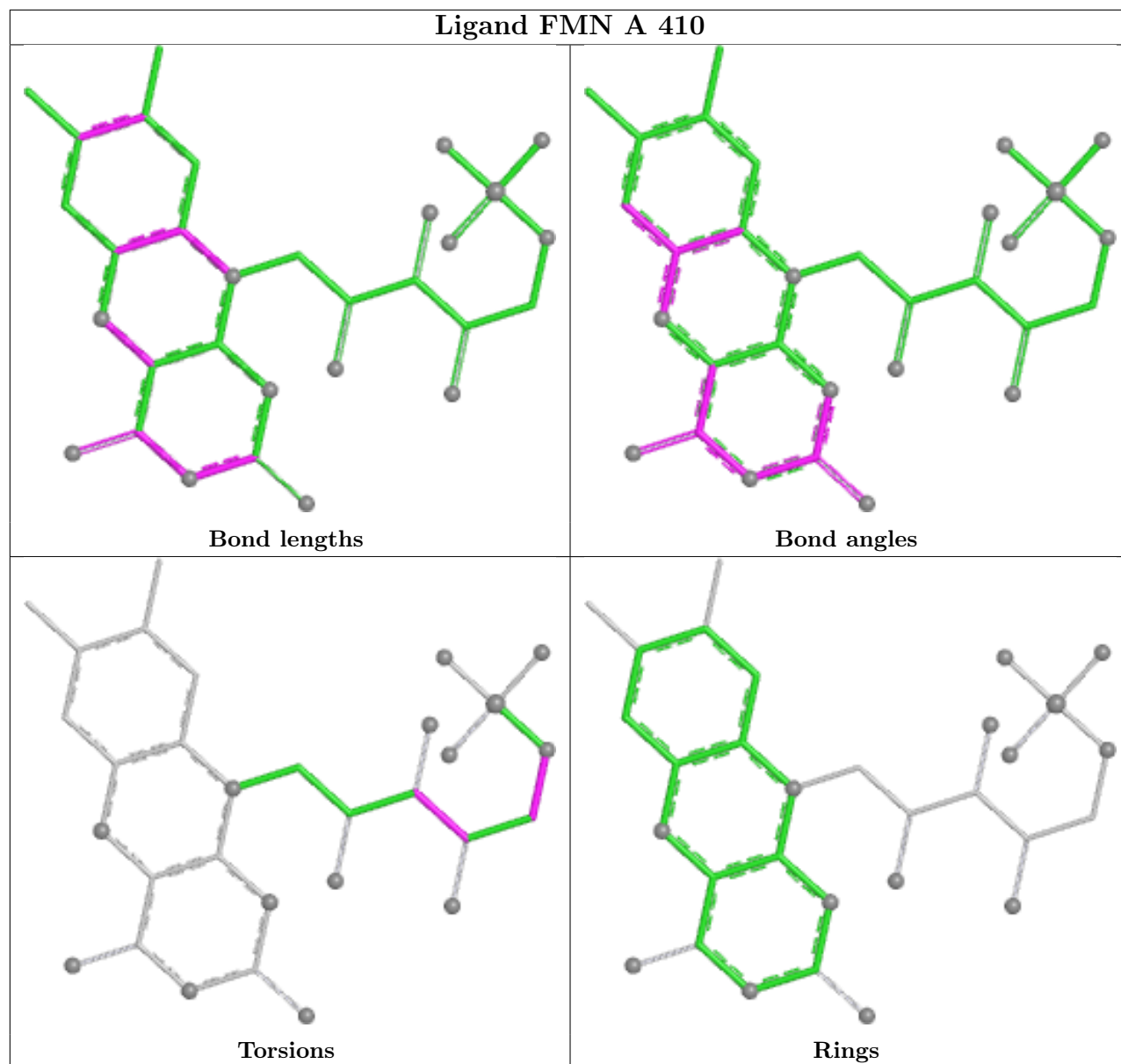
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	408	GOL	5	0
3	A	409	GOL	3	0
3	B	403	GOL	1	0
2	A	401	W73	4	0
3	B	408	GOL	3	0
4	A	410	FMN	1	0
3	B	407	GOL	3	0

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%)	0.01	6 (1%) 66 67	6, 13, 31, 51	0
1	B	313/313 (100%)	-0.11	3 (0%) 82 82	6, 12, 24, 55	0
All	All	626/626 (100%)	-0.05	9 (1%) 75 75	6, 12, 27, 55	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	VAL	7.6
1	A	134	PRO	5.9
1	A	131	PRO	4.4
1	B	312	GLU	4.2
1	A	135	GLY	4.1
1	A	312	GLU	3.8
1	B	130	CYS	3.6
1	A	0	MET	2.3
1	B	131	PRO	2.1

### 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,



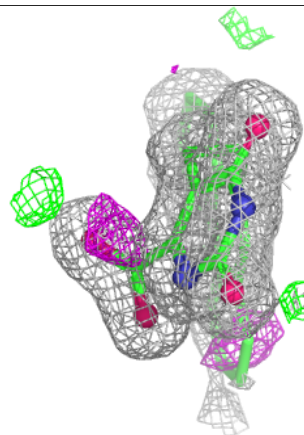
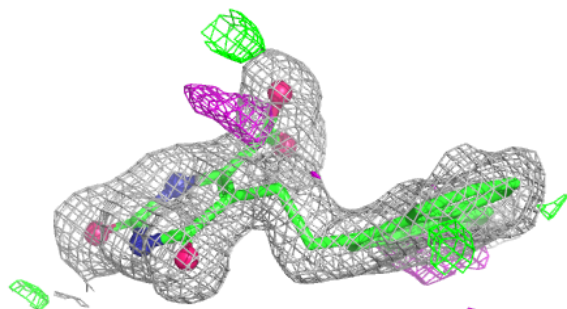
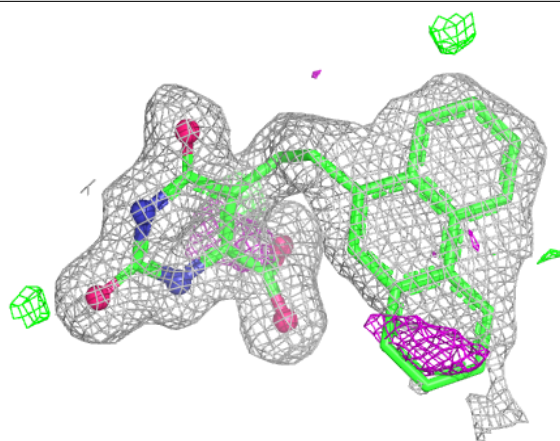
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	407	6/6	0.73	0.22	34,36,40,47	0
3	GOL	A	405	6/6	0.78	0.18	40,41,46,49	0
3	GOL	B	407	6/6	0.79	0.20	46,54,54,57	0
3	GOL	B	408	6/6	0.80	0.22	17,27,29,36	0
3	GOL	A	409	6/6	0.81	0.18	46,51,51,53	0
3	GOL	B	404	6/6	0.81	0.27	27,36,37,38	0
3	GOL	B	409	6/6	0.82	0.21	21,30,36,37	0
3	GOL	B	406	6/6	0.83	0.17	45,46,50,50	0
3	GOL	A	404	6/6	0.83	0.16	44,47,48,51	0
3	GOL	B	402	6/6	0.85	0.15	18,21,23,24	0
3	GOL	A	408	6/6	0.85	0.36	29,40,42,46	0
3	GOL	B	403	6/6	0.90	0.12	23,25,27,31	0
3	GOL	A	406	6/6	0.91	0.15	35,37,37,40	0
3	GOL	B	405	6/6	0.93	0.17	33,38,38,39	0
3	GOL	A	403	6/6	0.94	0.14	23,26,31,35	0
2	W73	A	401	27/27	0.94	0.12	8,15,39,39	0
2	W73	B	401	27/27	0.94	0.11	6,12,31,36	0
3	GOL	A	402	6/6	0.97	0.09	19,20,21,23	0
4	FMN	B	410	31/31	0.97	0.12	5,7,9,10	0
4	FMN	A	410	31/31	0.98	0.10	5,7,9,9	0
5	NCO	B	411	7/7	0.99	0.08	10,10,11,12	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.

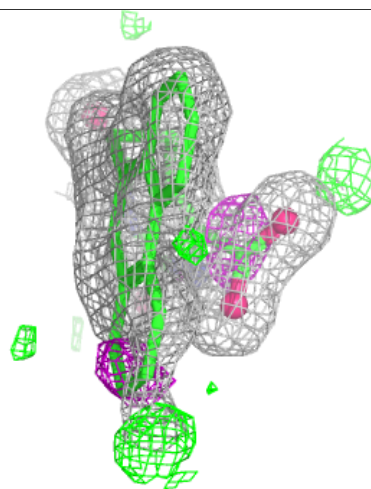
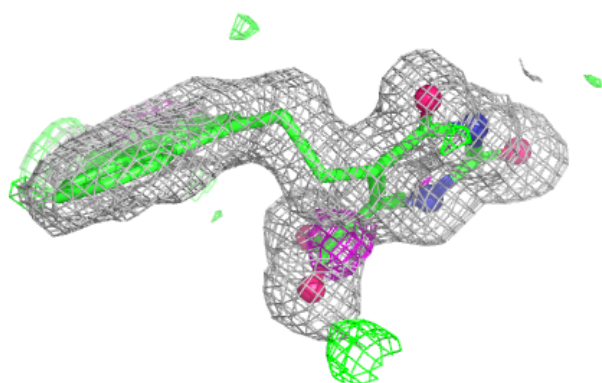
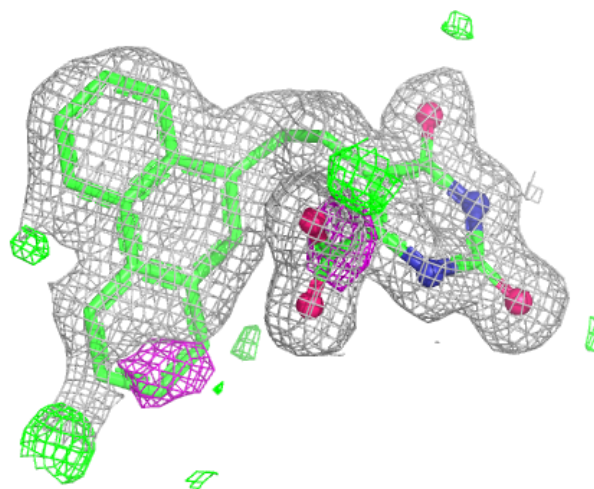
**Electron density around W73 A 401:**

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



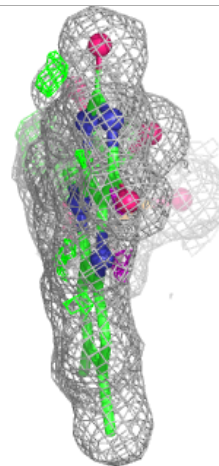
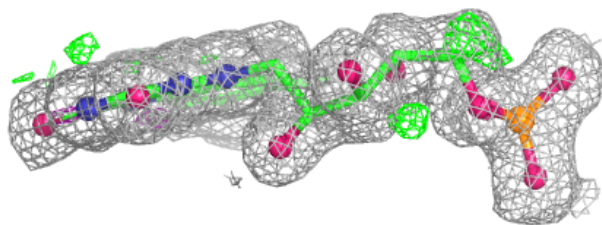
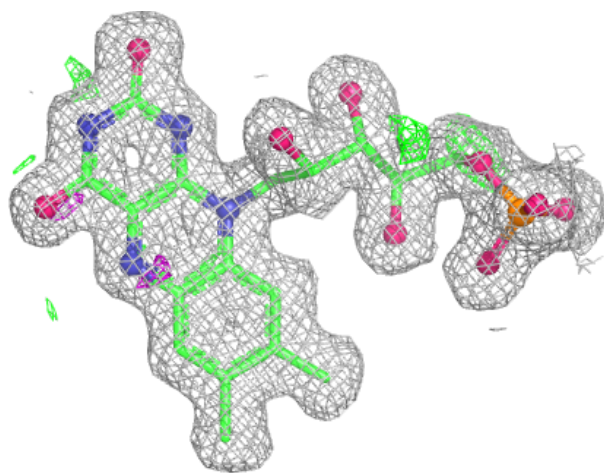
**Electron density around W73 B 401:**

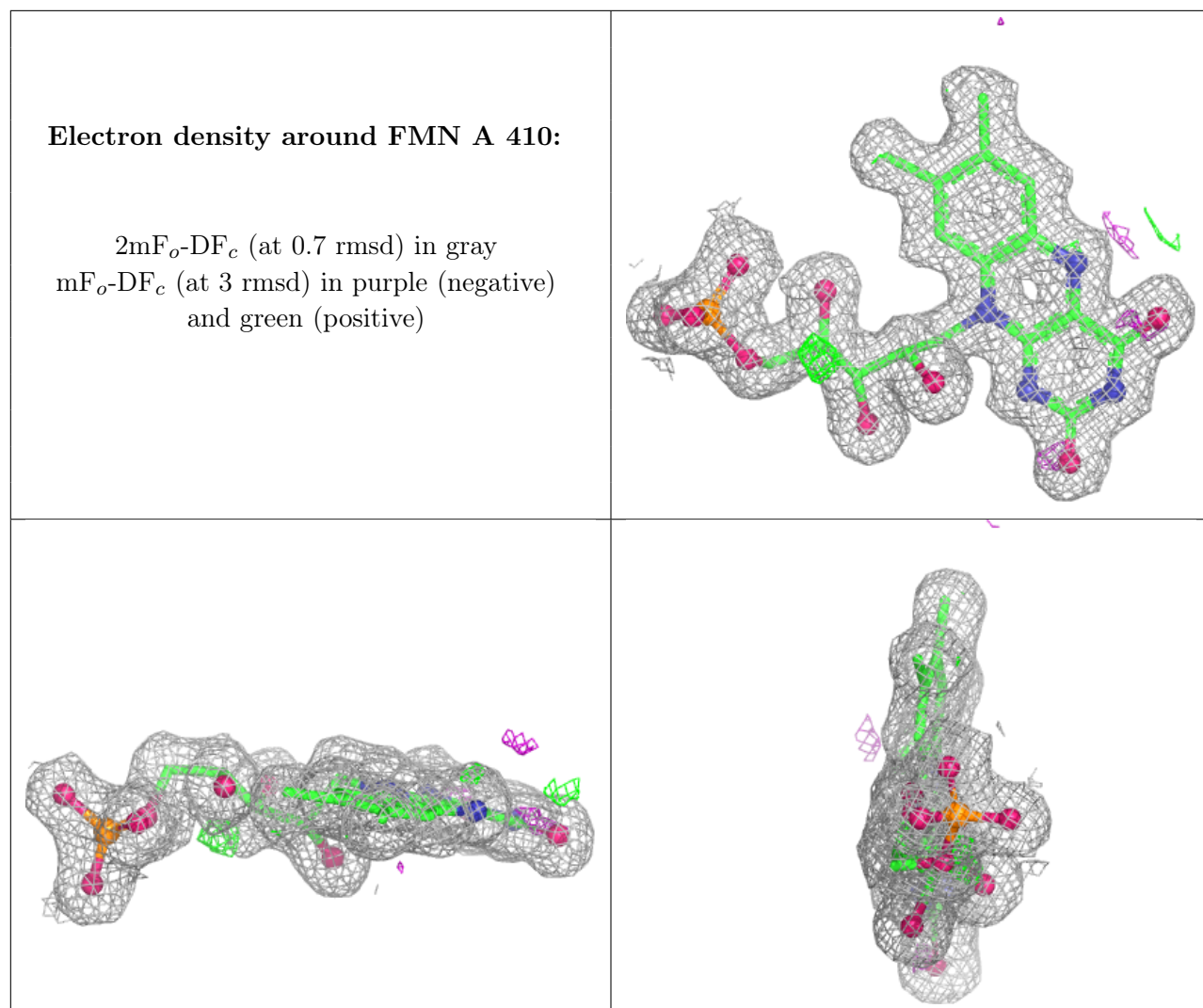
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN B 410:**

$2mF_o-DF_c$  (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.