



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 05:09 PM EDT

PDB ID : 7KYY
Title : Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM697 (3-methyl-N-(1-(5-methylisoxazol-3-yl)ethyl)-4-(6-(trifluoromethyl)-1H-indol-3-yl)-1H-pyrrole-2-carboxamide)
Authors : Deng, X.; Phillips, M.; Tomchick, D.
Deposited on : 2020-12-09
Resolution : 2.00 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

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>.

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 : 2.35.1
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) : 2.35.1

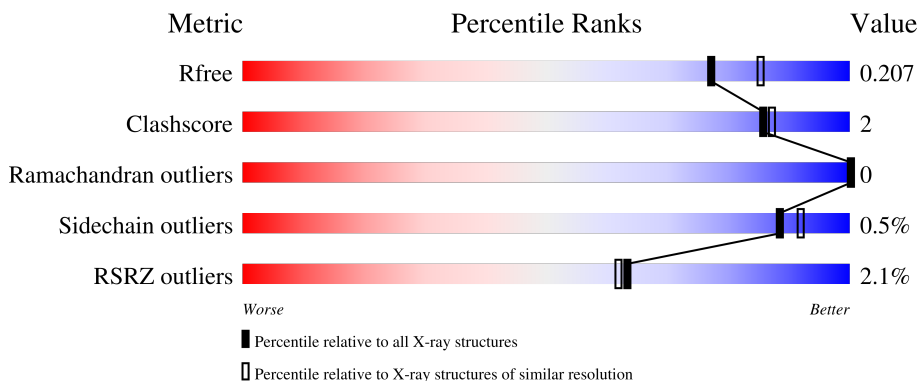
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	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 of 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 $\leq 5\%$. 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	401	 89% 6%
1	B	401	 84% 7% 9%
1	C	401	 90% 7%
1	D	401	 86% 6% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24683 atoms, of which 12139 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
			Total	C	H	N	O	S			
1	A	376	6002	1909	3020	498	561	14	0	0	0
1	B	364	5835	1845	2951	485	539	15	0	2	0
1	C	372	5968	1894	3010	495	554	15	0	3	0
1	D	371	5940	1886	2994	494	551	15	0	1	0

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q08210
A	-18	GLY	-	expression tag	UNP Q08210
A	-17	HIS	-	expression tag	UNP Q08210
A	-16	HIS	-	expression tag	UNP Q08210
A	-15	HIS	-	expression tag	UNP Q08210
A	-14	HIS	-	expression tag	UNP Q08210
A	-13	HIS	-	expression tag	UNP Q08210
A	-12	HIS	-	expression tag	UNP Q08210
A	-11	ALA	-	expression tag	UNP Q08210
A	-10	GLU	-	expression tag	UNP Q08210
A	-9	ASN	-	expression tag	UNP Q08210
A	-8	LEU	-	expression tag	UNP Q08210
A	-7	TYR	-	expression tag	UNP Q08210
A	-6	PHE	-	expression tag	UNP Q08210
A	-5	GLN	-	expression tag	UNP Q08210
A	-4	GLY	-	expression tag	UNP Q08210
A	-3	ALA	-	expression tag	UNP Q08210
A	-2	ASP	-	expression tag	UNP Q08210
A	-1	PRO	-	expression tag	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	THR	deletion	UNP Q08210

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
C	139	MET	-	initiating methionine	UNP Q08210
C	140	GLY	-	expression tag	UNP Q08210
C	141	HIS	-	expression tag	UNP Q08210
C	142	HIS	-	expression tag	UNP Q08210
C	143	HIS	-	expression tag	UNP Q08210
C	144	HIS	-	expression tag	UNP Q08210
C	145	HIS	-	expression tag	UNP Q08210

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Chain	Residue	Modelled	Actual	Comment	Reference
C	146	HIS	-	expression tag	UNP Q08210
C	147	ALA	-	expression tag	UNP Q08210
C	148	GLU	-	expression tag	UNP Q08210
C	149	ASN	-	expression tag	UNP Q08210
C	150	LEU	-	expression tag	UNP Q08210
C	151	TYR	-	expression tag	UNP Q08210
C	152	PHE	-	expression tag	UNP Q08210
C	153	GLN	-	expression tag	UNP Q08210
C	154	GLY	-	expression tag	UNP Q08210
C	155	ALA	-	expression tag	UNP Q08210
C	156	ASP	-	expression tag	UNP Q08210
C	157	PRO	-	expression tag	UNP Q08210
C	?	-	SER	deletion	UNP Q08210
C	?	-	THR	deletion	UNP Q08210
C	?	-	TYR	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210
C	?	-	GLU	deletion	UNP Q08210
C	?	-	ASP	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210
C	?	-	LYS	deletion	UNP Q08210
C	?	-	ILE	deletion	UNP Q08210
C	?	-	VAL	deletion	UNP Q08210
C	?	-	GLU	deletion	UNP Q08210
C	?	-	LYS	deletion	UNP Q08210
C	?	-	LYS	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210
C	?	-	PHE	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210
C	?	-	LYS	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210
C	?	-	SER	deletion	UNP Q08210
C	?	-	HIS	deletion	UNP Q08210
C	?	-	MET	deletion	UNP Q08210
C	?	-	MET	deletion	UNP Q08210
C	?	-	LYS	deletion	UNP Q08210
C	?	-	ASP	deletion	UNP Q08210
C	?	-	ALA	deletion	UNP Q08210
C	?	-	LYS	deletion	UNP Q08210
C	?	-	ASP	deletion	UNP Q08210
C	?	-	ASN	deletion	UNP Q08210

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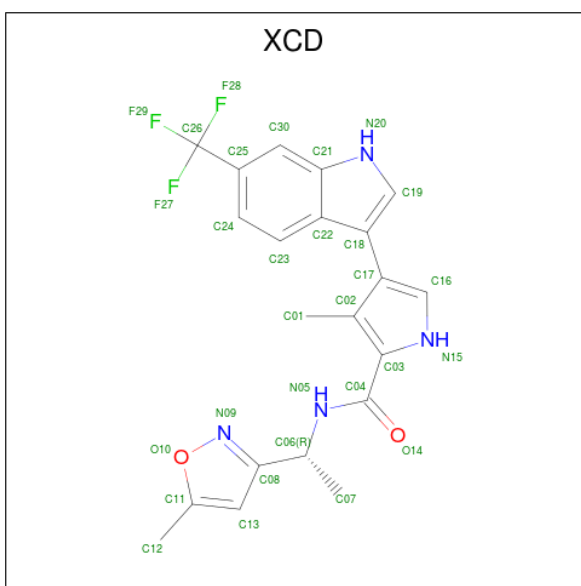
Chain	Residue	Modelled	Actual	Comment	Reference
D	139	MET	-	initiating methionine	UNP Q08210
D	140	GLY	-	expression tag	UNP Q08210
D	141	HIS	-	expression tag	UNP Q08210
D	142	HIS	-	expression tag	UNP Q08210
D	143	HIS	-	expression tag	UNP Q08210
D	144	HIS	-	expression tag	UNP Q08210
D	145	HIS	-	expression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

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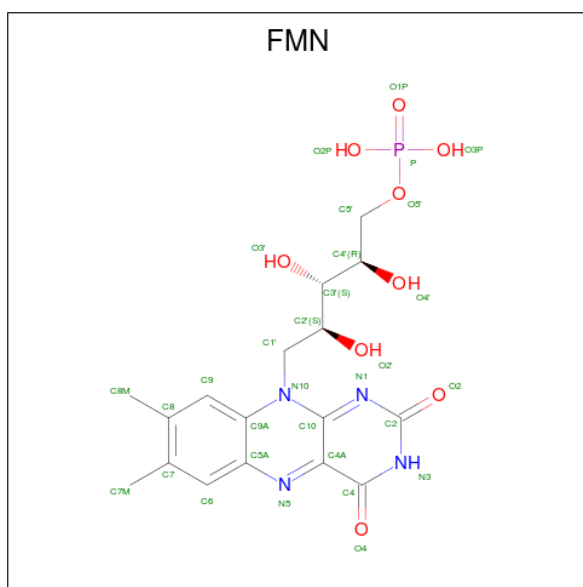
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	MET	deletion	UNP Q08210
D	?	-	LYS	deletion	UNP Q08210
D	?	-	ASP	deletion	UNP Q08210
D	?	-	ALA	deletion	UNP Q08210
D	?	-	LYS	deletion	UNP Q08210
D	?	-	ASP	deletion	UNP Q08210
D	?	-	ASN	deletion	UNP Q08210

- Molecule 2 is 3-methyl-N-[(1R)-1-(5-methyl-1,2-oxazol-3-yl)ethyl]-4-[6-(trifluoromethyl)-1H-indol-3-yl]-1H-pyrrole-2-carboxamide (three-letter code: XCD) (formula: C₂₁H₁₉F₃N₄O₂) (labeled as "Ligand of Interest" by depositor).



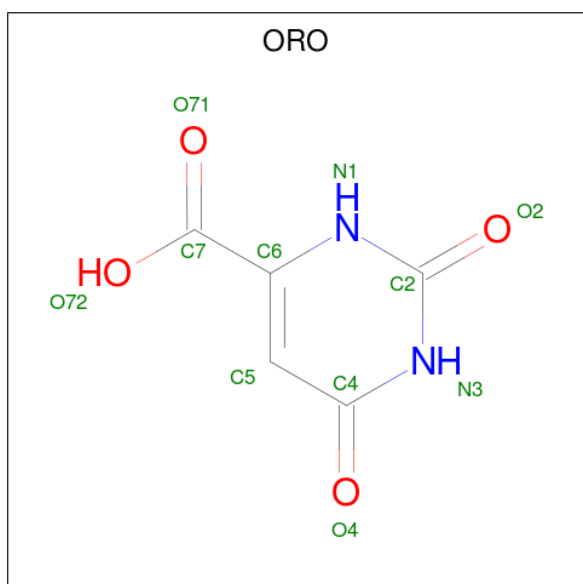
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			O
2	A	1	Total	C	F	H	N	O	0	0
			49	21	3	19	4	2		
2	B	1	Total	C	F	H	N	O	0	0
			49	21	3	19	4	2		
2	C	1	Total	C	F	H	N	O	0	0
			49	21	3	19	4	2		
2	D	1	Total	C	F	H	N	O	0	0
			49	21	3	19	4	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
3	A	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
3	B	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
3	C	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		
3	D	1	Total	C	H	N	O	P	0	0
			50	17	19	4	9	1		

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	B	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	C	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	D	1	Total	C	H	N	O	0	0
			14	5	3	2	4		

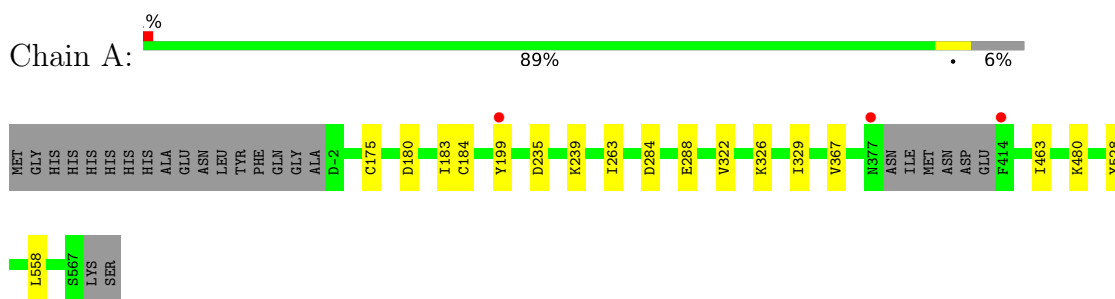
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	159	Total	O	0	0
			159	159		
5	B	142	Total	O	0	0
			142	142		
5	C	105	Total	O	0	0
			105	105		
5	D	80	Total	O	0	0
			80	80		

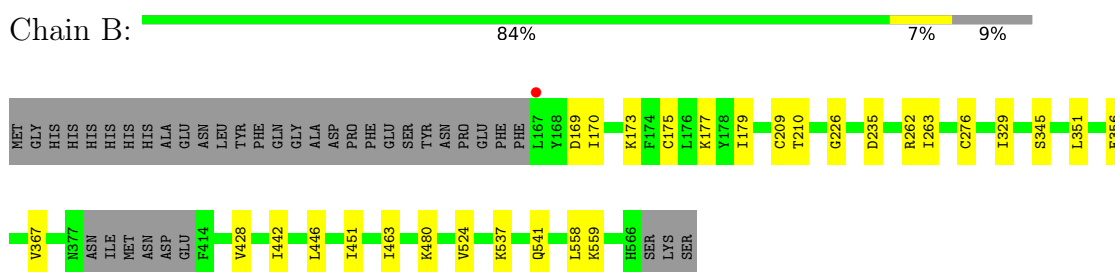
3 Residue-property plots [i](#)

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.

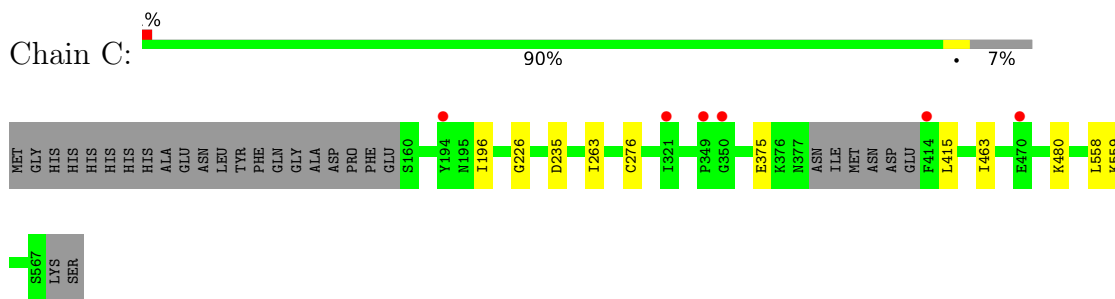
- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial



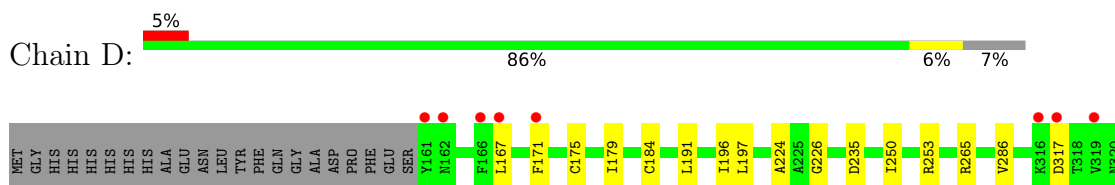
- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial

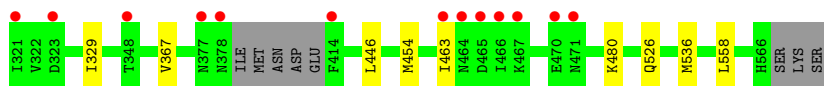


- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial



- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.06Å 97.25Å 186.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.06 – 2.00 47.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.7 (47.06-2.00) 87.7 (47.06-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.163 , 0.207 0.163 , 0.207	Depositor DCC
R_{free} test set	1008 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtrriage
Anisotropy	0.218	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24683	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ORO, FMN, XCD

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	0.46	0/3034	0.60	0/4085
1	B	0.46	0/2936	0.59	0/3951
1	C	0.42	0/3018	0.56	0/4064
1	D	0.40	0/2999	0.54	0/4037
All	All	0.44	0/11987	0.57	0/16137

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	2982	3020	3022	9	0
1	B	2884	2951	2951	19	0
1	C	2958	3010	3002	9	0
1	D	2946	2994	2994	16	0
2	A	30	19	0	1	0
2	B	30	19	0	0	0
2	C	30	19	0	2	0
2	D	30	19	0	0	0
3	A	31	19	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	19	19	1	0
3	C	31	19	19	1	0
3	D	31	19	19	1	0
4	A	11	3	3	0	0
4	B	11	3	3	0	0
4	C	11	3	3	0	0
4	D	11	3	3	0	0
5	A	159	0	0	0	0
5	B	142	0	0	2	0
5	C	105	0	0	0	0
5	D	80	0	0	0	0
All	All	12544	12139	12057	53	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 2.

All (53) 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:428[B]:VAL:HG23	1:B:451:ILE:HD11	1.58	0.82
1:B:428[B]:VAL:HG23	1:B:451:ILE:CD1	2.14	0.78
1:D:329:ILE:HD11	1:D:367:VAL:HG13	1.71	0.71
1:C:263:ILE:HD13	2:C:1001:XCD:O10	1.98	0.64
1:B:329:ILE:HD11	1:B:367:VAL:HG13	1.81	0.62
1:D:167:LEU:HD21	1:D:171:PHE:CZ	2.35	0.62
1:D:191:LEU:CD2	1:D:196:ILE:HD11	2.31	0.60
1:D:191:LEU:HD23	1:D:196:ILE:HD11	1.86	0.56
1:B:210:THR:HG21	1:B:524:VAL:HG12	1.88	0.55
1:B:345:SER:HB3	1:B:351:LEU:HD23	1.89	0.54
1:A:463:ILE:HD13	1:A:480:LYS:HB3	1.89	0.54
1:C:226:GLY:HA3	3:C:1002:FMN:N5	2.25	0.52
1:D:179:ILE:O	1:D:265:ARG:NH2	2.44	0.51
1:A:180:ASP:HB3	1:A:183:ILE:HD12	1.94	0.49
1:A:284:ASP:O	1:A:288:GLU:HG2	2.13	0.48
1:C:463:ILE:HD13	1:C:480:LYS:HB3	1.94	0.48
1:B:559:LYS:HG3	5:B:1123:HOH:O	2.14	0.48
1:C:558:LEU:C	1:C:558:LEU:HD23	2.34	0.48
1:A:329:ILE:HD11	1:A:367:VAL:HG13	1.96	0.48
1:A:263:ILE:HD13	2:A:1001:XCD:O10	2.14	0.47
1:A:558:LEU:C	1:A:558:LEU:HD23	2.35	0.47
1:B:262:ARG:HD2	1:B:276:CYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG12	1:A:326:LYS:HE2	1.97	0.46
1:D:224:ALA:HB2	1:D:526:GLN:HB3	1.98	0.46
1:B:558:LEU:C	1:B:558:LEU:HD23	2.36	0.46
1:B:169:ASP:O	1:B:173:LYS:HD3	2.16	0.45
1:C:263:ILE:HD13	2:C:1001:XCD:N09	2.32	0.45
1:B:175:CYS:HA	1:B:179:ILE:HD12	1.99	0.45
1:B:209[B]:CYS:SG	5:B:1142:HOH:O	2.61	0.45
1:D:253:ARG:NH2	1:D:317:ASP:OD1	2.44	0.45
1:B:537:LYS:HD2	1:B:541:GLN:OE1	2.16	0.45
1:A:199:TYR:CE1	1:A:239:LYS:HE2	2.52	0.45
1:D:250:ILE:HG21	1:D:286:VAL:HG11	1.98	0.44
1:B:210:THR:CG2	1:B:524:VAL:HG12	2.48	0.44
1:D:191:LEU:HD22	1:D:196:ILE:HD11	2.00	0.44
1:B:463:ILE:HD13	1:B:480:LYS:HB3	1.99	0.43
1:B:226:GLY:HA3	3:B:1002:FMN:N5	2.34	0.43
1:A:175:CYS:HB3	1:A:184:CYS:SG	2.59	0.43
1:D:558:LEU:C	1:D:558:LEU:HD23	2.39	0.43
1:B:173:LYS:O	1:B:177:LYS:HG2	2.19	0.42
1:C:196:ILE:HG22	1:C:196:ILE:O	2.17	0.42
1:D:175:CYS:HB3	1:D:184:CYS:SG	2.60	0.42
1:C:559:LYS:HZ3	1:C:559:LYS:H	1.66	0.42
1:C:263:ILE:HD11	1:C:276:CYS:SG	2.60	0.42
1:D:329:ILE:CD1	1:D:367:VAL:HG13	2.45	0.42
1:B:442:ILE:O	1:B:446:LEU:HG	2.20	0.41
1:B:262:ARG:HG3	1:B:263:ILE:HD12	2.02	0.41
1:D:197:LEU:HD22	1:D:536:MET:CE	2.51	0.41
1:C:375:GLU:HG3	1:C:415:LEU:HD21	2.03	0.41
1:D:446:LEU:HD12	1:D:454:MET:HE1	2.02	0.41
1:D:463:ILE:HD13	1:D:480:LYS:HB3	2.04	0.40
1:B:170:ILE:HD12	1:B:170:ILE:N	2.35	0.40
1:D:226:GLY:HA3	3:D:1002: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	372/401 (93%)	364 (98%)	8 (2%)	0	100	100
1	B	362/401 (90%)	355 (98%)	7 (2%)	0	100	100
1	C	371/401 (92%)	358 (96%)	13 (4%)	0	100	100
1	D	368/401 (92%)	358 (97%)	10 (3%)	0	100	100
All	All	1473/1604 (92%)	1435 (97%)	38 (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	333/354 (94%)	331 (99%)	2 (1%)	86	90
1	B	323/354 (91%)	321 (99%)	2 (1%)	86	90
1	C	332/354 (94%)	331 (100%)	1 (0%)	92	95
1	D	329/354 (93%)	328 (100%)	1 (0%)	92	95
All	All	1317/1416 (93%)	1311 (100%)	6 (0%)	88	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	A	528	TYR
1	B	235	ASP
1	B	356	GLU
1	C	235	ASP
1	D	235	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

12 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
2	XCD	A	1001	-	28,33,33	1.34	3 (10%)	29,50,50	1.11	2 (6%)
2	XCD	C	1001	-	28,33,33	1.32	2 (7%)	29,50,50	1.38	4 (13%)
3	FMN	B	1002	-	33,33,33	1.02	1 (3%)	48,50,50	1.18	3 (6%)
4	ORO	B	1003	-	9,11,11	1.29	0	8,15,15	2.22	2 (25%)
4	ORO	C	1003	-	9,11,11	1.34	0	8,15,15	2.70	3 (37%)
2	XCD	B	1001	-	28,33,33	1.26	3 (10%)	29,50,50	1.06	1 (3%)
3	FMN	A	1002	-	33,33,33	1.12	1 (3%)	48,50,50	1.16	5 (10%)
3	FMN	D	1002	-	33,33,33	1.03	2 (6%)	48,50,50	1.32	7 (14%)
4	ORO	D	1003	-	9,11,11	1.30	0	8,15,15	2.87	4 (50%)
2	XCD	D	1001	-	28,33,33	1.18	3 (10%)	29,50,50	1.17	2 (6%)
3	FMN	C	1002	-	33,33,33	1.21	2 (6%)	48,50,50	1.17	7 (14%)
4	ORO	A	1003	-	9,11,11	1.35	0	8,15,15	2.90	4 (50%)

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
2	XCD	A	1001	-	-	1/12/22/22	0/4/4/4
2	XCD	C	1001	-	-	1/12/22/22	0/4/4/4
3	FMN	B	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	B	1003	-	-	4/4/4/4	0/1/1/1
4	ORO	C	1003	-	-	4/4/4/4	0/1/1/1
2	XCD	B	1001	-	-	1/12/22/22	0/4/4/4
3	FMN	A	1002	-	-	1/18/18/18	0/3/3/3
3	FMN	D	1002	-	-	4/18/18/18	0/3/3/3
4	ORO	D	1003	-	-	4/4/4/4	0/1/1/1
2	XCD	D	1001	-	-	1/12/22/22	0/4/4/4
3	FMN	C	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	A	1003	-	-	4/4/4/4	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	FMN	C4A-N5	4.55	1.39	1.30
2	C	1001	XCD	C04-N05	4.41	1.43	1.34
3	A	1002	FMN	C4A-N5	3.90	1.38	1.30
3	D	1002	FMN	C4A-N5	3.67	1.37	1.30
2	B	1001	XCD	C04-N05	3.66	1.42	1.34
3	B	1002	FMN	C4A-N5	3.57	1.37	1.30
2	A	1001	XCD	C04-N05	3.47	1.41	1.34
2	D	1001	XCD	C04-N05	3.19	1.41	1.34
2	A	1001	XCD	C12-C11	3.11	1.52	1.48
2	C	1001	XCD	C12-C11	3.08	1.52	1.48
3	C	1002	FMN	C10-N1	2.91	1.39	1.33
2	A	1001	XCD	C06-N05	-2.53	1.41	1.47
2	B	1001	XCD	C12-C11	2.52	1.51	1.48
2	D	1001	XCD	C12-C11	2.47	1.51	1.48
2	D	1001	XCD	C06-N05	-2.41	1.42	1.47
3	D	1002	FMN	C10-N1	2.10	1.37	1.33
2	B	1001	XCD	C06-N05	-2.04	1.42	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1003	ORO	C6-C5-C4	5.40	120.22	116.73
4	D	1003	ORO	C6-C5-C4	4.97	119.94	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	ORO	C5-C4-N3	-4.68	118.61	124.08
4	A	1003	ORO	O72-C7-C6	4.18	124.20	114.69
4	B	1003	ORO	C6-C5-C4	4.15	119.41	116.73
4	C	1003	ORO	C5-C4-N3	-3.83	119.61	124.08
4	A	1003	ORO	C6-C5-C4	3.79	119.18	116.73
4	B	1003	ORO	C5-C4-N3	-3.79	119.66	124.08
4	D	1003	ORO	C5-C4-N3	-3.79	119.66	124.08
4	D	1003	ORO	O72-C7-C6	3.62	122.92	114.69
2	C	1001	XCD	F28-C26-C25	-3.22	105.86	112.93
3	A	1002	FMN	C4-N3-C2	-3.21	119.71	125.64
3	D	1002	FMN	C4A-C10-N10	3.19	121.15	116.48
3	A	1002	FMN	C4A-C10-N10	3.09	120.99	116.48
4	A	1003	ORO	O71-C7-C6	-3.08	114.99	121.24
3	B	1002	FMN	C4A-C10-N10	2.98	120.84	116.48
3	D	1002	FMN	C4-N3-C2	-2.81	120.44	125.64
3	A	1002	FMN	C4A-C4-N3	2.79	120.28	113.19
3	C	1002	FMN	C4-N3-C2	-2.77	120.53	125.64
3	B	1002	FMN	C5A-C9A-N10	2.75	120.79	117.95
3	D	1002	FMN	C4A-C4-N3	2.72	120.11	113.19
2	C	1001	XCD	C07-C06-C08	2.72	114.10	110.95
3	C	1002	FMN	C4A-C4-N3	2.61	119.81	113.19
2	B	1001	XCD	C13-C08-N09	-2.60	106.77	110.36
3	D	1002	FMN	C5A-C9A-N10	2.59	120.63	117.95
3	A	1002	FMN	O4-C4-C4A	-2.51	119.95	126.60
3	C	1002	FMN	C5A-C9A-N10	2.48	120.52	117.95
3	C	1002	FMN	C4A-C10-N10	2.38	119.96	116.48
3	C	1002	FMN	O4-C4-C4A	-2.34	120.40	126.60
2	A	1001	XCD	F28-C26-C25	-2.30	107.89	112.93
4	D	1003	ORO	O71-C7-C6	-2.26	116.66	121.24
2	C	1001	XCD	C23-C22-C21	2.23	121.13	118.17
2	D	1001	XCD	C23-C22-C18	-2.21	132.48	135.63
3	B	1002	FMN	C4-N3-C2	-2.19	121.59	125.64
3	D	1002	FMN	O4-C4-C4A	-2.16	120.86	126.60
3	C	1002	FMN	C9A-C5A-N5	-2.13	120.12	122.43
4	C	1003	ORO	C5-C6-N1	-2.11	119.59	123.40
3	D	1002	FMN	C10-C4A-N5	-2.08	120.44	124.86
3	A	1002	FMN	C4A-C10-N1	-2.07	119.92	124.73
2	D	1001	XCD	C23-C22-C21	2.06	120.90	118.17
2	C	1001	XCD	C23-C22-C18	-2.05	132.71	135.63
3	D	1002	FMN	C4A-C10-N1	-2.05	119.98	124.73
2	A	1001	XCD	C13-C08-C06	-2.00	126.17	129.25
3	C	1002	FMN	C10-C4A-N5	-2.00	120.61	124.86

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	XCD	C16-C17-C18-C19
2	B	1001	XCD	C16-C17-C18-C19
2	C	1001	XCD	C16-C17-C18-C19
2	D	1001	XCD	C16-C17-C18-C19
3	D	1002	FMN	C5'-O5'-P-O1P
3	D	1002	FMN	C5'-O5'-P-O2P
4	A	1003	ORO	N1-C6-C7-O71
4	A	1003	ORO	C5-C6-C7-O71
4	A	1003	ORO	C5-C6-C7-O72
4	B	1003	ORO	C5-C6-C7-O72
4	C	1003	ORO	N1-C6-C7-O71
4	C	1003	ORO	N1-C6-C7-O72
4	C	1003	ORO	C5-C6-C7-O71
4	C	1003	ORO	C5-C6-C7-O72
4	D	1003	ORO	N1-C6-C7-O71
4	D	1003	ORO	N1-C6-C7-O72
4	D	1003	ORO	C5-C6-C7-O71
4	D	1003	ORO	C5-C6-C7-O72
4	A	1003	ORO	N1-C6-C7-O72
4	B	1003	ORO	N1-C6-C7-O72
4	B	1003	ORO	C5-C6-C7-O71
4	B	1003	ORO	N1-C6-C7-O71
3	B	1002	FMN	C4'-C5'-O5'-P
3	C	1002	FMN	C4'-C5'-O5'-P
3	A	1002	FMN	C4'-C5'-O5'-P
3	D	1002	FMN	C4'-C5'-O5'-P
3	D	1002	FMN	C5'-O5'-P-O3P

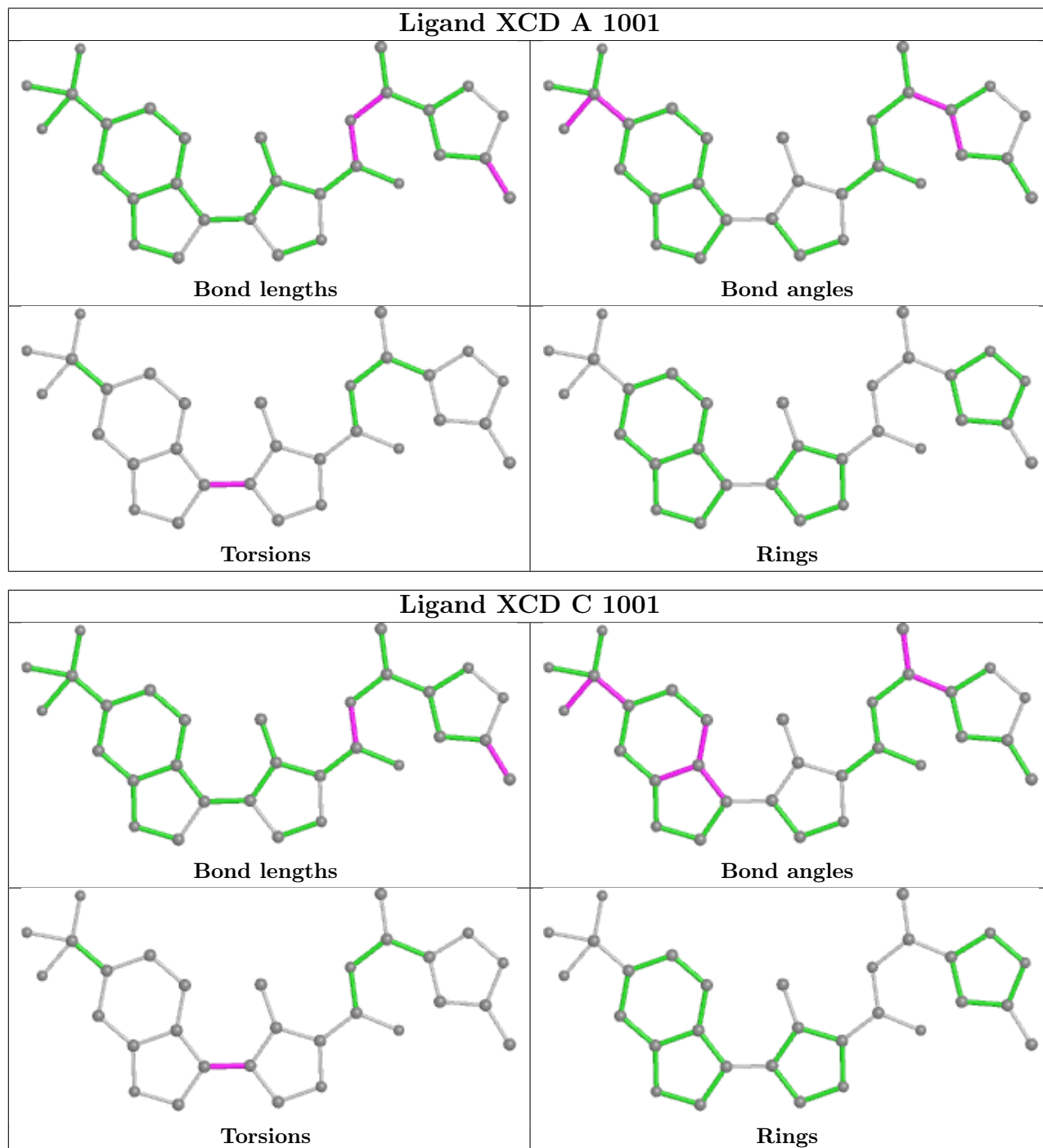
There are no ring outliers.

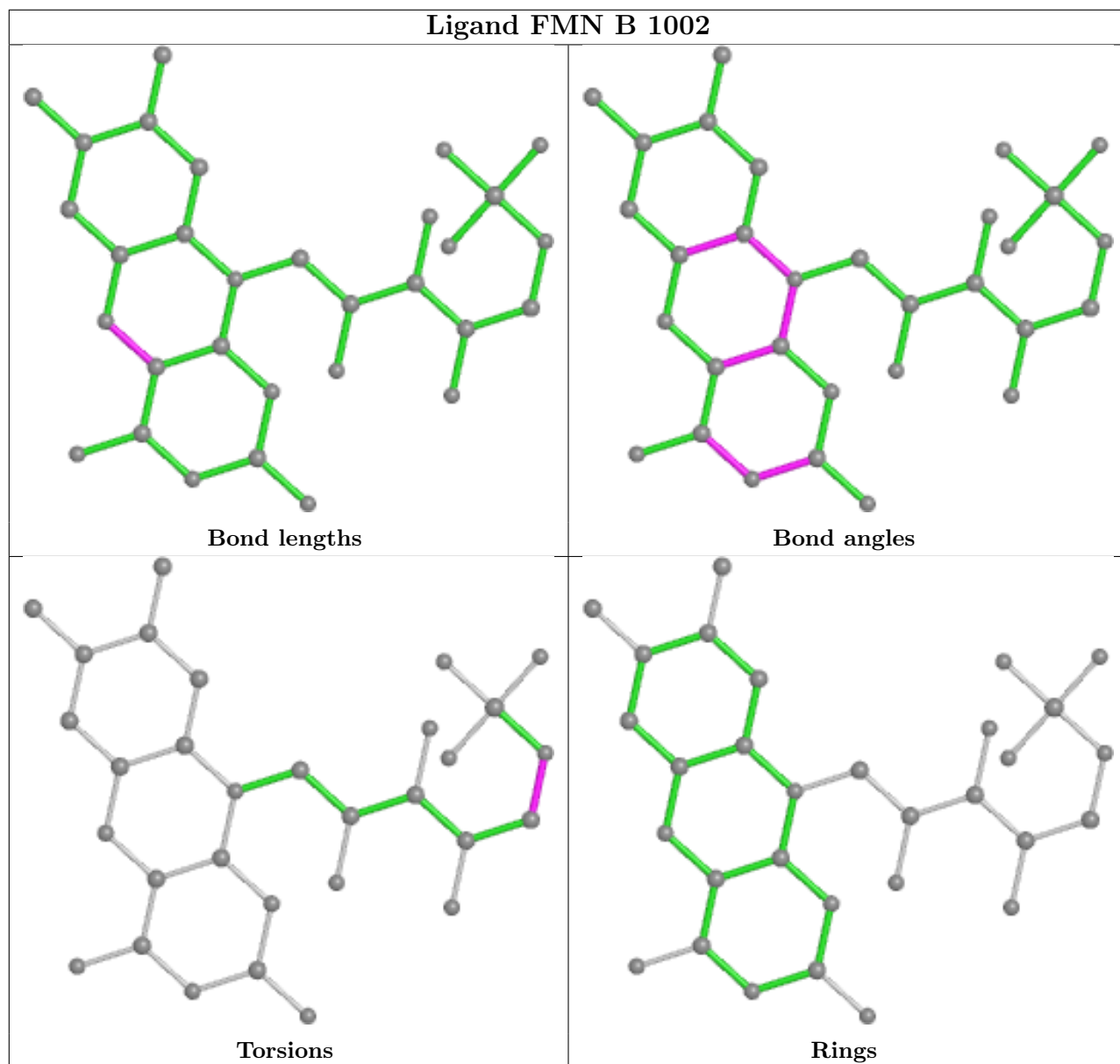
5 monomers are involved in 6 short contacts:

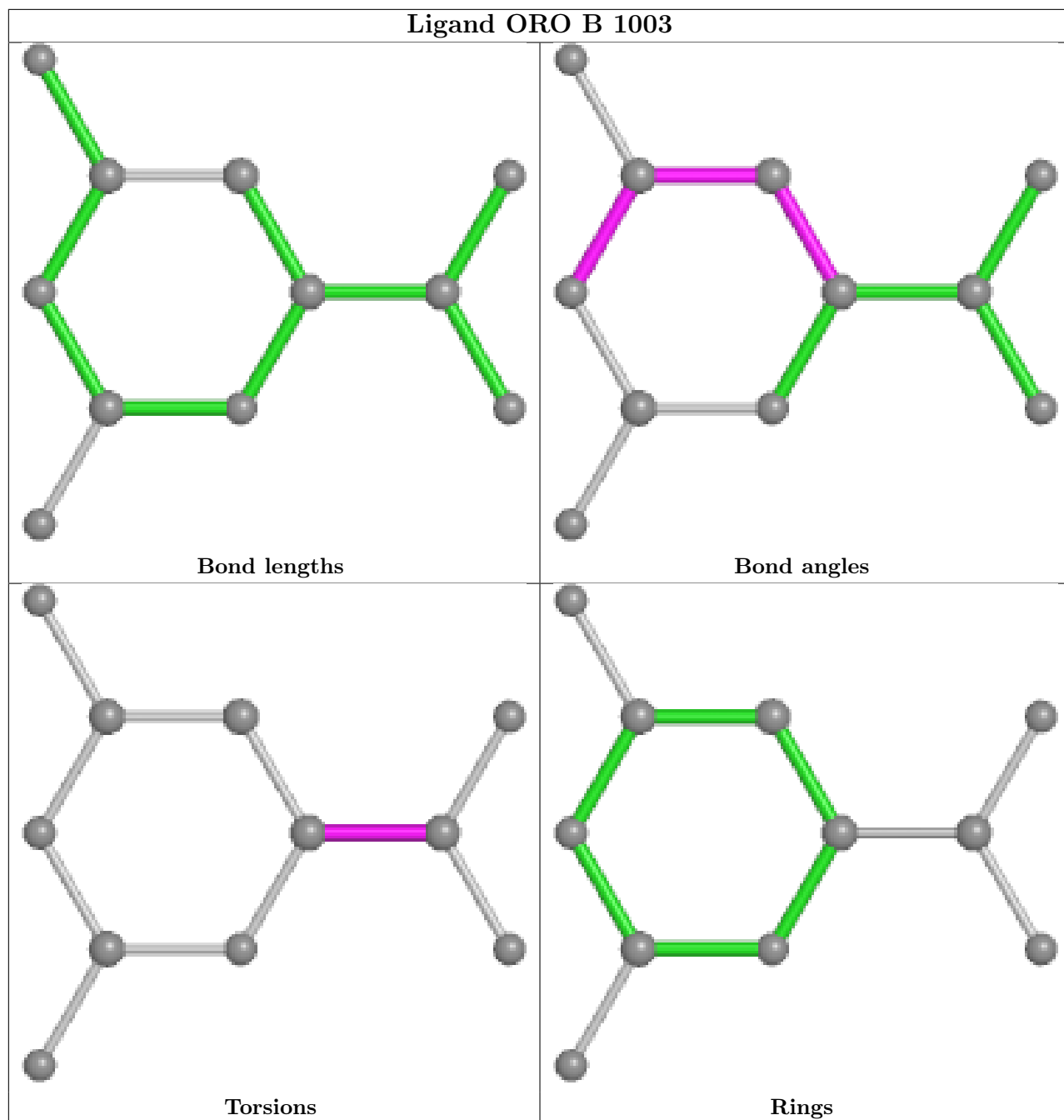
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	XCD	1	0
2	C	1001	XCD	2	0
3	B	1002	FMN	1	0
3	D	1002	FMN	1	0
3	C	1002	FMN	1	0

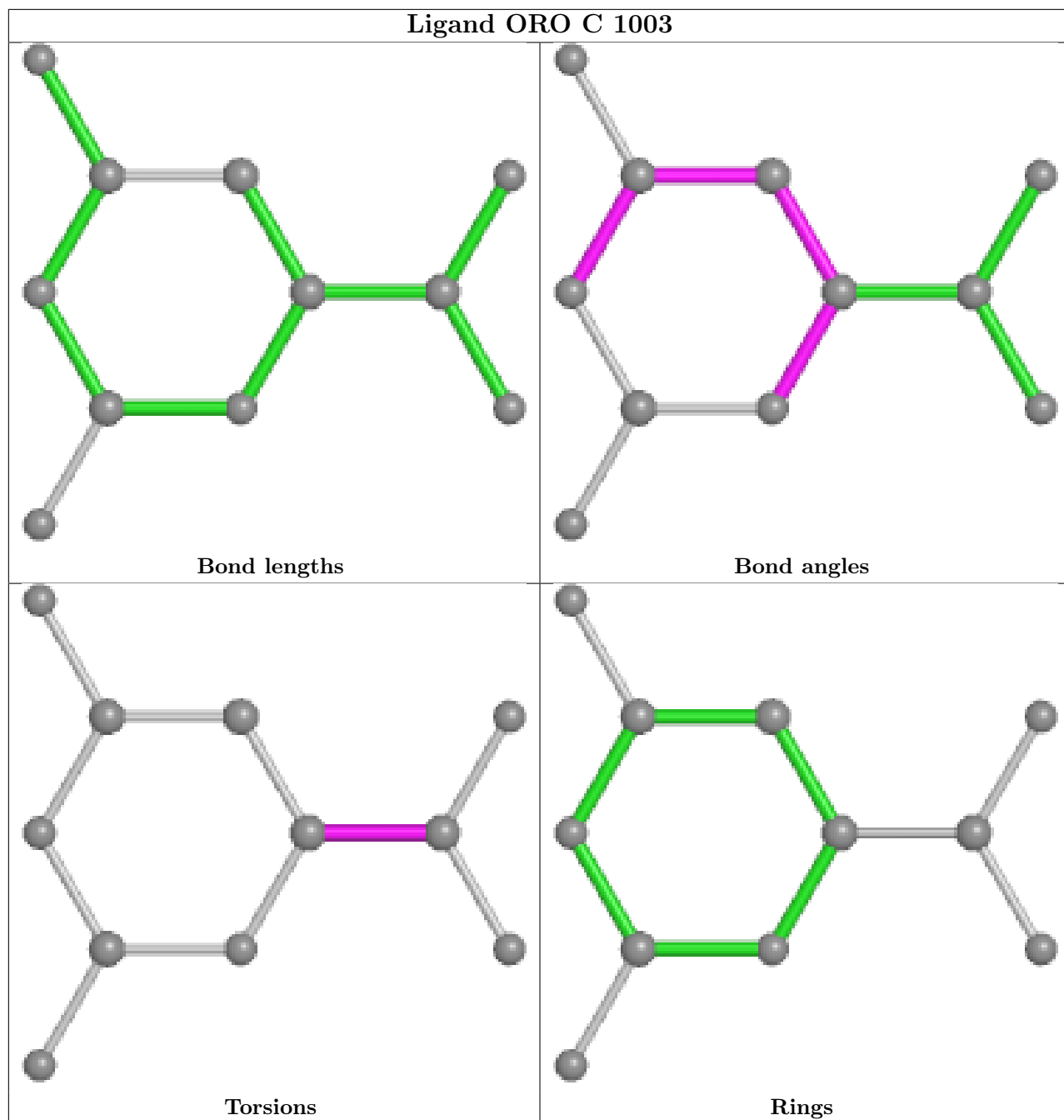
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

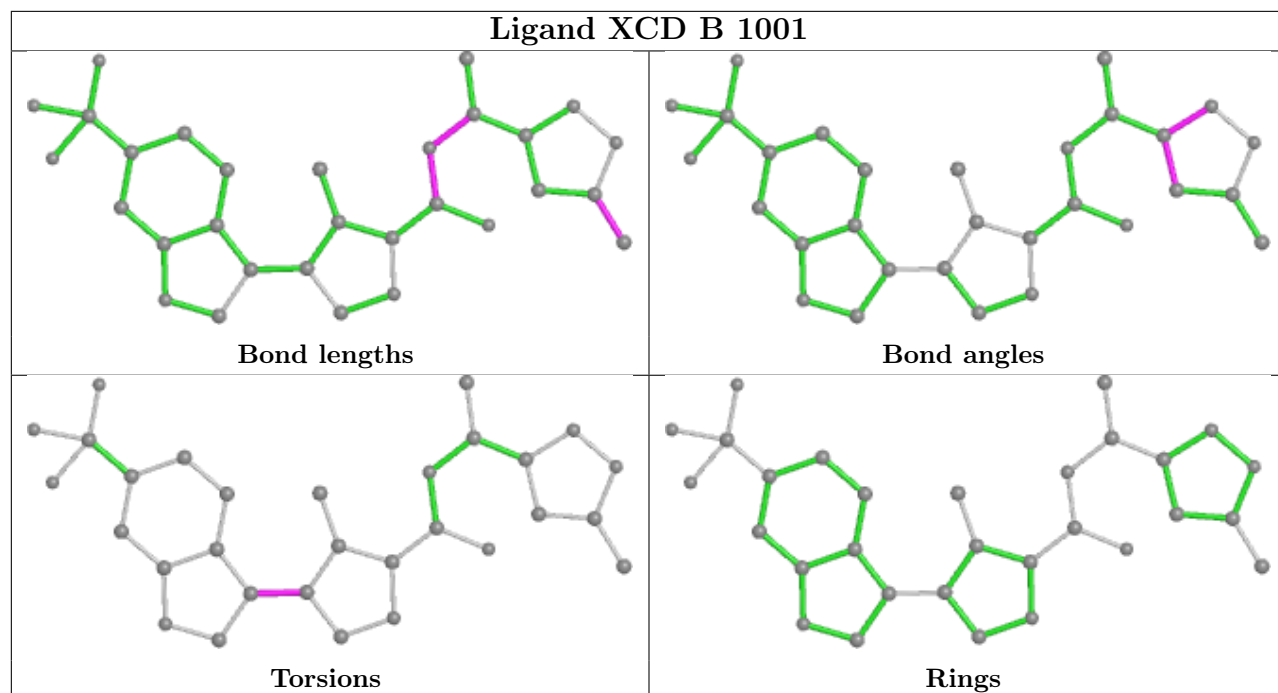
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

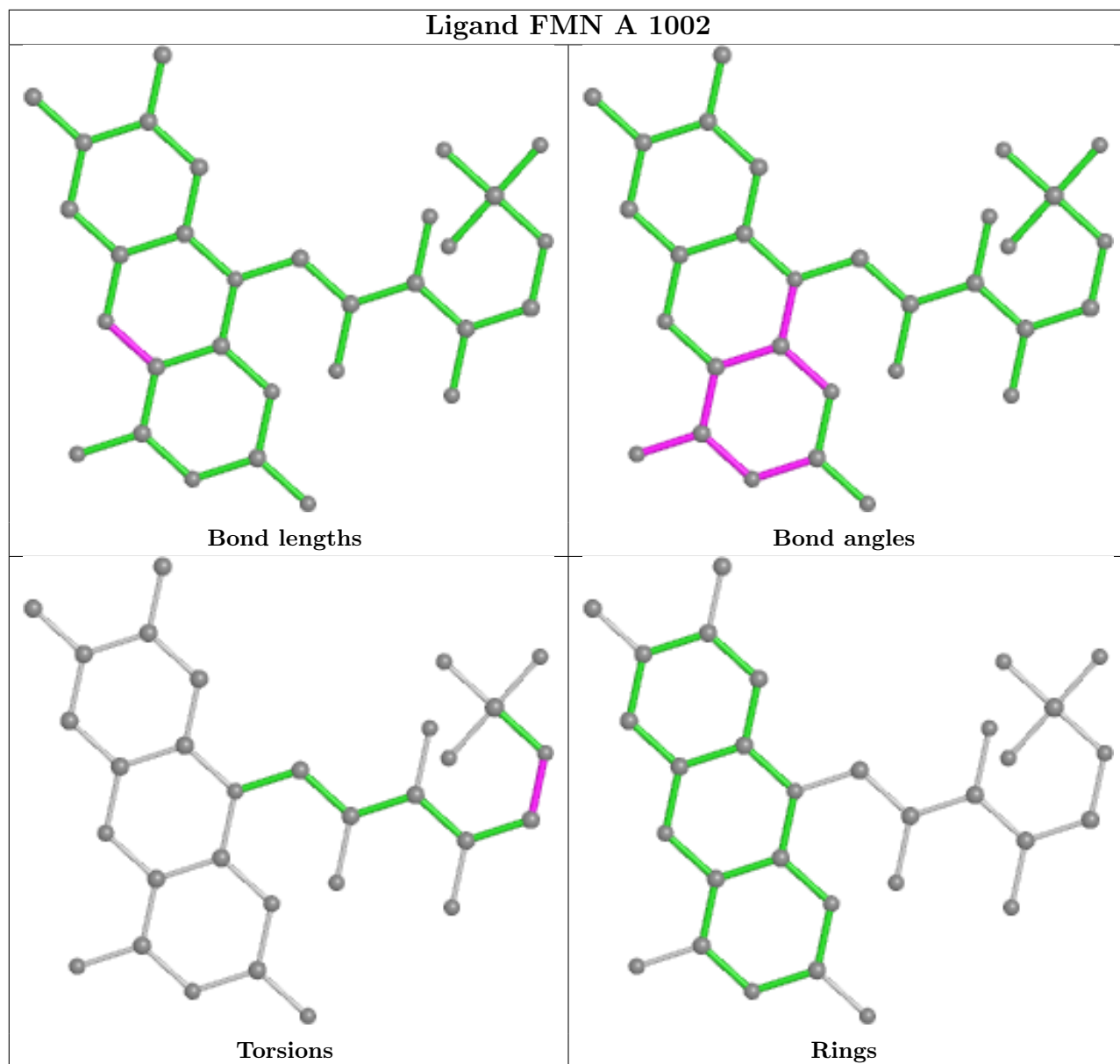


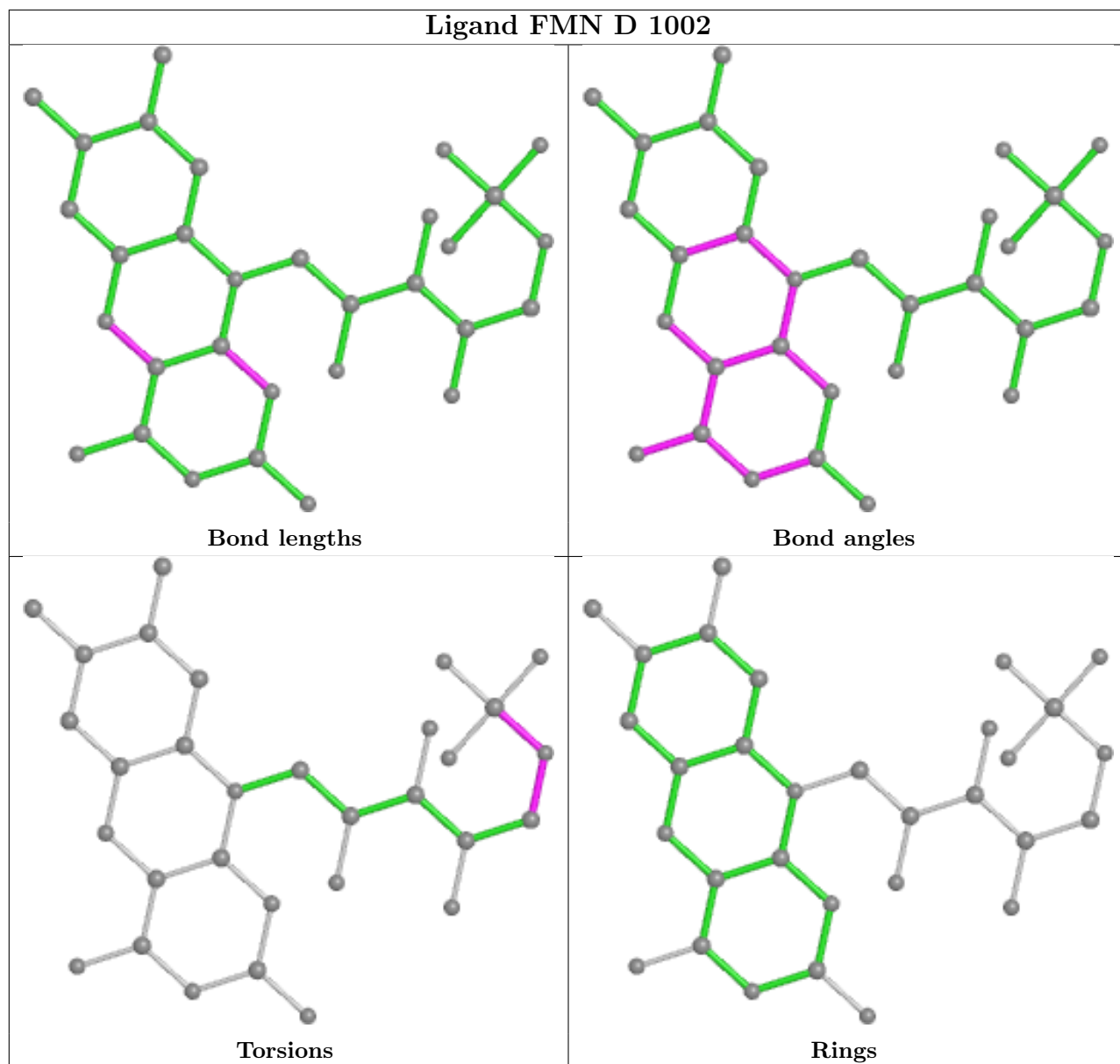


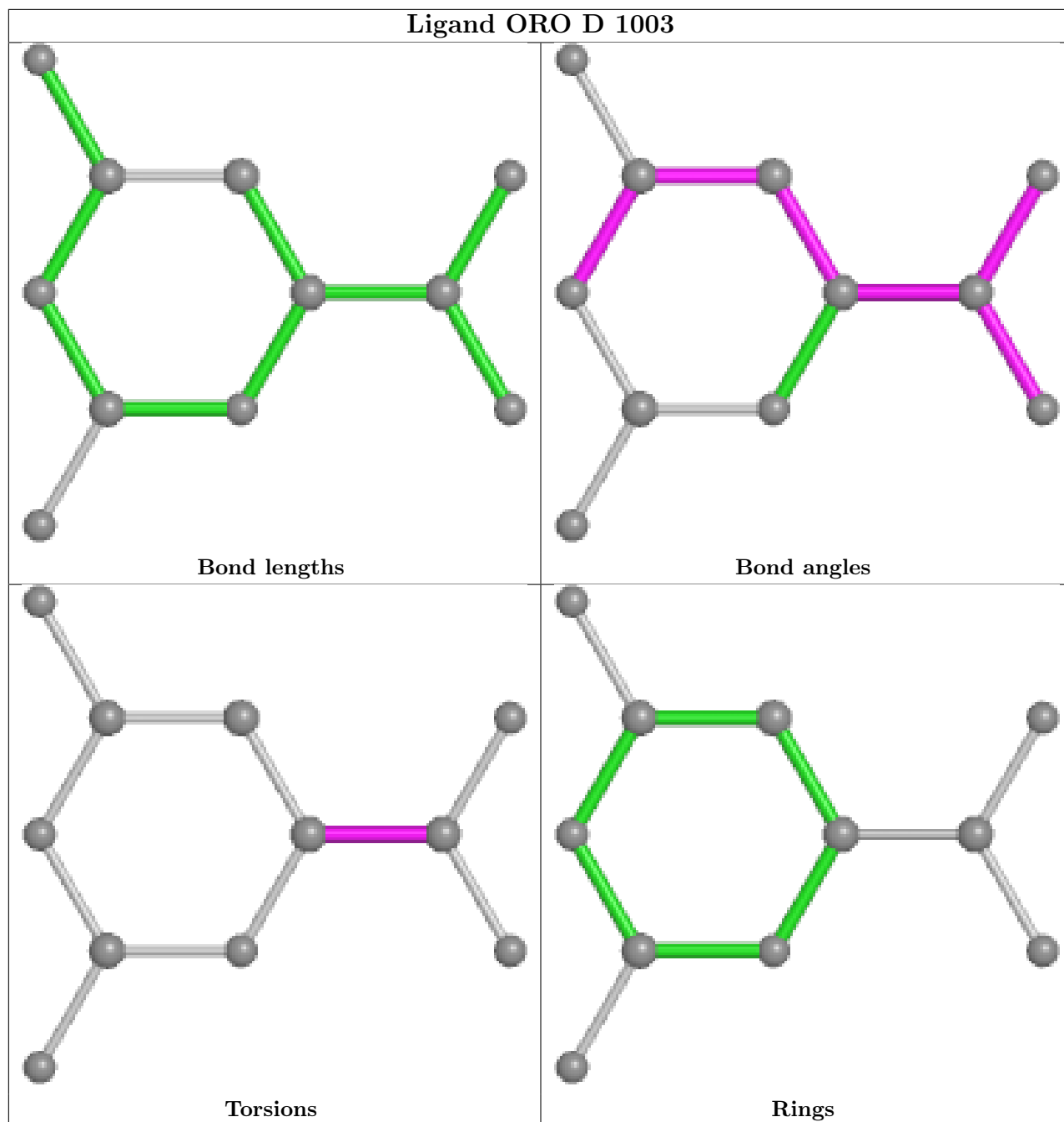


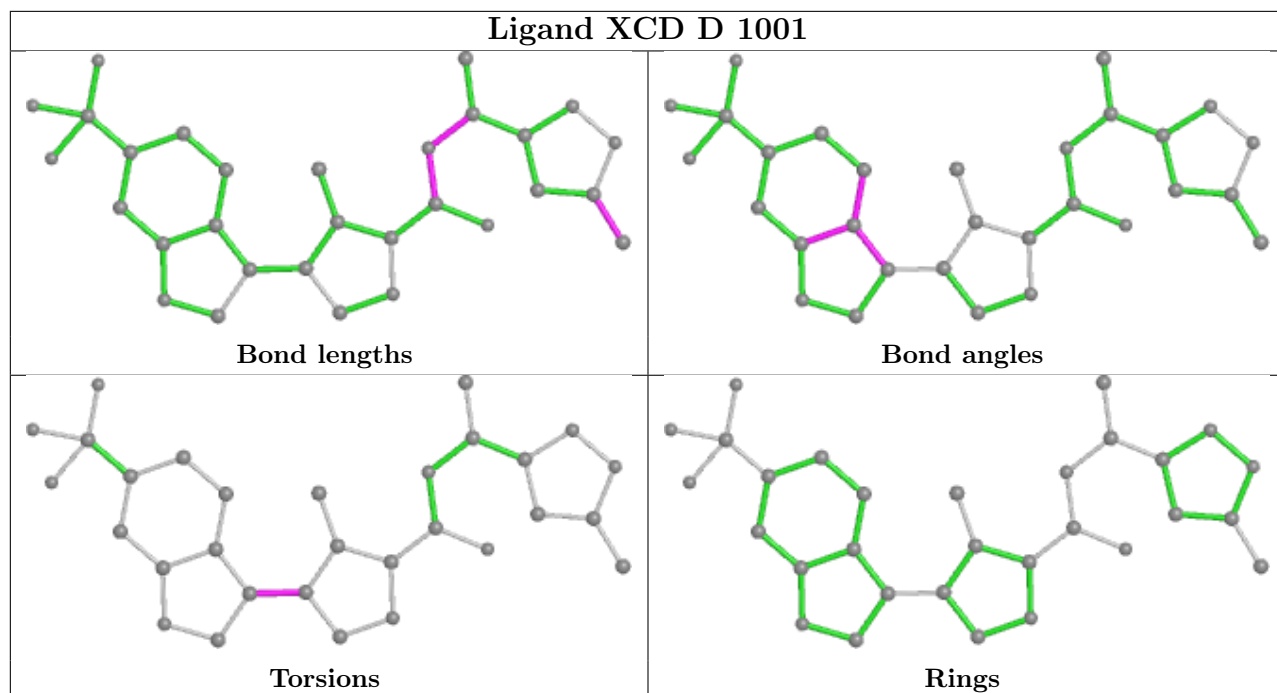


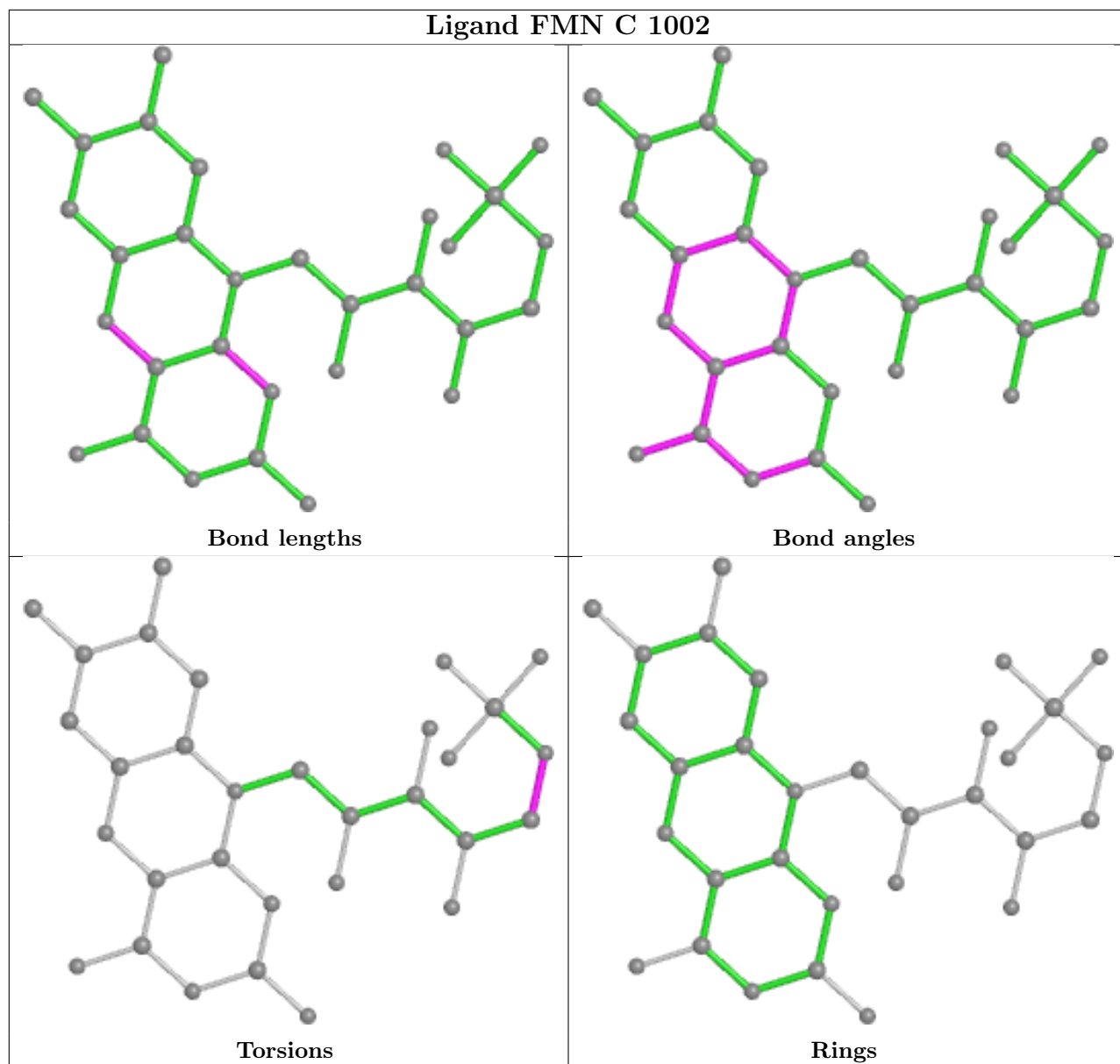


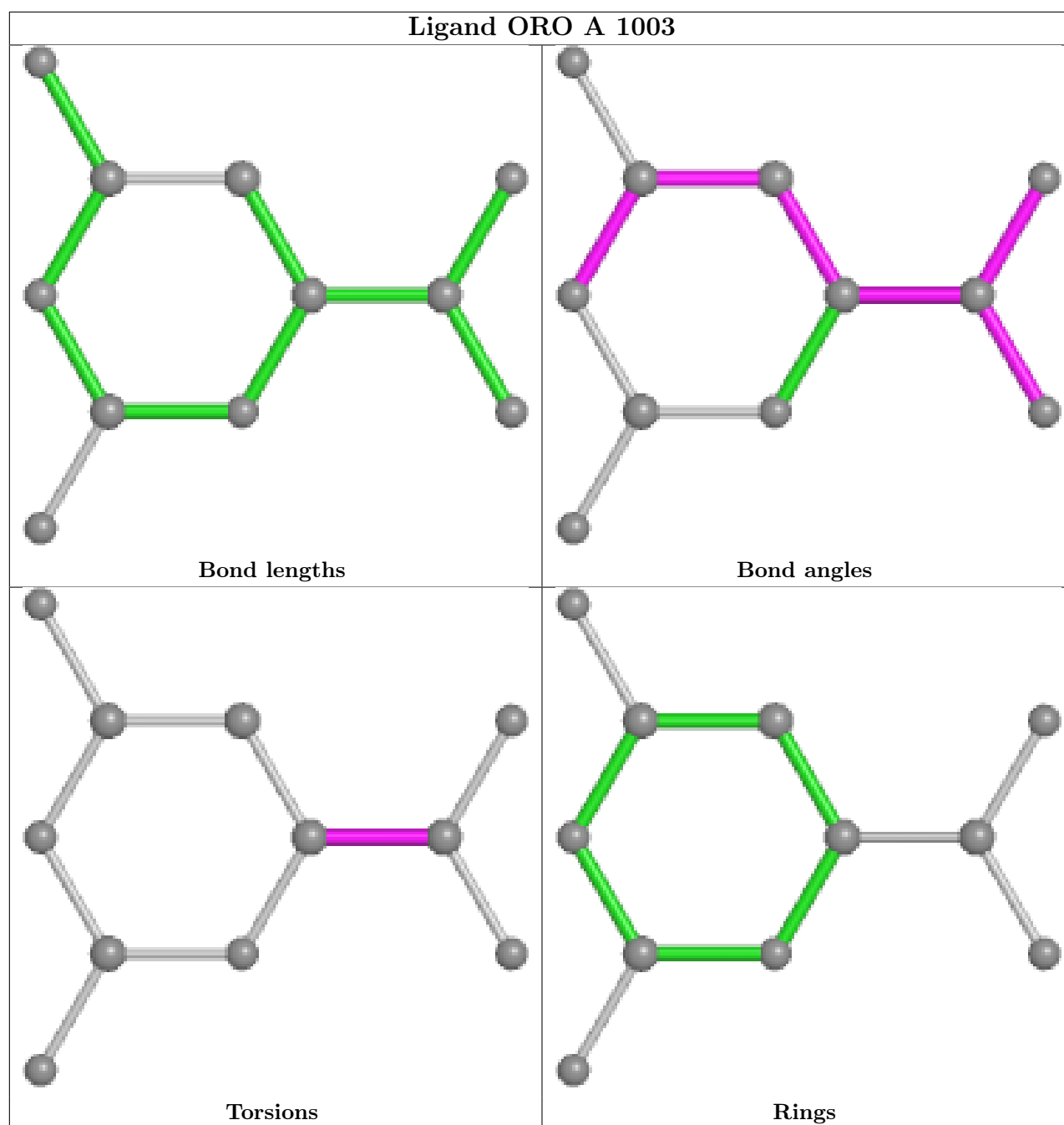












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	376/401 (93%)	-0.15	3 (0%) 86 85	9, 23, 41, 59	0
1	B	364/401 (90%)	-0.16	1 (0%) 94 93	10, 23, 45, 75	0
1	C	372/401 (92%)	0.04	6 (1%) 72 70	15, 32, 56, 73	0
1	D	371/401 (92%)	0.23	21 (5%) 23 23	12, 34, 68, 93	0
All	All	1483/1604 (92%)	-0.01	31 (2%) 63 62	9, 27, 57, 93	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	414	PHE	5.9
1	A	414	PHE	5.7
1	D	161	TYR	4.7
1	D	471	ASN	4.6
1	D	467	LYS	4.5
1	D	166	PHE	4.2
1	D	162	ASN	4.2
1	D	377	ASN	3.6
1	B	167	LEU	3.5
1	D	321	ILE	3.1
1	D	465	ASP	3.0
1	D	414	PHE	3.0
1	D	464	ASN	2.7
1	C	321	ILE	2.6
1	D	463	ILE	2.5
1	C	470	GLU	2.5
1	D	378	ASN	2.5
1	A	199	TYR	2.4
1	D	171	PHE	2.4
1	D	323	ASP	2.4
1	D	167	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	349	PRO	2.3
1	C	350	GLY	2.3
1	A	377	ASN	2.2
1	C	194	TYR	2.2
1	D	317	ASP	2.2
1	D	319	VAL	2.1
1	D	348	THR	2.1
1	D	470	GLU	2.0
1	D	316	LYS	2.0
1	D	466	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](#)

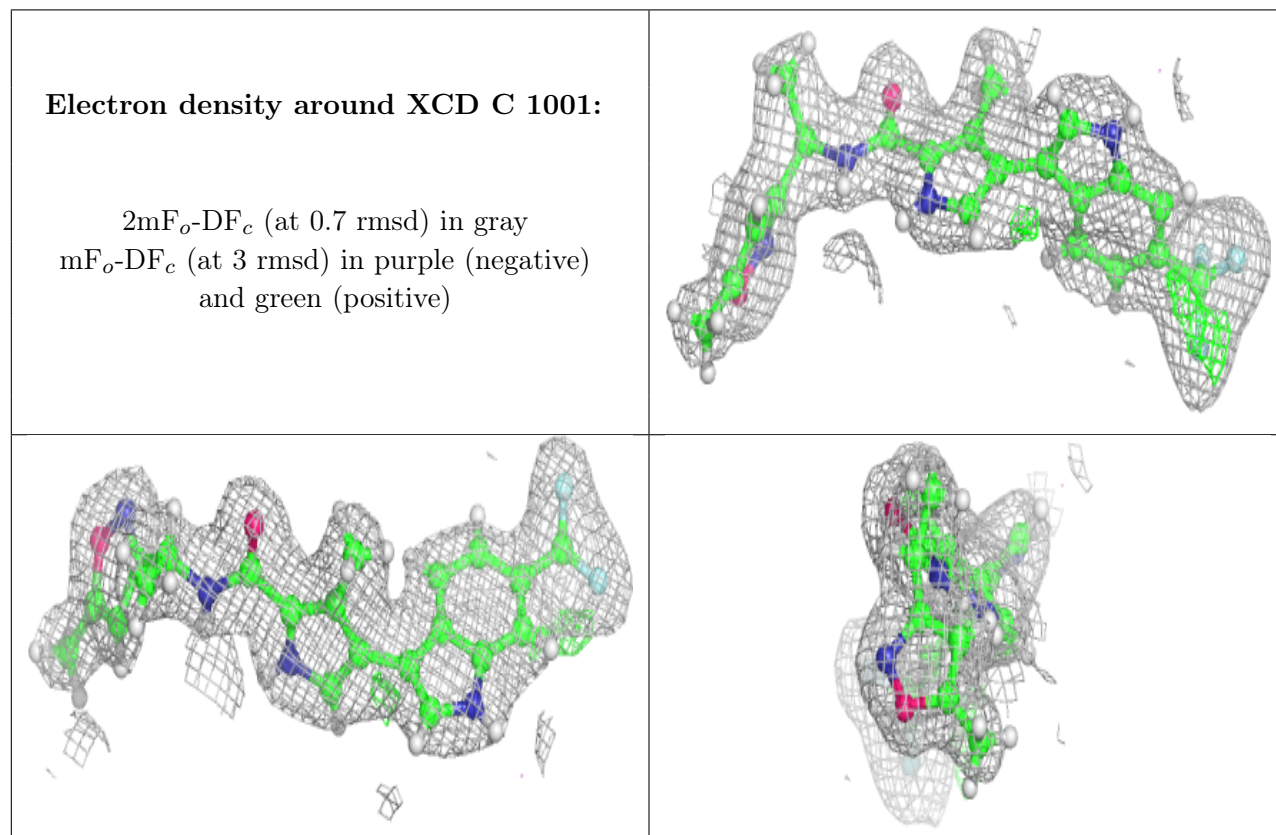
There are no monosaccharides in this entry.

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, 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.

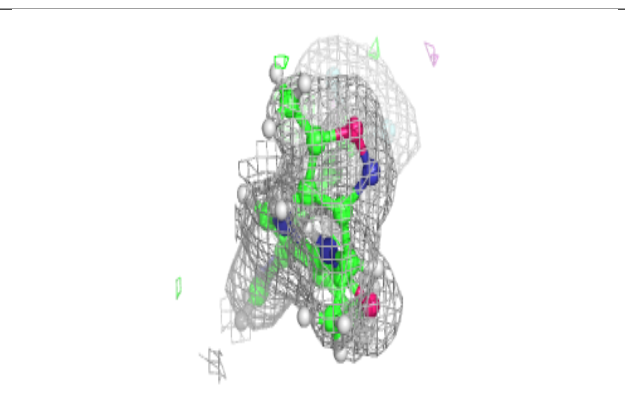
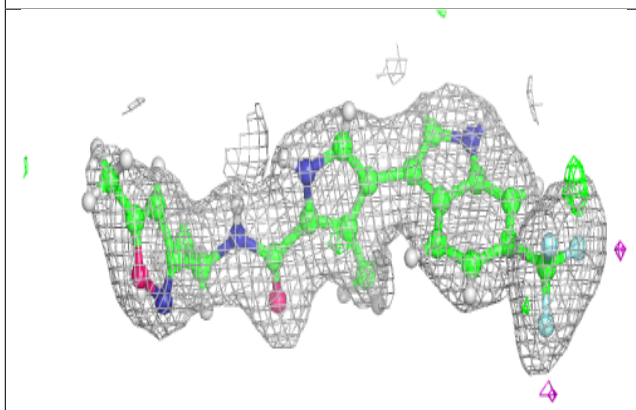
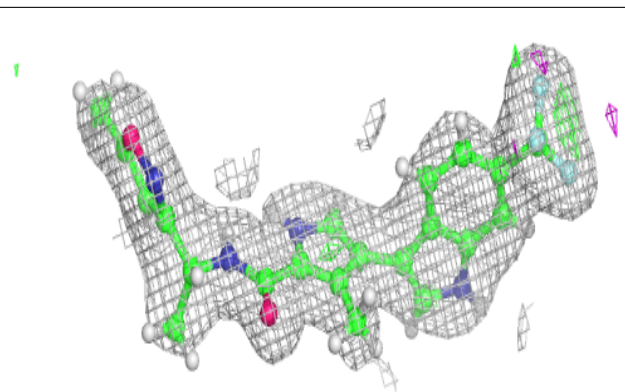
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XCD	C	1001	30/30	0.95	0.11	25,32,40,42	0
2	XCD	B	1001	30/30	0.96	0.11	18,30,38,42	0
4	ORO	C	1003	11/11	0.96	0.10	23,30,39,40	0
4	ORO	D	1003	11/11	0.96	0.10	26,32,39,43	0
3	FMN	C	1002	31/31	0.97	0.11	13,20,36,38	0
2	XCD	A	1001	30/30	0.97	0.09	14,21,26,31	0
2	XCD	D	1001	30/30	0.97	0.11	22,31,37,41	0
3	FMN	D	1002	31/31	0.98	0.13	18,24,32,38	0
4	ORO	A	1003	11/11	0.98	0.11	8,13,18,20	0
4	ORO	B	1003	11/11	0.98	0.11	11,16,24,24	0
3	FMN	B	1002	31/31	0.98	0.13	10,13,23,28	0
3	FMN	A	1002	31/31	0.98	0.13	7,10,17,20	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.



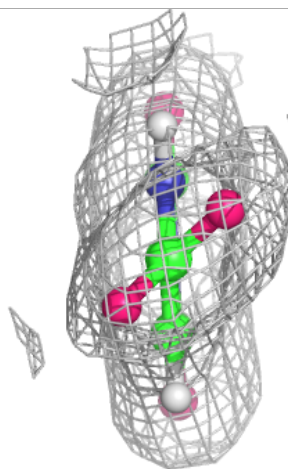
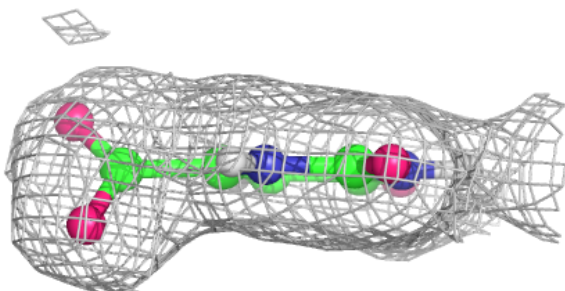
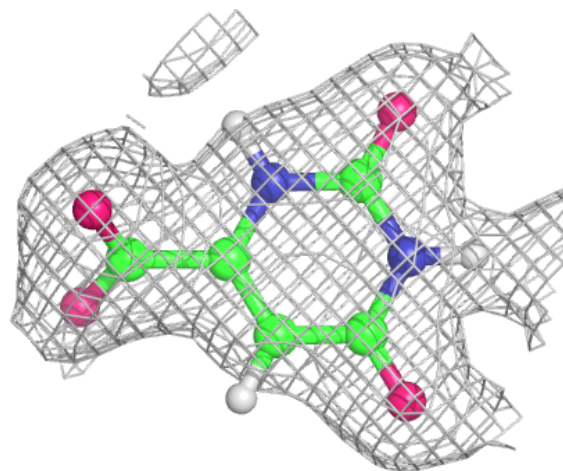
Electron density around XCD B 1001:

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



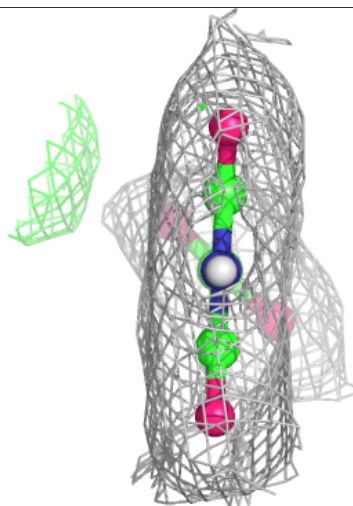
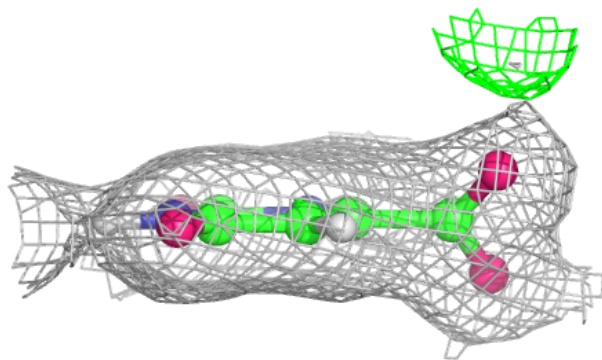
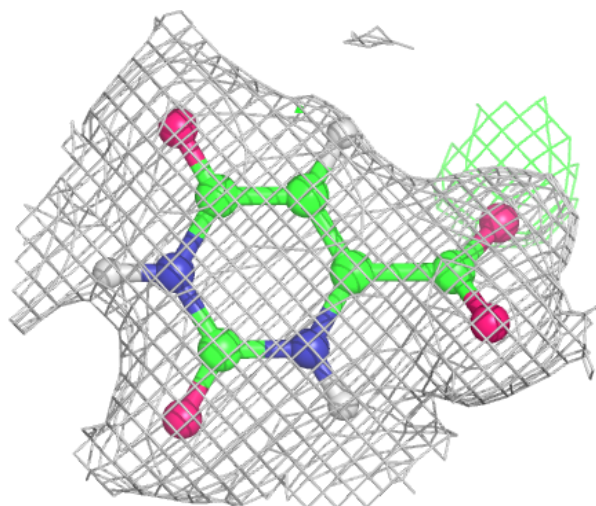
Electron density around ORO C 1003:

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



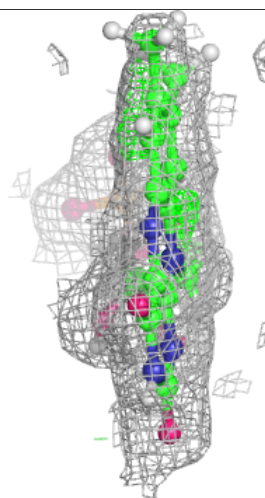
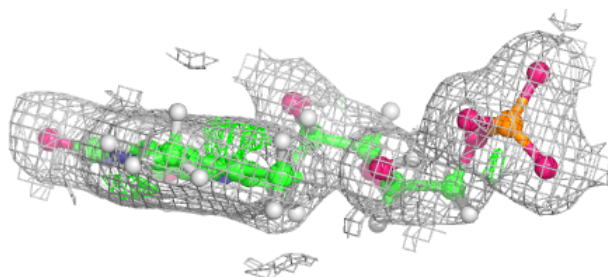
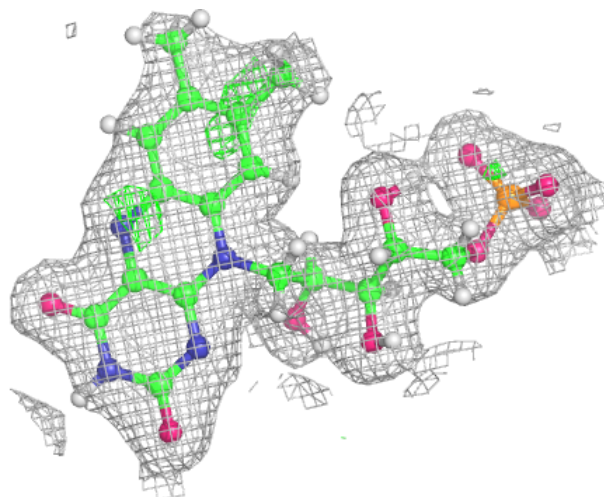
Electron density around ORO D 1003:

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



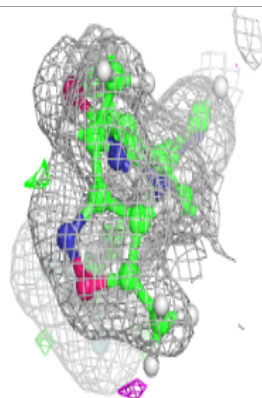
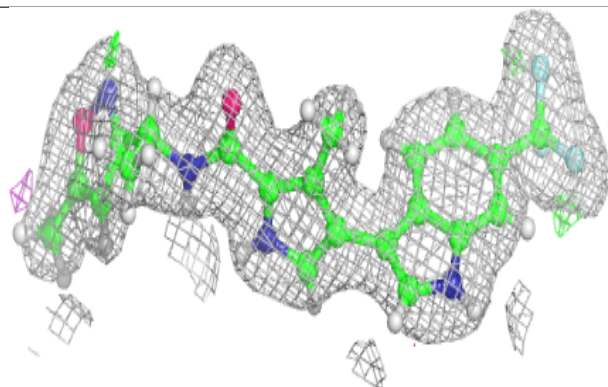
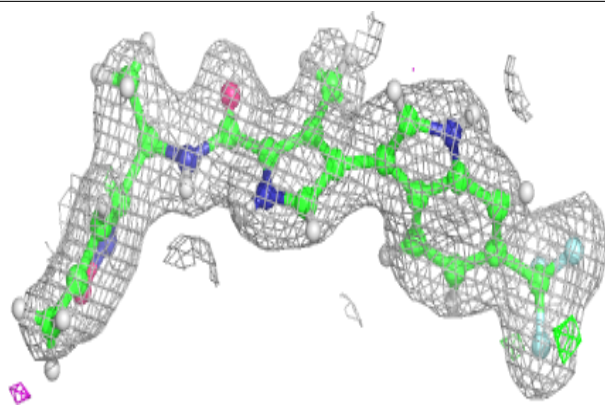
Electron density around FMN C 1002:

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

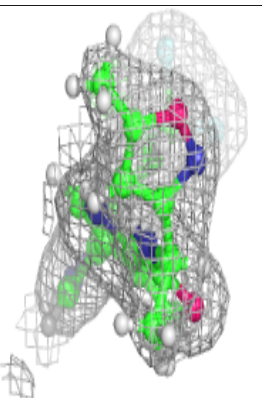
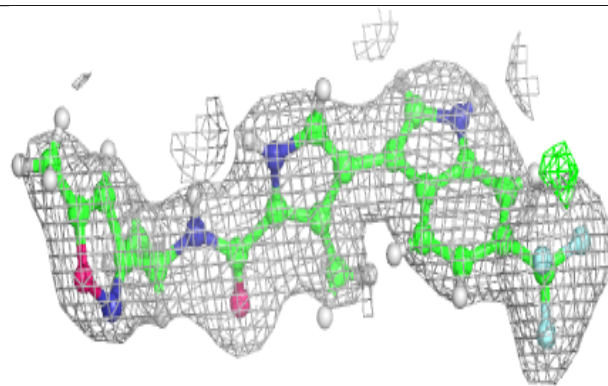
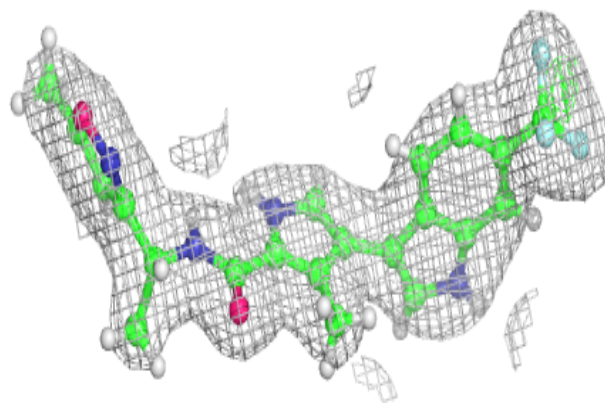


Electron density around XCD A 1001:

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

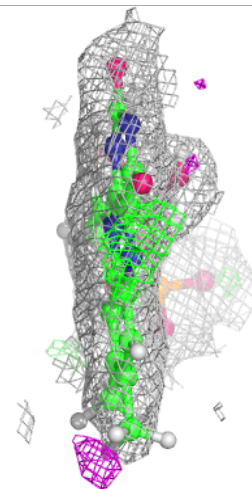
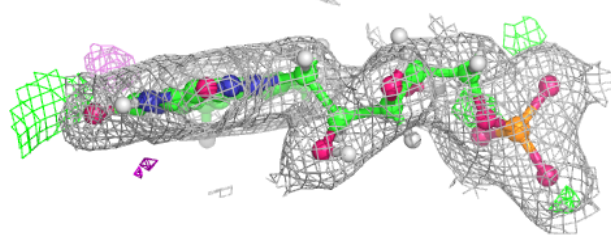
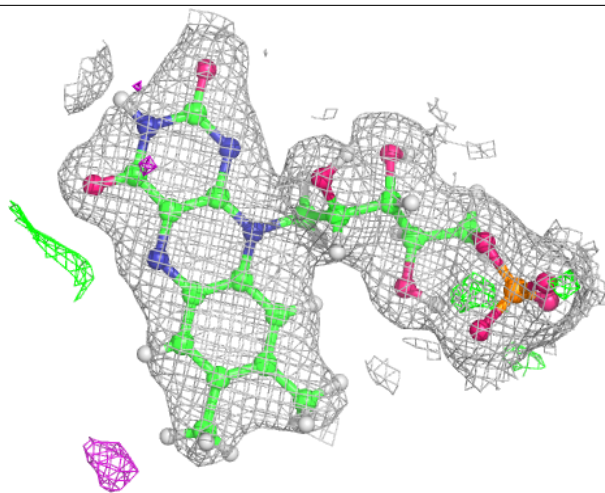
**Electron density around XCD D 1001:**

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



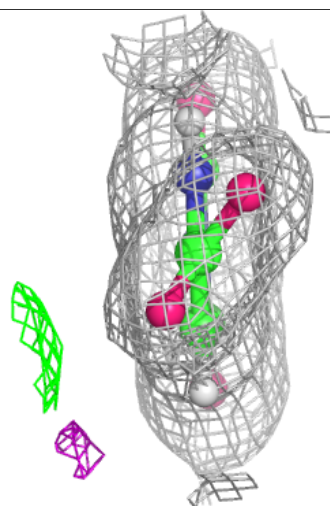
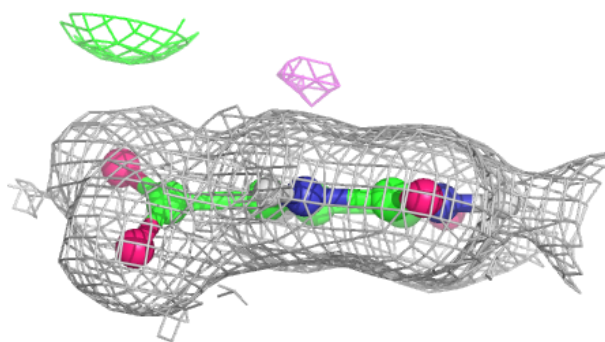
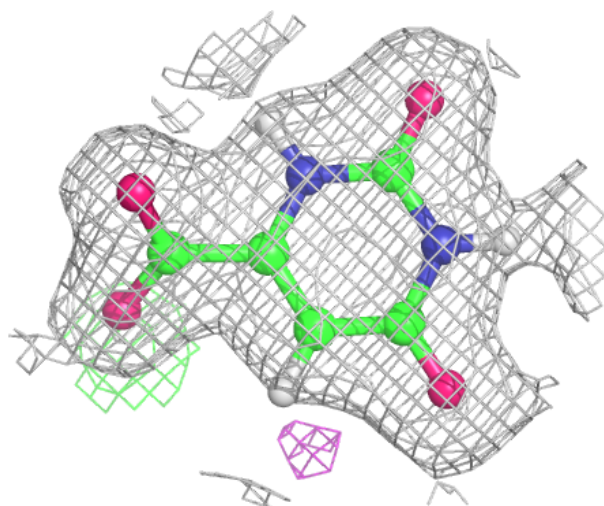
Electron density around FMN D 1002:

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



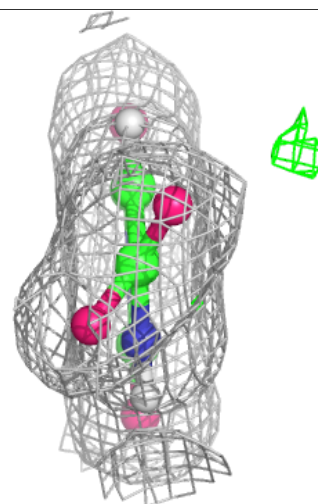
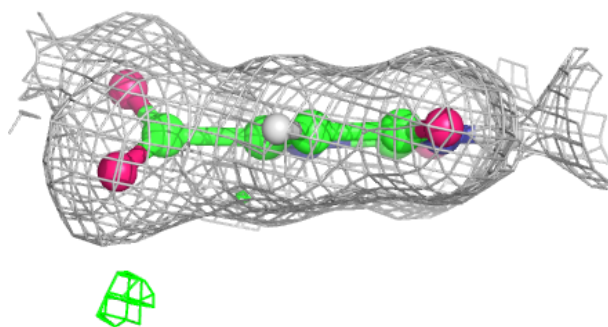
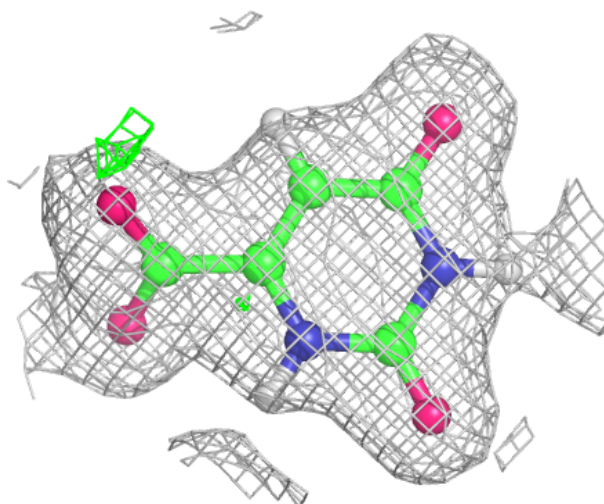
Electron density around ORO A 1003:

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



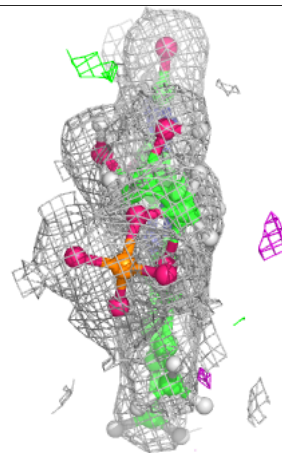
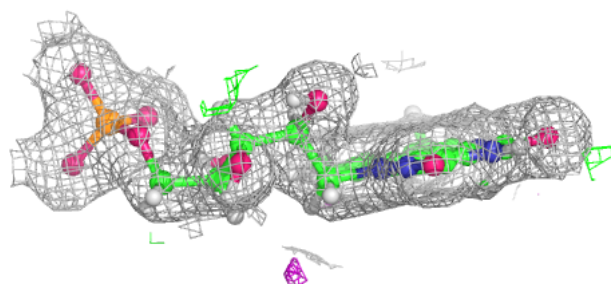
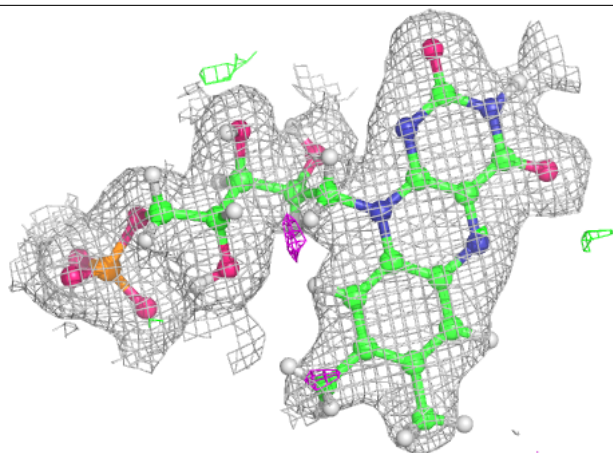
Electron density around ORO B 1003:

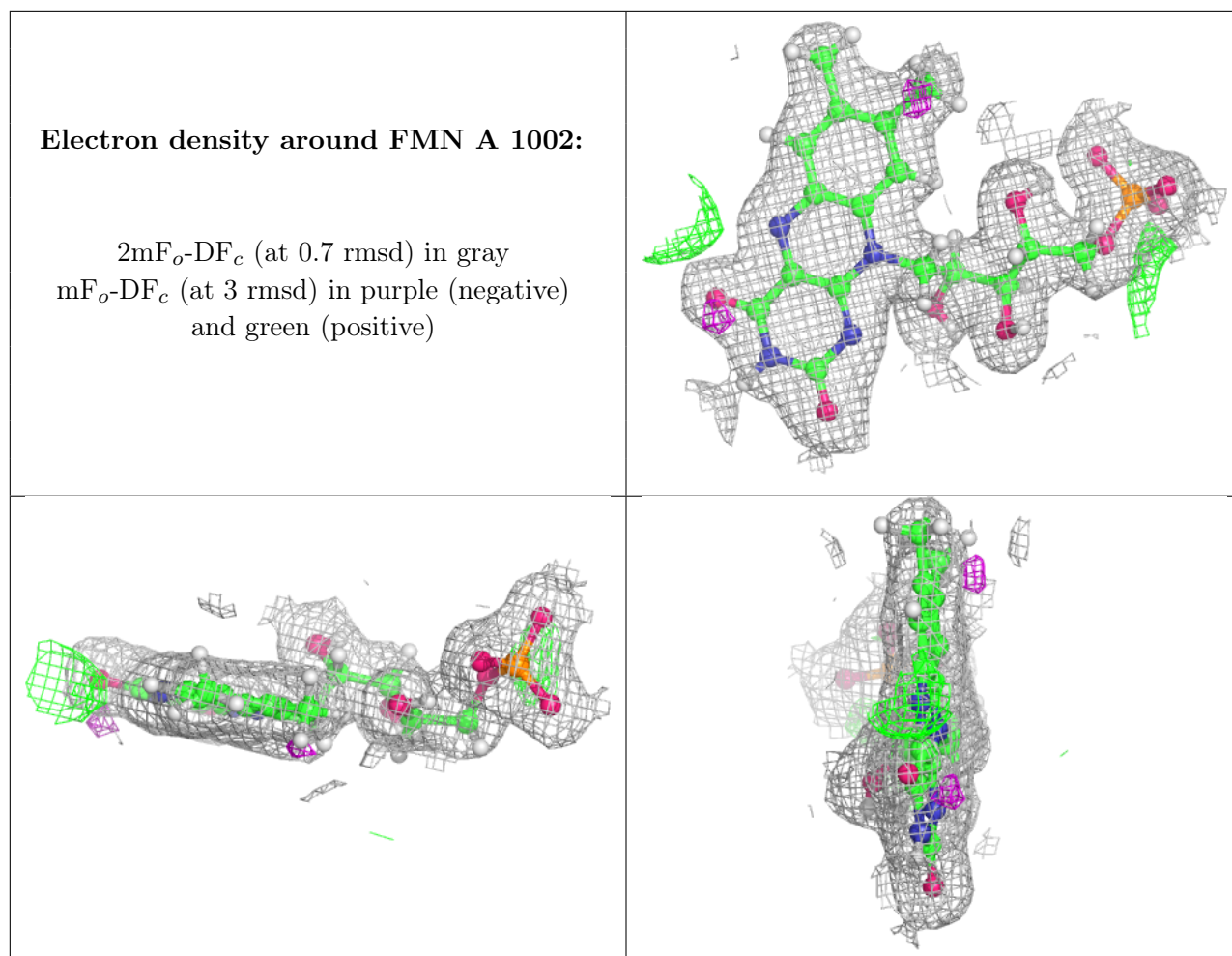
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN B 1002:

$2mF_o-DF_c$ (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.