Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2020 – 05:23 pm BST

PDB ID	:	6GJG
Title	:	Plasmodium falciparum dihydroorotate dehydrogenase DHODH in complex with 3,6-dimethyl-N-(4-(trifluoromethyl)phenyl)-(1,2)oxazolo(5,4-d)pyrimidin -4-amine
Authors	:	Rowland, P.
Deposited on	:	2018-05-16
Resolution	:	1.99 Å(reported)

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

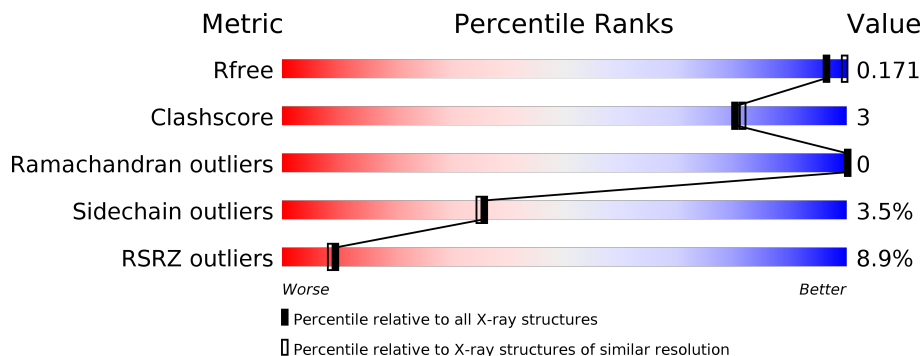|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	Percentile Ranks	Value
Rfree		0.171
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		3.5%
RSRZ outliers		8.9%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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 <=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	401	6% / 83% / 9% / 7%
1	B	401	10% / 85% / 7% · 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6488 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 (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total 2937	C 1878	N 494	O 551	S 14	0	0	0
1	B	373	Total 2954	C 1887	N 496	O 557	S 14	0	0	0

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP Q08210
A	140	GLY	-	expression tag	UNP Q08210
A	141	HIS	-	expression tag	UNP Q08210
A	142	HIS	-	expression tag	UNP Q08210
A	143	HIS	-	expression tag	UNP Q08210
A	144	HIS	-	expression tag	UNP Q08210
A	145	HIS	-	expression tag	UNP Q08210
A	146	HIS	-	expression tag	UNP Q08210
A	147	ALA	-	expression tag	UNP Q08210
A	148	GLU	-	expression tag	UNP Q08210
A	149	ASN	-	expression tag	UNP Q08210
A	150	LEU	-	expression tag	UNP Q08210
A	151	TYR	-	expression tag	UNP Q08210
A	152	PHE	-	expression tag	UNP Q08210
A	153	GLN	-	expression tag	UNP Q08210
A	154	GLY	-	expression tag	UNP Q08210
A	155	ALA	-	expression tag	UNP Q08210
A	156	ASP	-	expression tag	UNP Q08210
A	157	PRO	-	expression tag	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	THR	deletion	UNP Q08210
A	?	-	TYR	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ILE	deletion	UNP Q08210
A	?	-	VAL	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	PHE	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	HIS	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ALA	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
B	139	MET	-	initiating methionine	UNP Q08210
B	140	GLY	-	expression tag	UNP Q08210
B	141	HIS	-	expression tag	UNP Q08210
B	142	HIS	-	expression tag	UNP Q08210
B	143	HIS	-	expression tag	UNP Q08210
B	144	HIS	-	expression tag	UNP Q08210
B	145	HIS	-	expression tag	UNP Q08210
B	146	HIS	-	expression tag	UNP Q08210
B	147	ALA	-	expression tag	UNP Q08210
B	148	GLU	-	expression tag	UNP Q08210
B	149	ASN	-	expression tag	UNP Q08210
B	150	LEU	-	expression tag	UNP Q08210
B	151	TYR	-	expression tag	UNP Q08210
B	152	PHE	-	expression tag	UNP Q08210
B	153	GLN	-	expression tag	UNP Q08210
B	154	GLY	-	expression tag	UNP Q08210
B	155	ALA	-	expression tag	UNP Q08210
B	156	ASP	-	expression tag	UNP Q08210

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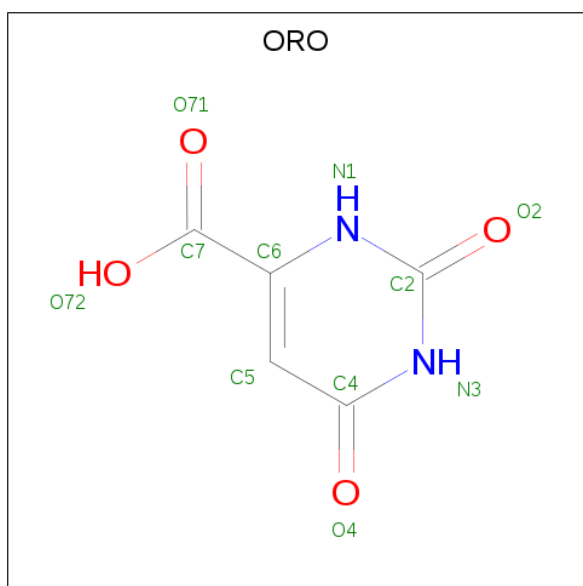
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Chain	Residue	Modelled	Actual	Comment	Reference
B	157	PRO	-	expression tag	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	THR	deletion	UNP Q08210
B	?	-	TYR	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ILE	deletion	UNP Q08210
B	?	-	VAL	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	PHE	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	HIS	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ALA	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by author).
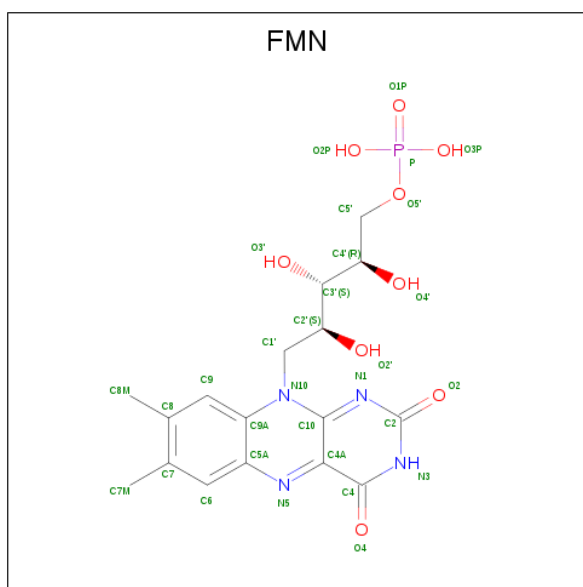
FMN

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

- Molecule 3 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$) (labeled as "Ligand of Interest" by author).
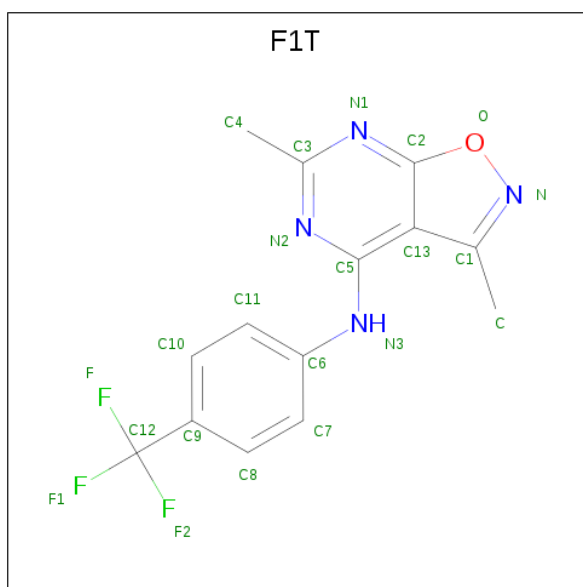

ORO

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 11	C 5	N 2	O 4	0	0

- Molecule 4 is 3,6-dimethyl- {N}-[4-(trifluoromethyl)phenyl]-[1,2]oxazolo[5,4-d]pyrimidin-4-a mine (three-letter code: F1T) (formula: $C_{14}H_{11}F_3N_4O$) (labeled as "Ligand of Interest" by author).

F1T

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 22	C 14	F 3	N 4	O 1	0	0
4	B	1	Total 22	C 14	F 3	N 4	O 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	247	Total 247	O 247	0	0
5	B	222	Total 222	O 222	0	0

3 Residue-property plots ⓘ

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 (quinone), mitochondrial
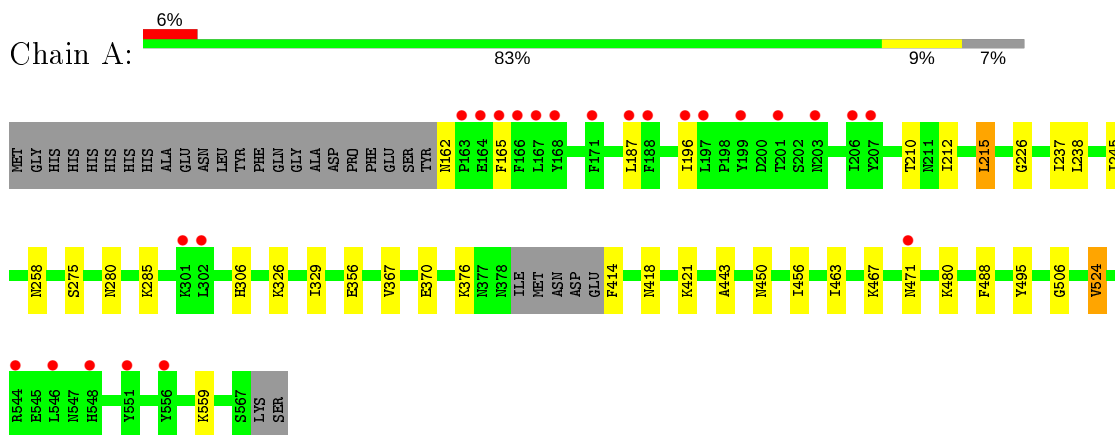
- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial
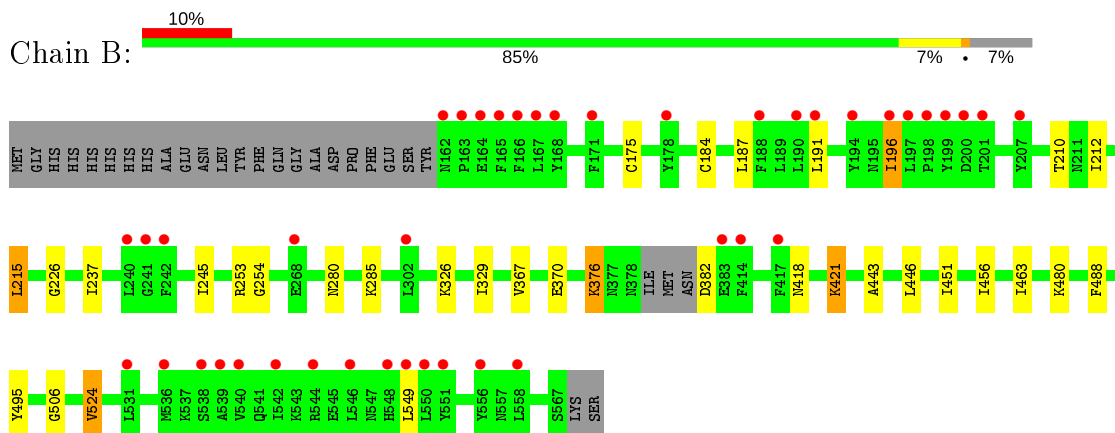
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.73Å 162.95Å 64.74Å 90.00° 112.90° 90.00°	Depositor
Resolution (Å)	21.80 – 1.99	Depositor
	59.64 – 1.99	EDS
% Data completeness	46.9 (21.80-1.99)	Depositor
(in resolution range)	46.8 (59.64-1.99)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.163 , 0.206	Depositor
	0.174 , 0.171	DCC
R_{free} test set	1830 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 65.4	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ORO, F1T

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.51	0/2986	0.71	0/4019
1	B	0.50	0/3003	0.71	0/4042
All	All	0.50	0/5989	0.71	0/8061

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2937	0	2985	17	0
1	B	2954	0	2995	18	0
2	A	31	0	19	1	0
2	B	31	0	19	1	0
3	A	11	0	3	0	0
3	B	11	0	3	0	0
4	A	22	0	0	0	0
4	B	22	0	0	0	0
5	A	247	0	0	2	0
5	B	222	0	0	1	0
All	All	6488	0	6024	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (33) 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:326:LYS:HG2	1:B:370:GLU:HG3	1.66	0.77
1:A:326:LYS:HG2	1:A:370:GLU:HG3	1.68	0.74
1:A:506:GLY:HA2	5:A:712:HOH:O	1.94	0.67
1:B:329:ILE:HD11	1:B:367:VAL:HG13	1.85	0.58
1:B:326:LYS:HG2	1:B:370:GLU:CG	2.34	0.58
1:A:329:ILE:HD11	1:A:367:VAL:HG13	1.87	0.56
1:A:559:LYS:HG2	5:A:848:HOH:O	2.07	0.55
1:A:450:ASN:OD1	1:B:253:ARG:HD2	2.07	0.54
1:A:326:LYS:HG2	1:A:370:GLU:CG	2.38	0.53
1:B:175:CYS:HB3	1:B:184:CYS:SG	2.48	0.53
1:A:212:ILE:O	1:A:215:LEU:HB2	2.10	0.51
1:B:212:ILE:O	1:B:215:LEU:HB2	2.11	0.50
1:A:463:ILE:HD13	1:A:480:LYS:HB3	1.93	0.50
1:B:463:ILE:HD13	1:B:480:LYS:HB3	1.93	0.50
1:B:506:GLY:HA2	5:B:705:HOH:O	2.12	0.49
1:B:443:ALA:CB	1:B:495:TYR:HB3	2.43	0.48
1:B:456:ILE:HG23	1:B:488:PHE:CD1	2.50	0.47
1:B:418:ASN:O	1:B:421:LYS:HE3	2.15	0.46
1:A:443:ALA:CB	1:A:495:TYR:HB3	2.45	0.46
1:A:456:ILE:HG23	1:A:488:PHE:CD1	2.51	0.46
1:B:237:ILE:HG21	1:B:245:ILE:HD12	1.99	0.45
1:A:418:ASN:O	1:A:421:LYS:HE3	2.18	0.43
1:B:446:LEU:HD22	1:B:451:ILE:HG21	2.01	0.42
1:A:226:GLY:HA3	2:A:601:FMN:N5	2.35	0.42
1:A:237:ILE:HG21	1:A:245:ILE:HD12	2.01	0.42
1:A:450:ASN:HB2	1:B:254:GLY:O	2.19	0.42
1:A:210:THR:CG2	1:A:524:VAL:HG13	2.50	0.41
1:A:238:LEU:HD13	1:A:306:HIS:HB3	2.03	0.41
1:B:191:LEU:HD22	1:B:196:ILE:HD11	2.03	0.41
1:B:376:LYS:H	1:B:376:LYS:HG2	1.54	0.41
1:A:258:ASN:HB2	1:A:275:SER:O	2.21	0.41
1:B:210:THR:CG2	1:B:524:VAL:HG13	2.50	0.41
1:B:226:GLY:HA3	2:B:601:FMN:N5	2.36	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	367/401 (92%)	352 (96%)	15 (4%)	0	100	100
1	B	369/401 (92%)	352 (95%)	17 (5%)	0	100	100
All	All	736/802 (92%)	704 (96%)	32 (4%)	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	328/354 (93%)	315 (96%)	13 (4%)	31	29
1	B	330/354 (93%)	320 (97%)	10 (3%)	41	41
All	All	658/708 (93%)	635 (96%)	23 (4%)	36	35

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	165	PHE
1	A	187	LEU
1	A	196	ILE
1	A	215	LEU
1	A	280	ASN
1	A	285	LYS
1	A	356	GLU

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Mol	Chain	Res	Type
1	A	376	LYS
1	A	414	PHE
1	A	467	LYS
1	A	471	ASN
1	A	524	VAL
1	B	187	LEU
1	B	196	ILE
1	B	215	LEU
1	B	280	ASN
1	B	285	LYS
1	B	376	LYS
1	B	382	ASP
1	B	421	LYS
1	B	524	VAL
1	B	549	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	494	ASN
1	B	162	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	ORO	A	602	-	6,11,11	2.09	2 (33%)	3,15,15	4.87	2 (66%)
2	FMN	B	601	-	31,33,33	1.83	5 (16%)	40,50,50	2.68	7 (17%)
2	FMN	A	601	-	31,33,33	1.93	5 (16%)	40,50,50	2.69	7 (17%)
3	ORO	B	602	-	6,11,11	2.25	2 (33%)	3,15,15	4.87	2 (66%)
4	F1T	A	603	-	21,24,24	0.63	0	26,36,36	0.80	1 (3%)
4	F1T	B	603	-	21,24,24	0.64	0	26,36,36	0.73	1 (3%)

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	ORO	A	602	-	-	0/0/4/4	0/1/1/1
2	FMN	B	601	-	-	1/18/18/18	0/3/3/3
2	FMN	A	601	-	-	1/18/18/18	0/3/3/3
3	ORO	B	602	-	-	0/0/4/4	0/1/1/1
4	F1T	A	603	-	-	1/10/10/10	0/3/3/3
4	F1T	B	603	-	-	2/10/10/10	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FMN	C4A-C10	7.37	1.46	1.38
2	B	601	FMN	C4A-C10	6.34	1.45	1.38
2	B	601	FMN	C4-C4A	5.16	1.50	1.41
3	B	602	ORO	C4-N3	4.35	1.40	1.33
2	A	601	FMN	C4-C4A	4.19	1.48	1.41
2	A	601	FMN	C4-N3	3.78	1.39	1.33
2	B	601	FMN	C4-N3	3.74	1.39	1.33
3	A	602	ORO	C4-N3	3.73	1.39	1.33
2	A	601	FMN	C5A-N5	3.64	1.41	1.35
2	B	601	FMN	C5A-N5	3.15	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ORO	C6-N1	3.08	1.39	1.34
3	B	602	ORO	C6-N1	3.06	1.39	1.34
2	A	601	FMN	C9A-N10	2.88	1.42	1.38
2	B	601	FMN	C9A-N10	2.68	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FMN	C4-N3-C2	12.78	125.93	115.14
2	B	601	FMN	C4-N3-C2	12.69	125.85	115.14
2	B	601	FMN	C4A-C4-N3	-7.40	113.31	123.43
2	A	601	FMN	C4A-C4-N3	-7.29	113.46	123.43
3	A	602	ORO	C5-C4-N3	-7.03	115.87	124.08
3	B	602	ORO	C5-C4-N3	-7.02	115.89	124.08
3	B	602	ORO	C4-C5-C6	4.51	119.64	116.73
3	A	602	ORO	C4-C5-C6	4.45	119.61	116.73
2	B	601	FMN	C10-C4A-N5	4.35	124.27	121.26
2	A	601	FMN	C10-C4A-N5	4.29	124.23	121.26
2	B	601	FMN	C4-C4A-C10	-4.09	117.25	119.95
2	A	601	FMN	C4-C4A-C10	-4.08	117.25	119.95
2	B	601	FMN	C1'-N10-C9A	3.72	121.22	118.29
2	A	601	FMN	C1'-N10-C9A	3.64	121.16	118.29
4	A	603	F1T	C3-N1-C2	-3.23	112.90	115.52
4	B	603	F1T	C3-N1-C2	-3.01	113.08	115.52
2	B	601	FMN	C4A-C10-N10	-2.92	117.30	120.30
2	A	601	FMN	C4A-C10-N10	-2.86	117.36	120.30
2	B	601	FMN	O5'-P-O1P	2.20	112.64	106.47
2	A	601	FMN	O5'-P-O1P	2.06	112.26	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

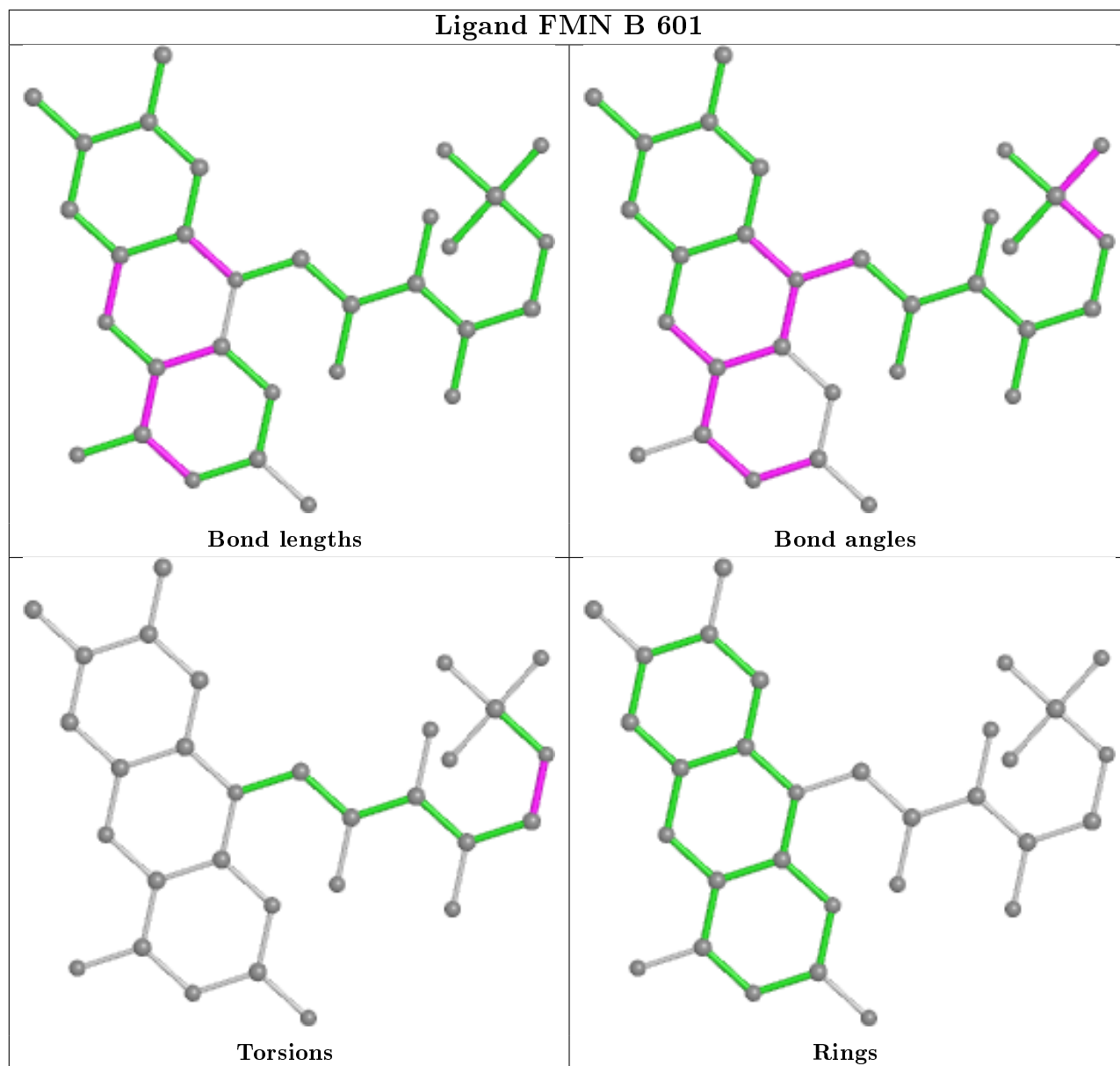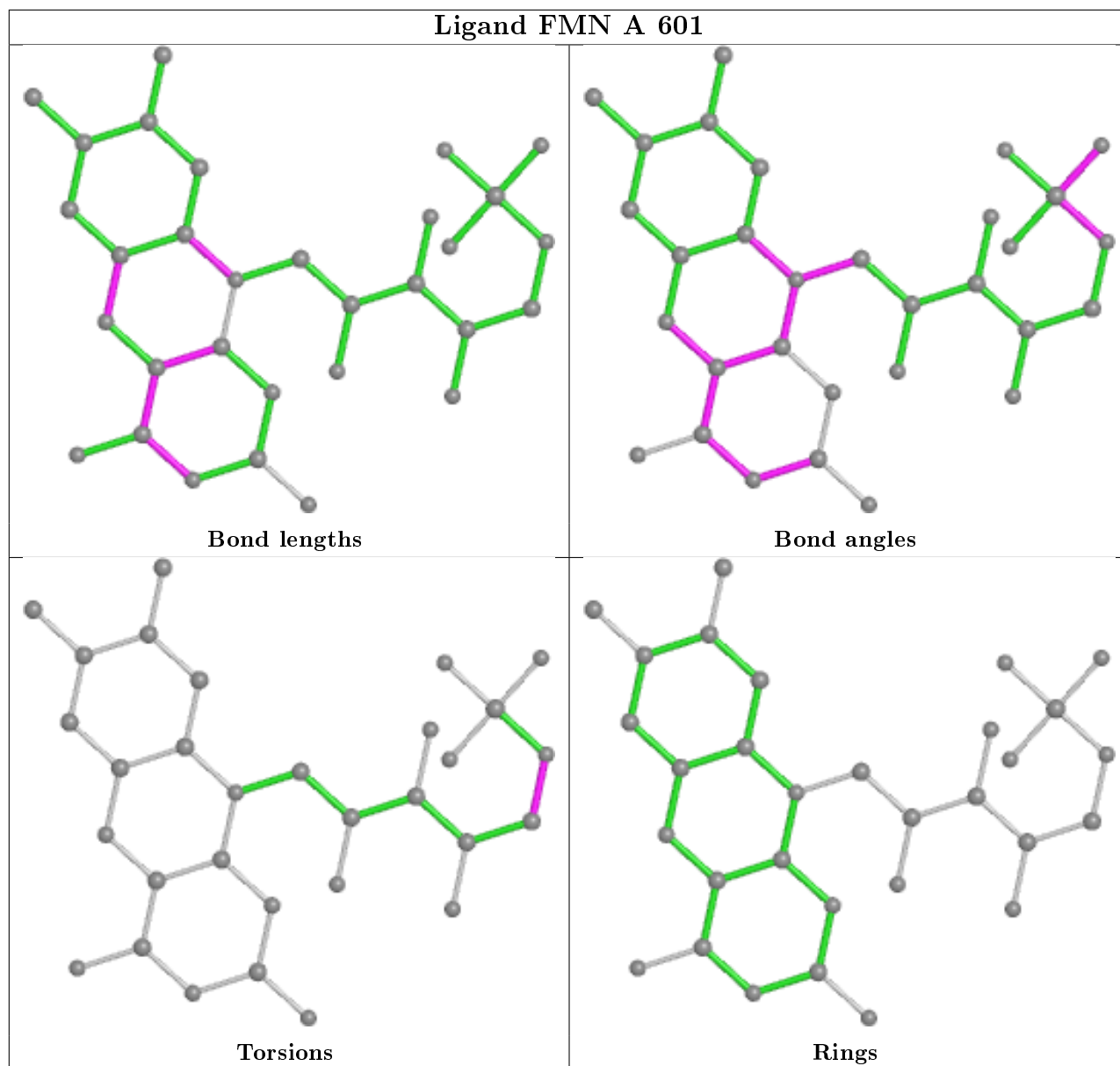| Mol	Chain	Res	Type	Atoms
4	B	603	F1T	N2-C5-N3-C6
4	B	603	F1T	C13-C5-N3-C6
2	B	601	FMN	C4'-C5'-O5'-P
2	A	601	FMN	C4'-C5'-O5'-P
4	A	603	F1T	N2-C5-N3-C6

There are no ring outliers.
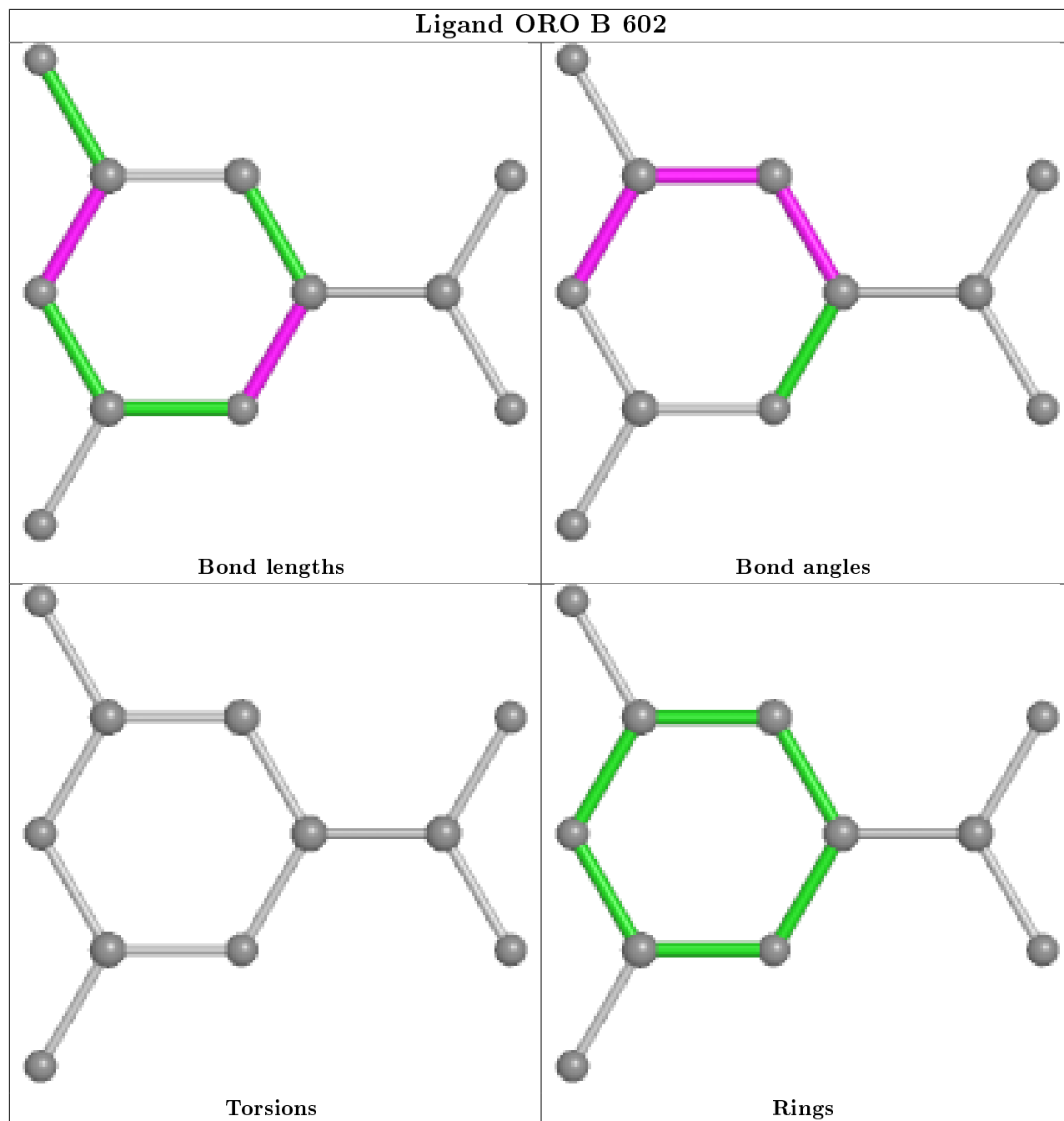
2 monomers are involved in 2 short contacts:

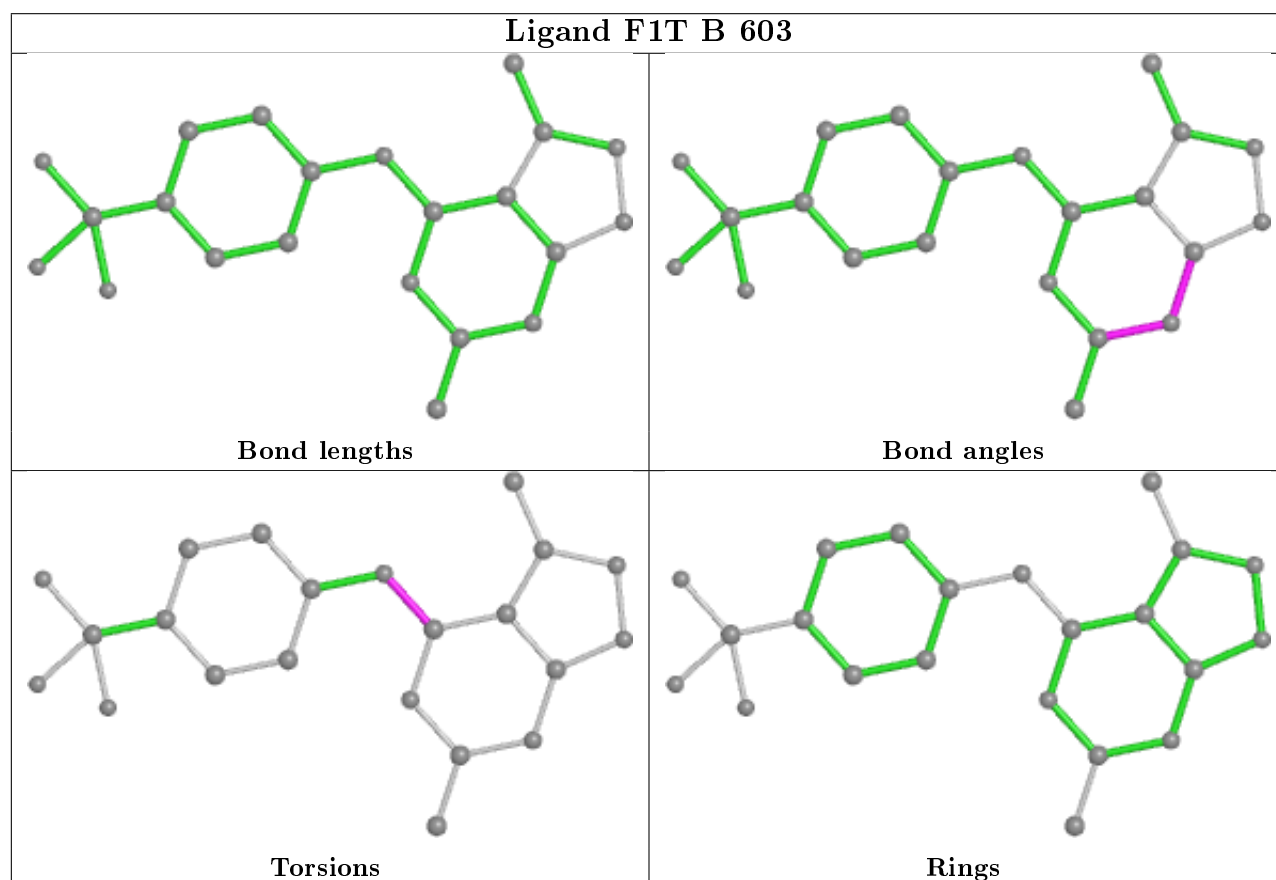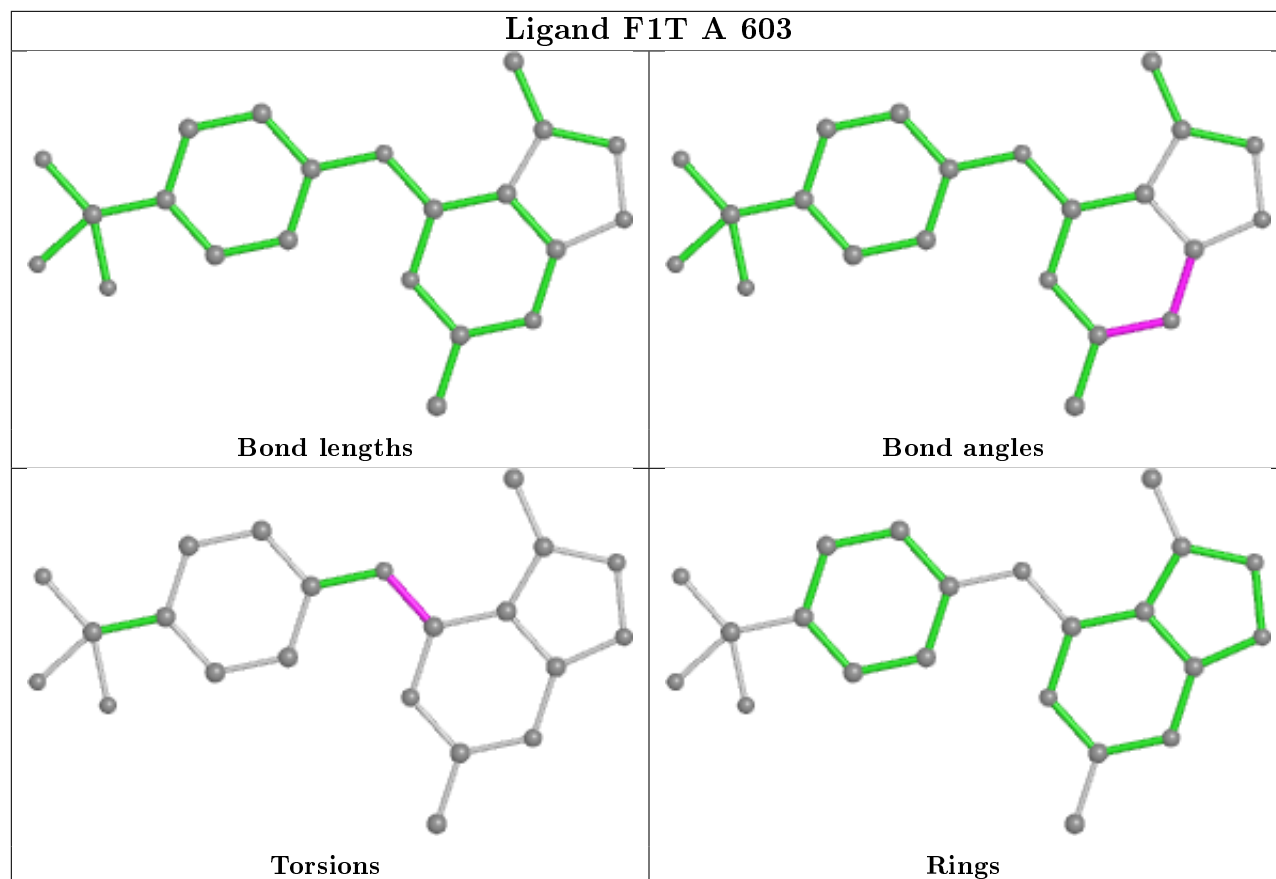| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FMN	1	0
2	A	601	FMN	1	0

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 then 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.

Ligand ORO A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand FMN A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ORO B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand F1T A 603

Bond lengths

Bond angles

Torsions

Rings

Ligand F1T B 603

Bond lengths

Bond angles

Torsions

Rings
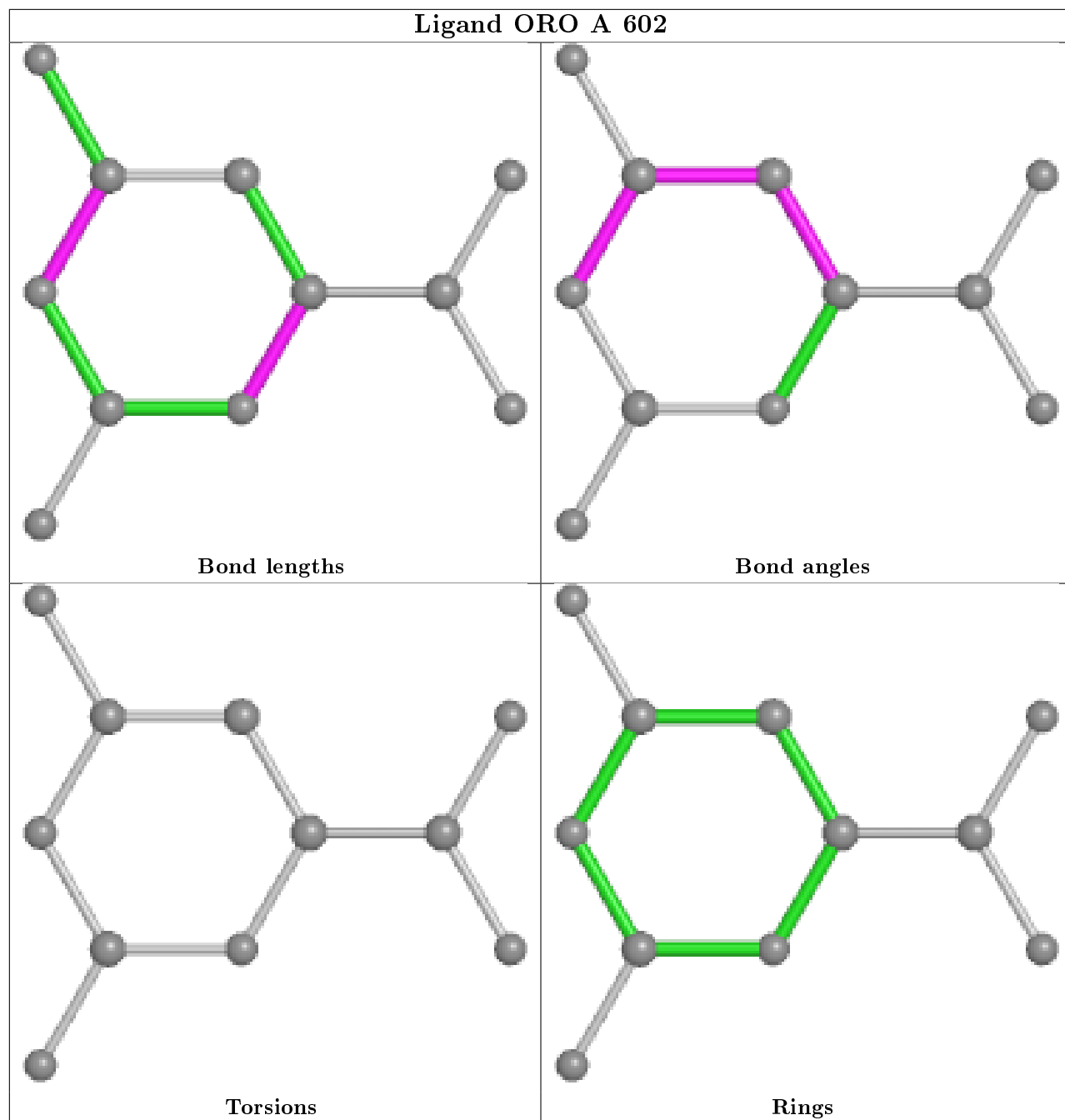
5.7 Other polymers (i)

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, 95th 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^2)	Q<0.9
1	A	371/401 (92%)	0.13	24 (6%)	18	18	12, 36, 87, 126	1 (0%)
1	B	373/401 (93%)	0.37	42 (11%)	5	4	13, 41, 100, 138	1 (0%)
All	All	744/802 (92%)	0.25	66 (8%)	9	8	12, 39, 93, 138	2 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	PHE	9.6
1	B	383	GLU	7.0
1	B	201	THR	6.2
1	A	165	PHE	5.1
1	B	199	TYR	5.0
1	A	171	PHE	4.9
1	A	556	TYR	4.9
1	B	302	LEU	4.7
1	A	544	ARG	4.5
1	A	166	PHE	4.4
1	B	548	HIS	4.3
1	B	163	PRO	4.3
1	B	556	TYR	4.2
1	B	167	LEU	4.2
1	A	167	LEU	4.2
1	B	540	VAL	4.2
1	B	546	LEU	4.0
1	B	166	PHE	4.0
1	A	196	ILE	4.0
1	B	197	LEU	3.8
1	B	207	TYR	3.8
1	B	414	PHE	3.6
1	A	548	HIS	3.5
1	A	203	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	191	LEU	3.5
1	A	188	PHE	3.4
1	A	163	PRO	3.3
1	B	544	ARG	3.2
1	B	188	PHE	3.2
1	A	201	THR	3.2
1	B	531	LEU	3.1
1	B	551	TYR	3.1
1	B	268	GLU	3.1
1	B	539	ALA	3.1
1	B	542	ILE	3.0
1	A	551	TYR	3.0
1	B	168	TYR	2.9
1	A	302	LEU	2.9
1	B	171	PHE	2.9
1	B	550	LEU	2.8
1	B	178	TYR	2.8
1	A	471	ASN	2.8
1	B	162	ASN	2.8
1	A	301	LYS	2.7
1	A	164	GLU	2.7
1	B	417	PHE	2.6
1	A	199	TYR	2.6
1	A	546	LEU	2.6
1	B	200	ASP	2.5
1	B	549	LEU	2.5
1	B	536	MET	2.5
1	A	187	LEU	2.4
1	B	241	GLY	2.4
1	B	240	LEU	2.4
1	B	196	ILE	2.3
1	B	164	GLU	2.2
1	A	207	TYR	2.2
1	B	538	SER	2.1
1	A	197	LEU	2.1
1	B	190	LEU	2.1
1	B	194	TYR	2.1
1	B	558	LEU	2.1
1	B	198	PRO	2.1
1	A	168	TYR	2.1
1	B	242	PHE	2.0
1	A	206	ILE	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 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, 95th 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^2)	Q<0.9
4	F1T	B	603	22/22	0.94	0.19	49,65,78,83	0
4	F1T	A	603	22/22	0.97	0.14	29,51,65,69	0
2	FMN	B	601	31/31	0.97	0.09	25,32,40,41	0
2	FMN	A	601	31/31	0.98	0.08	14,19,30,34	0
3	ORO	B	602	11/11	0.98	0.09	21,28,31,32	0
3	ORO	A	602	11/11	0.99	0.09	16,18,21,23	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 F1T B 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
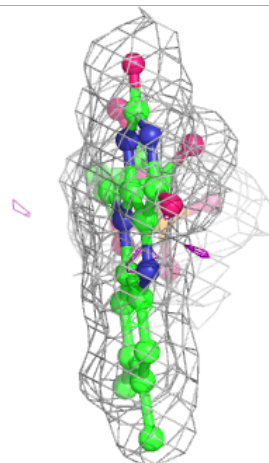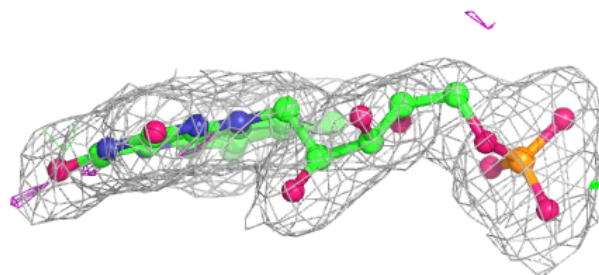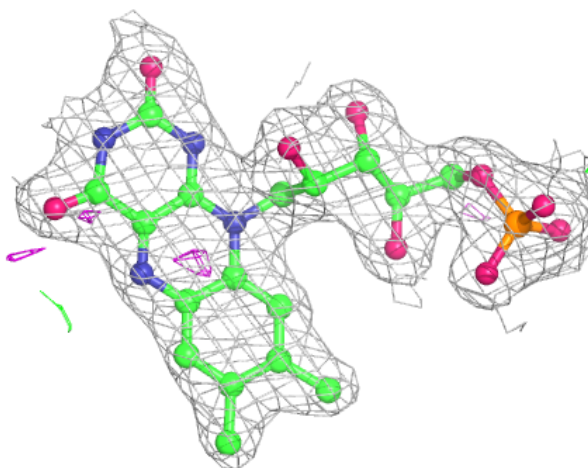and green (positive)
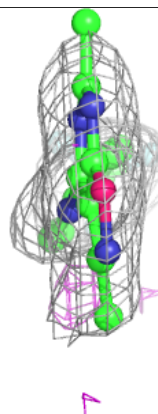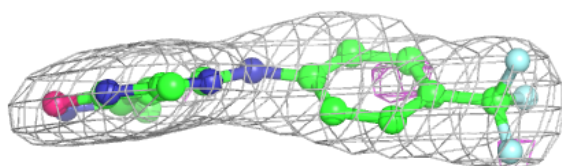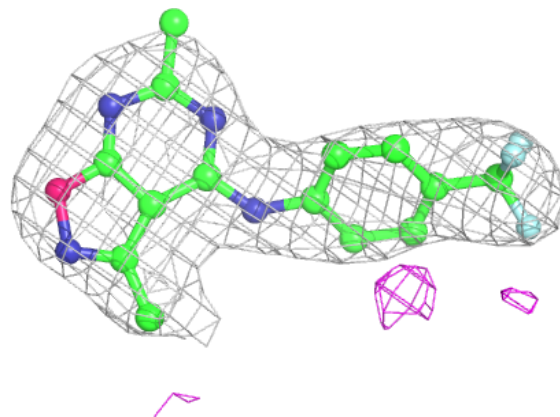
Electron density around F1T A 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
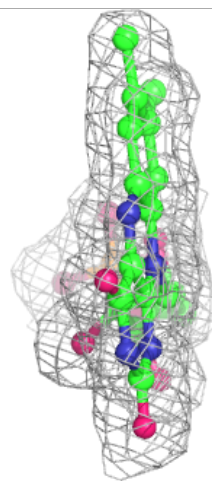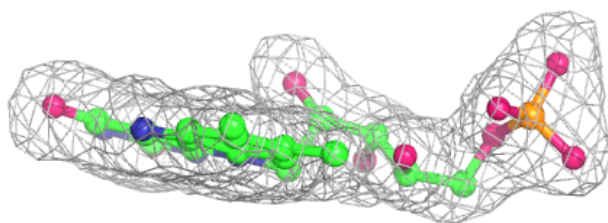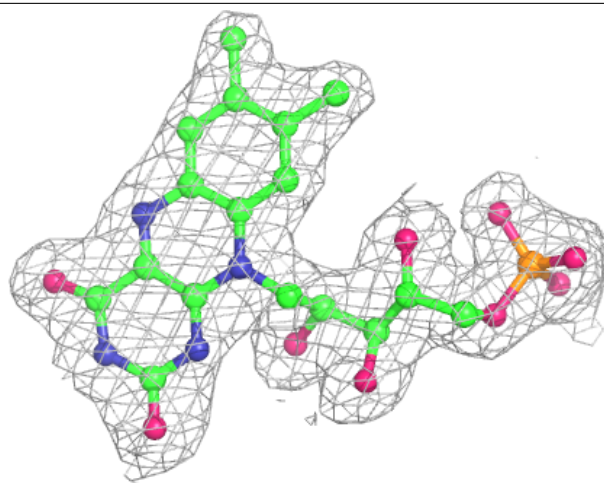$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
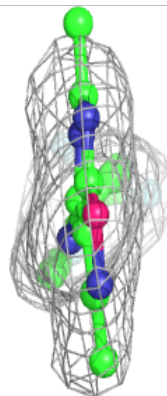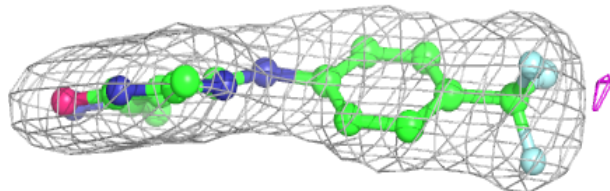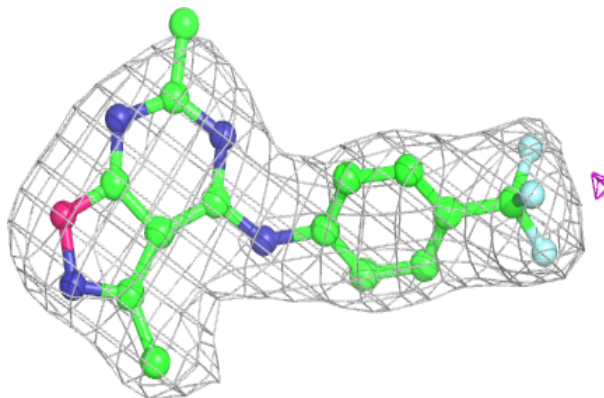
Electron density around FMN B 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
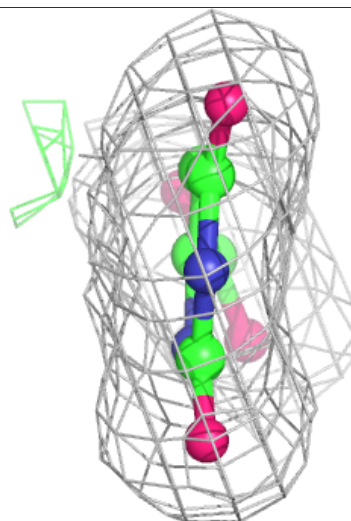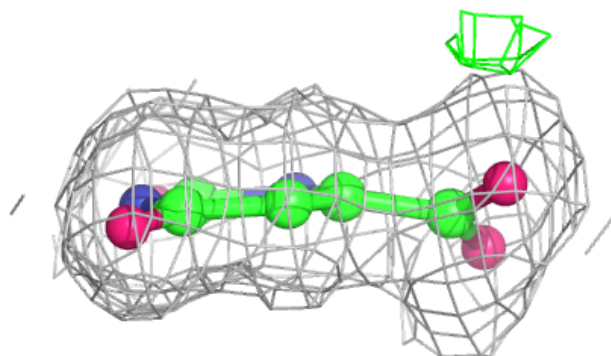mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
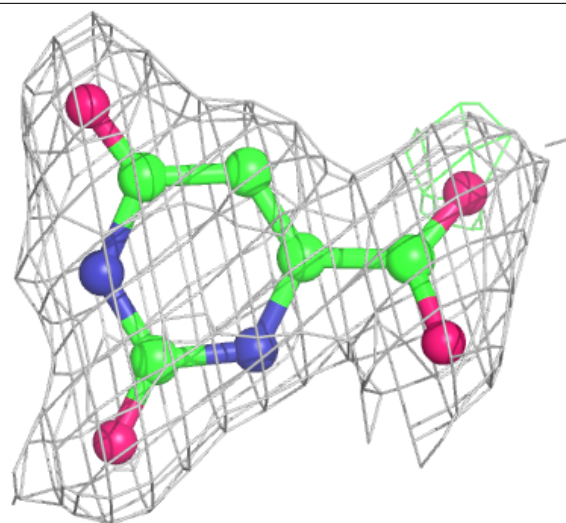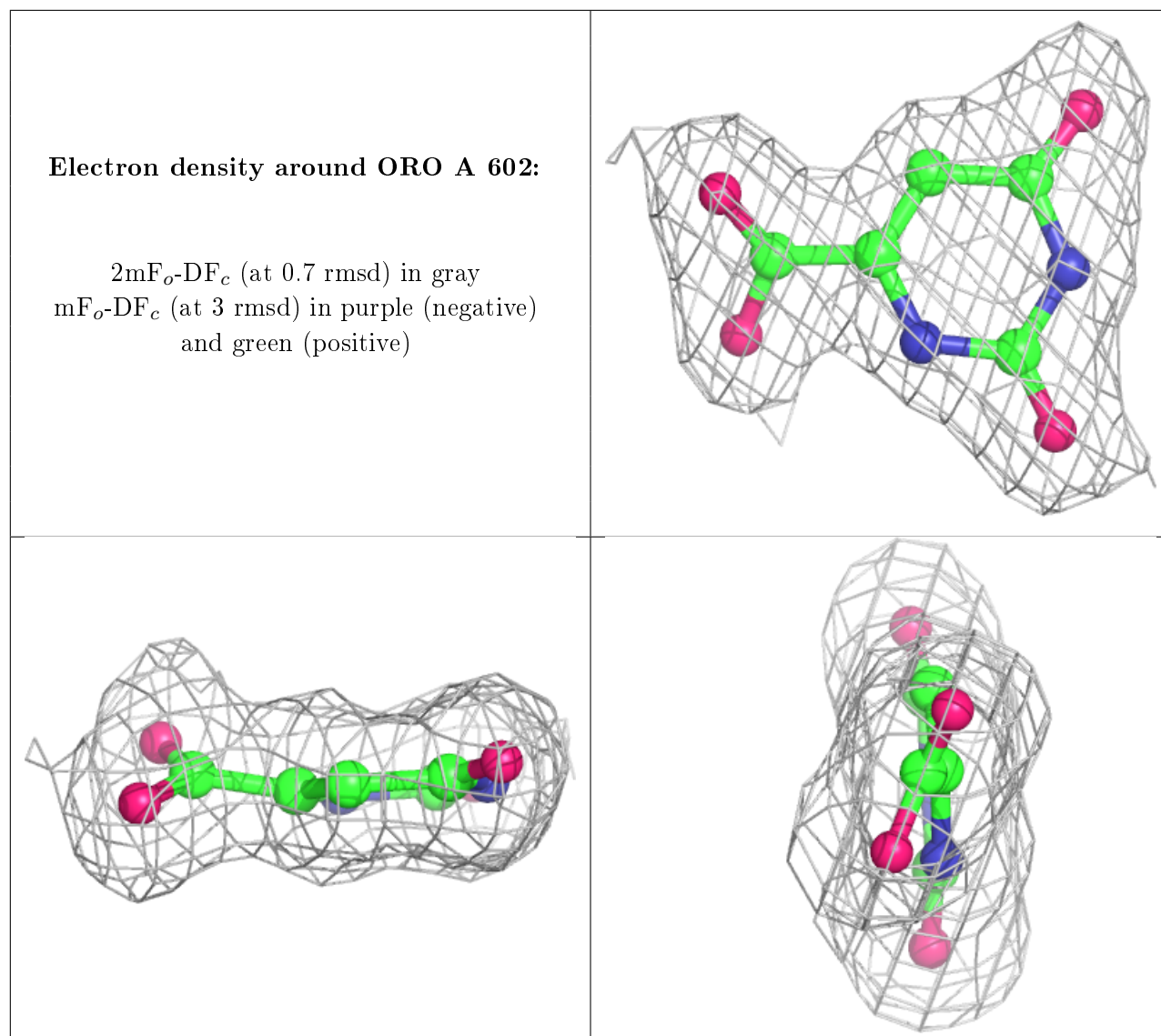and green (positive)

Electron density around FMN A 601:

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 ORO B 602:

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

Electron density around ORO A 602:

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

6.5 Other polymers (i)

There are no such residues in this entry.