Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 02:24 PM EDT

PDB ID	:	7L01
Title	:	Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM782 (N-(1-(5-cyano-1H-pyrazol-3-yl)ethyl)-3-methyl-4-(1-(6-(trifluoromethyl)pyridin-3-yl)cyclopropyl)-1H-pyrrole-2-carboxamide)
Authors	:	Deng, X.; Phillips, M.; Tomchick, D.
Deposited on	:	2020-12-10
Resolution	:	1.60 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 (1)) were used in the production of this report:

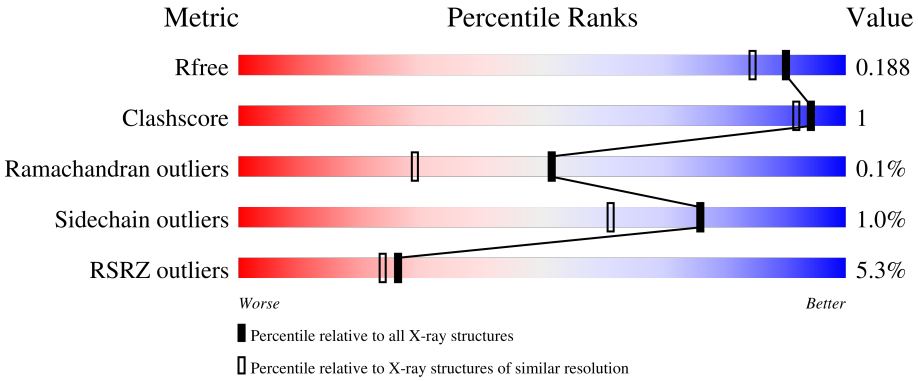
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

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

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 <=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	4% 89% · 7%
1	B	401	6% 92% · ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12988 atoms, of which 6191 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	372	Total	C	H	N	O	S	0	4	0
			5986	1899	3019	497	556	15			
1	B	385	Total	C	H	N	O	S	0	3	0
			6160	1955	3092	518	579	16			

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	-12	MET	-	initiating methionine	UNP Q08210
B	-11	GLY	-	expression tag	UNP Q08210
B	-10	HIS	-	expression tag	UNP Q08210
B	-9	HIS	-	expression tag	UNP Q08210
B	-8	HIS	-	expression tag	UNP Q08210
B	-7	HIS	-	expression tag	UNP Q08210
B	-6	HIS	-	expression tag	UNP Q08210
B	-5	HIS	-	expression tag	UNP Q08210
B	-4	ALA	-	expression tag	UNP Q08210
B	-3	GLU	-	expression tag	UNP Q08210
B	-2	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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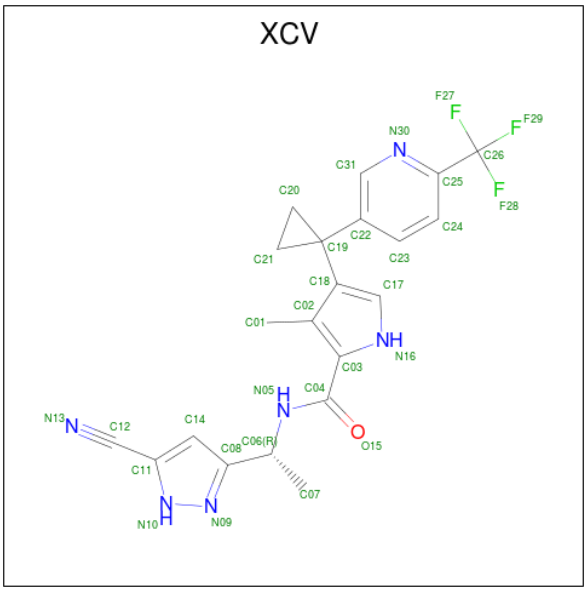
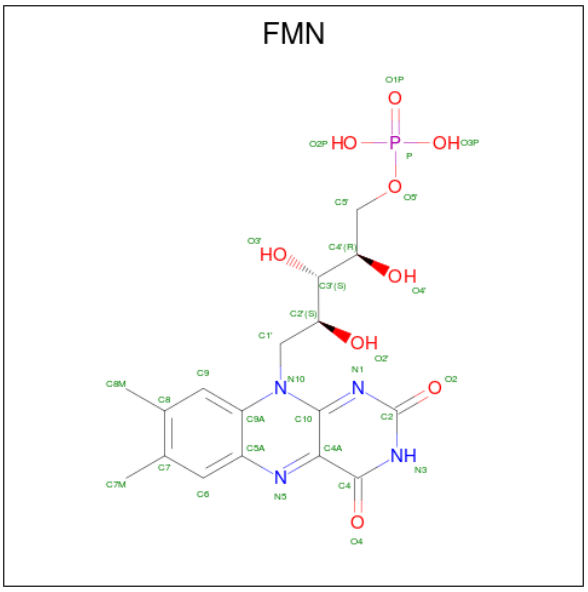
Chain	Residue	Modelled	Actual	Comment	Reference
B	157	PRO	-	expression tag	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	THR	deletion	UNP Q08210
B	?	-	TYR	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	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 N-[(1R)-1-(5-cyano-1H-pyrazol-3-yl)ethyl]-3-methyl-4-{1-[6-(trifluoromethyl)pyridin-3-yl]cyclopropyl}-1H-pyrrole-2-carboxamide (three-letter code: XCV) (formula: $C_{21}H_{19}F_3N_6O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			50	21	3	19	6	1		
2	B	1	Total	C	F	H	N	O	0	0
			50	21	3	19	6	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		

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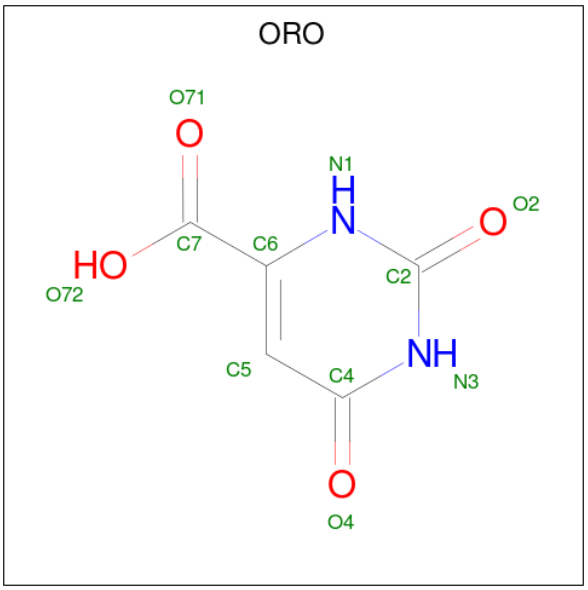
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		

- 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		

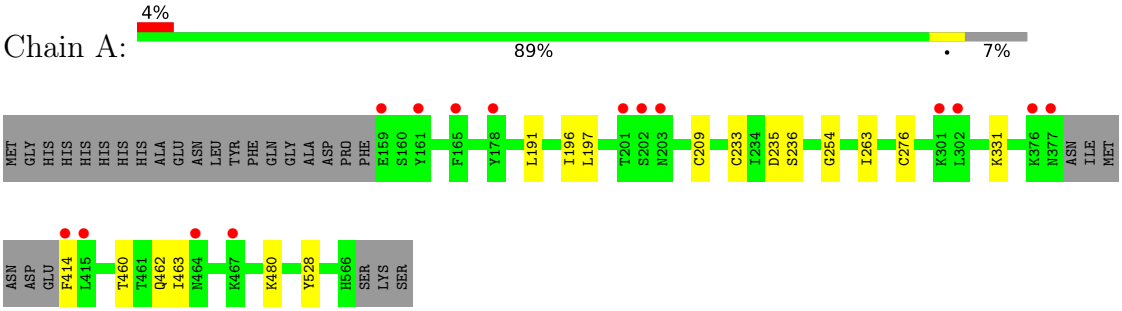
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	293	Total	O	0	0
			293	293		
5	B	323	Total	O	0	0
			323	323		

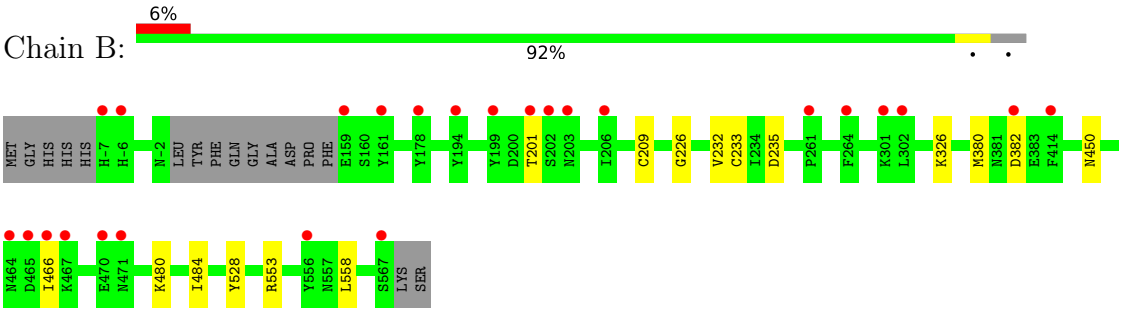
3 Residue-property plots (i)

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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.06Å 158.03Å 61.05Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	33.39 – 1.60 33.39 – 1.60	Depositor EDS
% Data completeness (in resolution range)	80.5 (33.39-1.60) 80.5 (33.39-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.164 , 0.188 0.164 , 0.188	Depositor DCC
R_{free} test set	1260 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12988	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ORO, FMN, XCV

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	0.53	1/3031 (0.0%)	0.65	0/4079
1	B	0.57	1/3137 (0.0%)	0.65	0/4224
All	All	0.55	2/6168 (0.0%)	0.65	0/8303

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	CYS	CB-SG	-14.24	1.58	1.82
1	A	233	CYS	CB-SG	-6.12	1.71	1.82

There are no bond angle outliers.

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	2967	3019	3007	8	0
1	B	3068	3092	3084	9	0
2	A	31	19	0	0	0
2	B	31	19	0	0	0
3	A	31	18	19	0	0
3	B	31	18	19	1	0
4	A	11	3	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	3	3	0	0
5	A	293	0	0	2	0
5	B	323	0	0	5	0
All	All	6797	6191	6135	16	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 1.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ILE:HD13	1:A:480:LYS:HB3	1.79	0.65
1:A:263:ILE:HD11	1:A:276:CYS:SG	2.45	0.57
1:A:331[B]:LYS:HG2	5:A:1249:HOH:O	2.05	0.56
1:A:209[B]:CYS:SG	5:A:1165:HOH:O	2.58	0.55
1:A:197:LEU:HD12	1:A:236:SER:HB3	1.96	0.47
1:B:326:LYS:HE2	5:B:1158:HOH:O	2.13	0.47
1:B:558:LEU:HD23	1:B:558:LEU:C	2.39	0.43
1:A:191:LEU:HD23	1:A:196:ILE:HD11	2.00	0.43
1:B:466:ILE:HD11	1:B:480:LYS:HD3	2.00	0.43
1:B:226:GLY:HA3	3:B:1002:FMN:N5	2.33	0.43
1:B:484:ILE:HG13	5:B:1241:HOH:O	2.17	0.42
1:A:254:GLY:O	1:B:450:ASN:HB2	2.19	0.42
1:B:232:VAL:HG23	5:B:1120:HOH:O	2.19	0.42
1:B:553:ARG:HD2	5:B:1144:HOH:O	2.18	0.42
1:A:460:THR:OG1	1:A:462:GLN:HG2	2.20	0.42
1:B:209[B]:CYS:SG	5:B:1176:HOH:O	2.62	0.41

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%)	366 (98%)	6 (2%)	0	100 100
1	B	384/401 (96%)	374 (97%)	9 (2%)	1 (0%)	41 21
All	All	756/802 (94%)	740 (98%)	15 (2%)	1 (0%)	51 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	THR

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%)	330 (99%)	3 (1%)	78 65
1	B	344/354 (97%)	340 (99%)	4 (1%)	71 54
All	All	677/708 (96%)	670 (99%)	7 (1%)	76 61

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

Mol	Chain	Res	Type
1	A	235	ASP
1	A	414	PHE
1	A	528	TYR
1	B	235	ASP
1	B	380	MET
1	B	382	ASP
1	B	528	TYR

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)

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	$\#\|Z\| > 2$
4	ORO	B	1003	-	9,11,11	1.43	1 (11%)	8,15,15	1.78	2 (25%)
2	XCV	A	1001	-	30,34,34	1.35	2 (6%)	33,52,52	1.61	7 (21%)
2	XCV	B	1001	-	30,34,34	1.44	6 (20%)	33,52,52	1.83	11 (33%)
3	FMN	B	1002	-	33,33,33	1.14	3 (9%)	48,50,50	1.25	7 (14%)
4	ORO	A	1003	-	9,11,11	1.49	1 (11%)	8,15,15	2.30	4 (50%)
3	FMN	A	1002	-	33,33,33	1.23	1 (3%)	48,50,50	1.20	4 (8%)

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
4	ORO	B	1003	-	-	4/4/4/4	0/1/1/1
2	XCV	A	1001	-	-	3/18/36/36	0/4/4/4
2	XCV	B	1001	-	-	2/18/36/36	0/4/4/4
3	FMN	B	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	A	1003	-	-	4/4/4/4	0/1/1/1
3	FMN	A	1002	-	-	1/18/18/18	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	XCV	C04-N05	4.55	1.44	1.34
2	A	1001	XCV	C04-N05	4.48	1.43	1.34
3	A	1002	FMN	C4A-N5	4.43	1.39	1.30
3	B	1002	FMN	C4A-N5	3.76	1.38	1.30
4	B	1003	ORO	C4-N3	3.00	1.38	1.33
2	B	1001	XCV	C11-C12	2.82	1.53	1.44
2	B	1001	XCV	C31-C22	2.54	1.41	1.38
2	B	1001	XCV	C03-C04	2.49	1.54	1.50
3	B	1002	FMN	C5'-C4'	2.47	1.55	1.51
2	A	1001	XCV	C11-C12	2.44	1.52	1.44
4	A	1003	ORO	O4-C4	-2.42	1.18	1.24
2	B	1001	XCV	C26-C25	2.08	1.54	1.50
3	B	1002	FMN	C10-N1	2.02	1.37	1.33
2	B	1001	XCV	C01-C02	2.00	1.55	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	XCV	O15-C04-C03	4.30	127.01	120.59
4	B	1003	ORO	C5-C4-N3	-4.09	119.31	124.08
2	A	1001	XCV	O15-C04-C03	3.78	126.24	120.59
4	A	1003	ORO	O71-C7-C6	-3.60	113.95	121.24
3	A	1002	FMN	C4A-C10-N10	3.46	121.54	116.48
3	B	1002	FMN	C4A-C10-N10	3.28	121.28	116.48
3	B	1002	FMN	O3P-P-O2P	3.22	119.94	107.64
4	A	1003	ORO	C5-C4-N3	-3.06	120.51	124.08
4	A	1003	ORO	C6-C5-C4	2.93	118.62	116.73
4	A	1003	ORO	O72-C7-C6	2.92	121.33	114.69
2	B	1001	XCV	F27-C26-C25	-2.92	107.48	112.47
4	B	1003	ORO	C6-C5-C4	2.79	118.53	116.73
2	B	1001	XCV	O15-C04-N05	-2.73	117.42	122.45
2	A	1001	XCV	C31-C22-C19	-2.72	117.68	121.97
2	B	1001	XCV	C31-C22-C19	-2.66	117.78	121.97
2	B	1001	XCV	C26-C25-N30	2.60	117.73	114.61
2	B	1001	XCV	C24-C23-C22	-2.59	117.75	121.22
2	A	1001	XCV	F29-C26-C25	-2.54	108.13	112.47
3	A	1002	FMN	C10-C4A-N5	-2.48	119.59	124.86
2	A	1001	XCV	C24-C23-C22	-2.45	117.94	121.22
2	A	1001	XCV	C21-C19-C18	-2.43	113.66	117.13
2	B	1001	XCV	F29-C26-C25	-2.33	108.48	112.47
2	B	1001	XCV	C21-C19-C18	-2.28	113.87	117.13
2	B	1001	XCV	C07-C06-C08	2.28	113.59	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	XCV	C21-C19-C20	2.16	60.03	58.70
3	B	1002	FMN	C10-C4A-N5	-2.15	120.29	124.86
3	B	1002	FMN	C4-C4A-C10	2.15	120.40	116.79
3	B	1002	FMN	C5A-C9A-N10	2.15	120.17	117.95
2	B	1001	XCV	F28-C26-C25	-2.12	108.84	112.47
2	A	1001	XCV	C21-C20-C19	-2.11	59.18	60.64
3	B	1002	FMN	C9-C9A-N10	-2.03	119.09	121.84
2	A	1001	XCV	C22-C31-N30	-2.03	121.40	123.34
3	A	1002	FMN	C5A-C9A-N10	2.02	120.04	117.95
3	B	1002	FMN	O2-C2-N1	-2.01	118.50	121.83
3	A	1002	FMN	C9A-C5A-N5	-2.00	120.25	122.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	A	1001	XCV	C18-C19-C22-C31
2	B	1001	XCV	C18-C19-C22-C31
4	A	1003	ORO	N1-C6-C7-O72
4	B	1003	ORO	N1-C6-C7-O72
2	B	1001	XCV	C18-C19-C22-C23
2	A	1001	XCV	C18-C19-C22-C23
4	B	1003	ORO	C5-C6-C7-O71
3	B	1002	FMN	C4'-C5'-O5'-P
3	A	1002	FMN	C4'-C5'-O5'-P
4	B	1003	ORO	N1-C6-C7-O71
2	A	1001	XCV	C08-C06-N05-C04

There are no ring outliers.

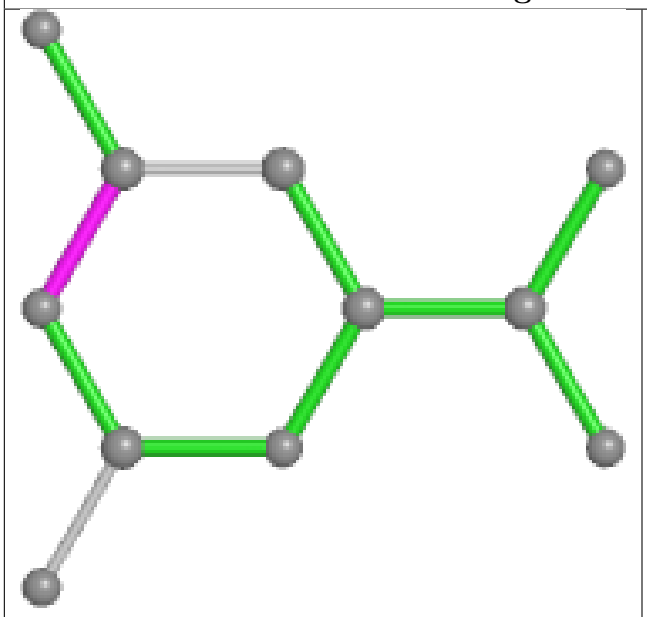
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	FMN	1	0

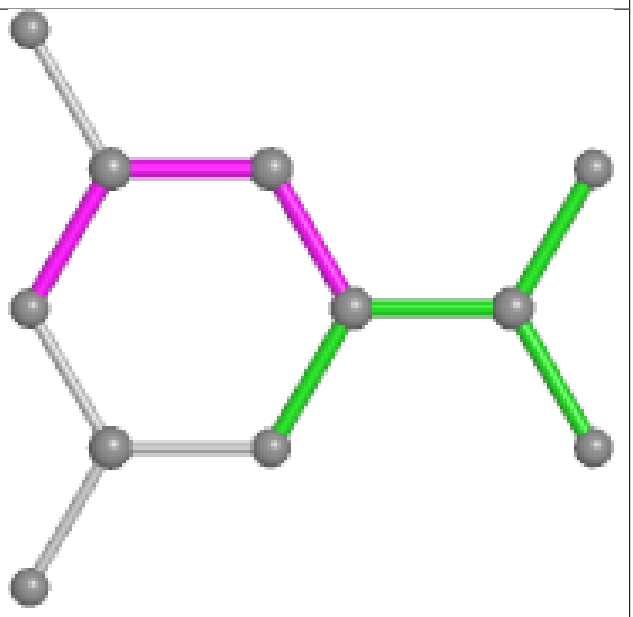
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

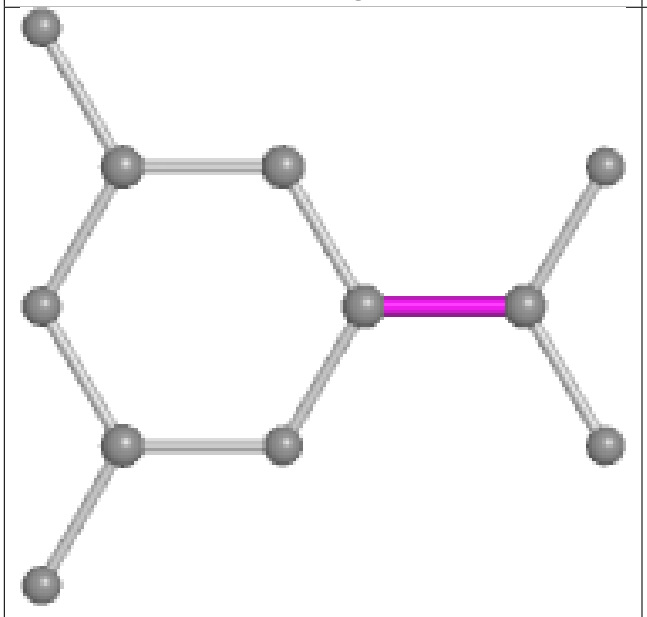
Ligand ORO B 1003



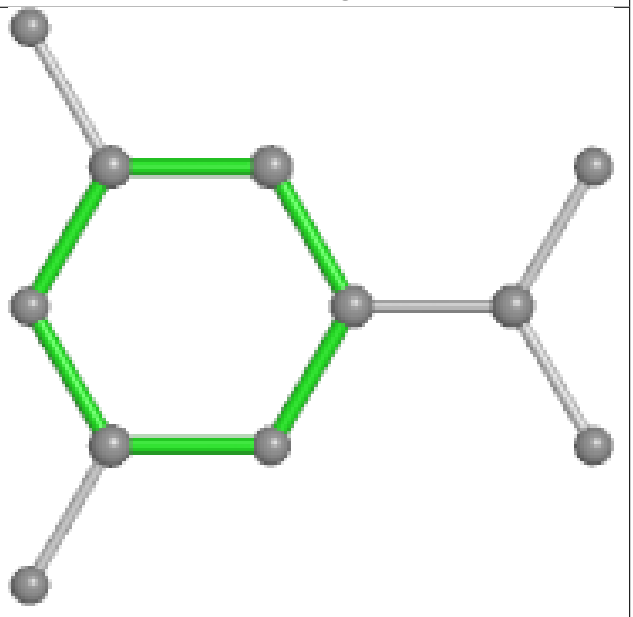
Bond lengths



Bond angles

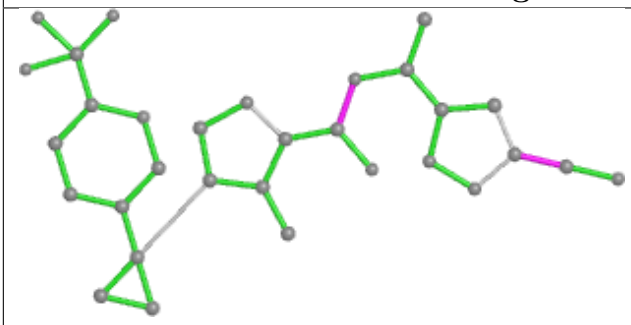


Torsions

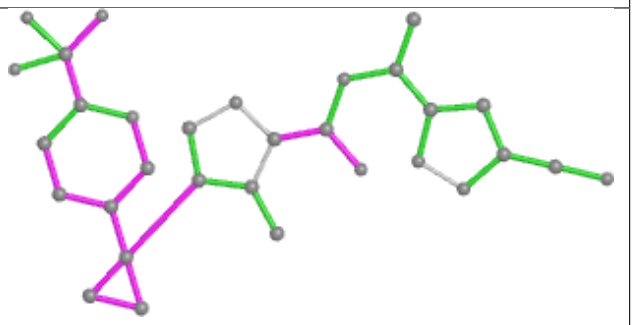


Rings

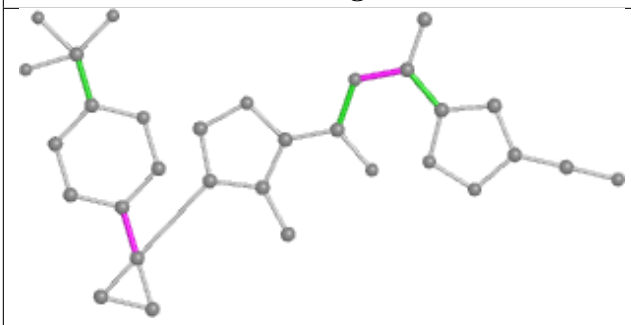
Ligand XCV A 1001



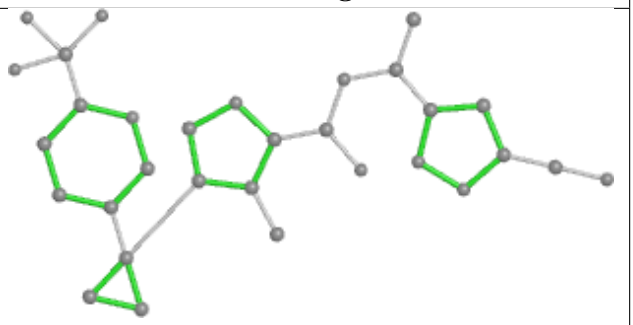
Bond lengths



Bond angles

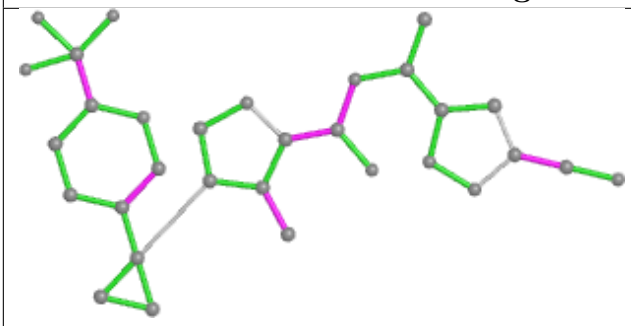


Torsions

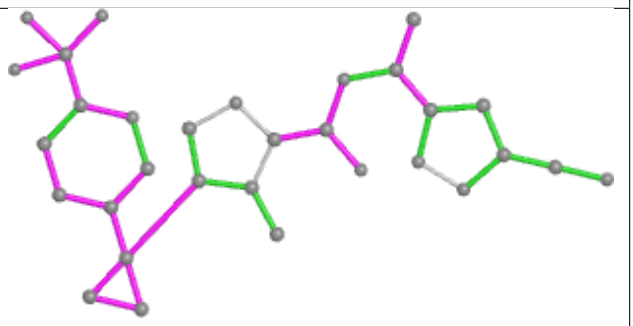


Rings

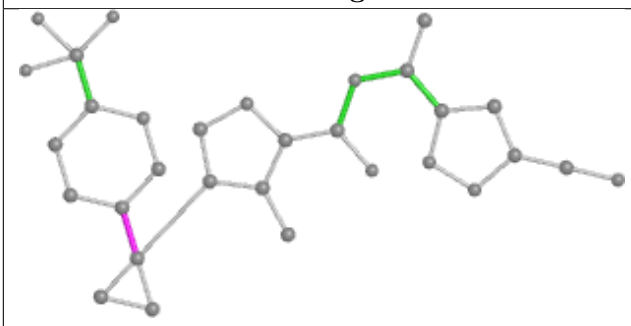
Ligand XCV B 1001



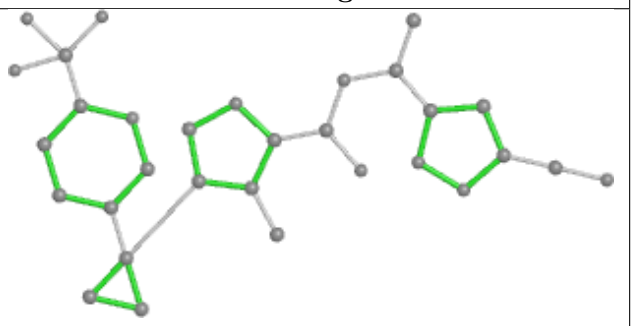
Bond lengths



Bond angles

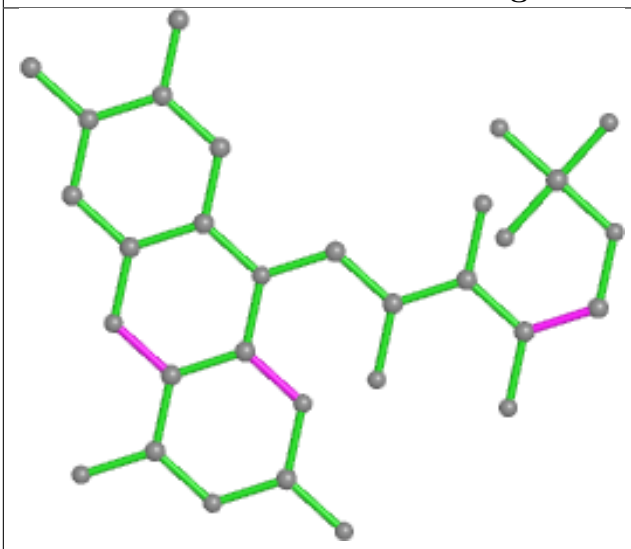


Torsions

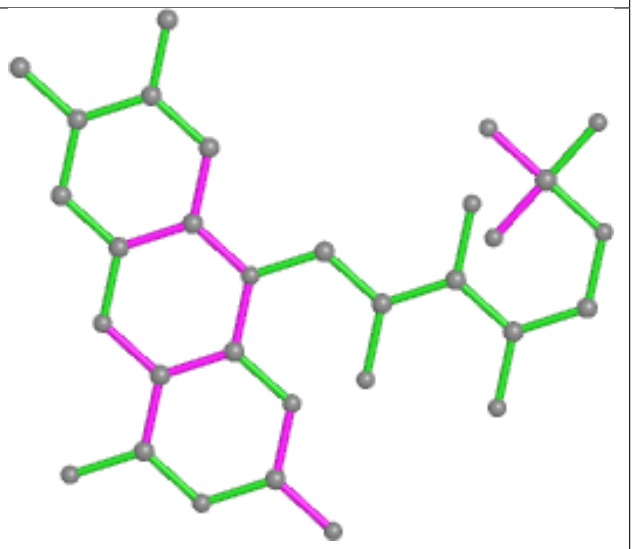


Rings

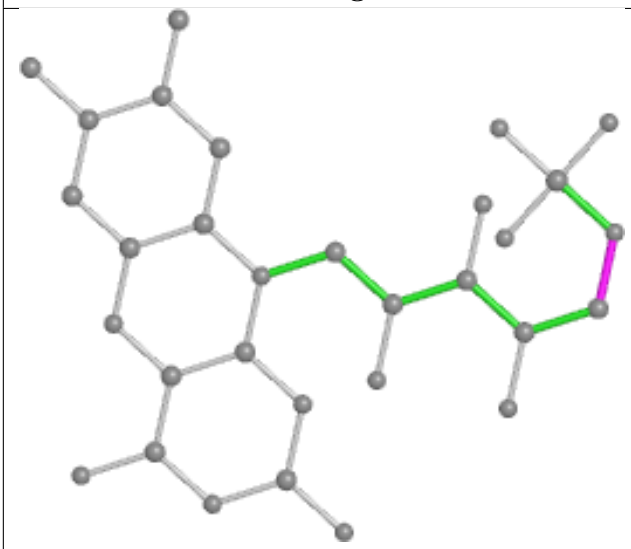
Ligand FMN B 1002



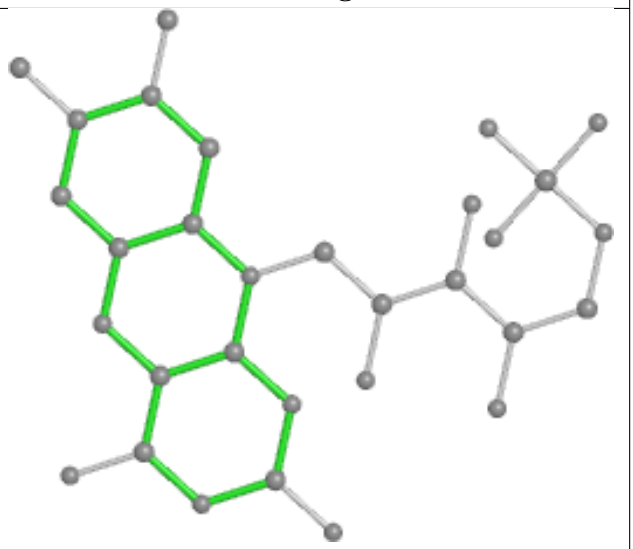
Bond lengths



Bond angles

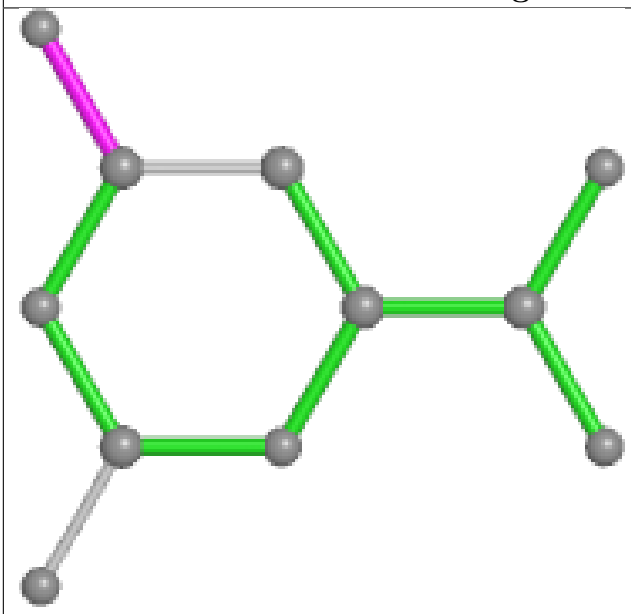


Torsions

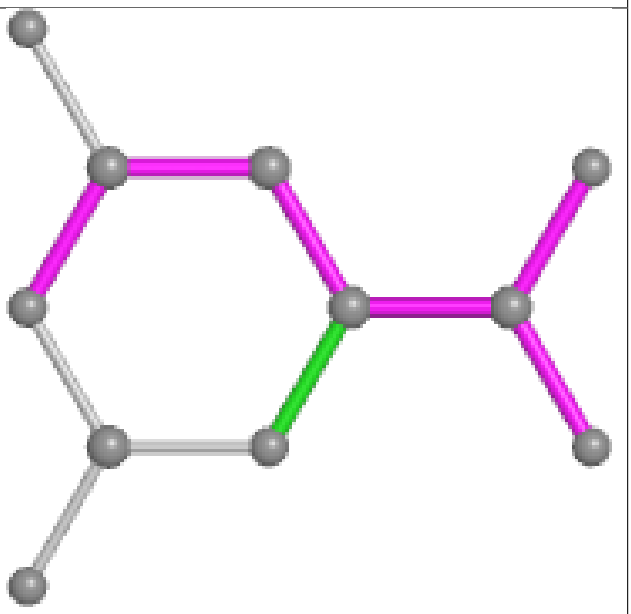


Rings

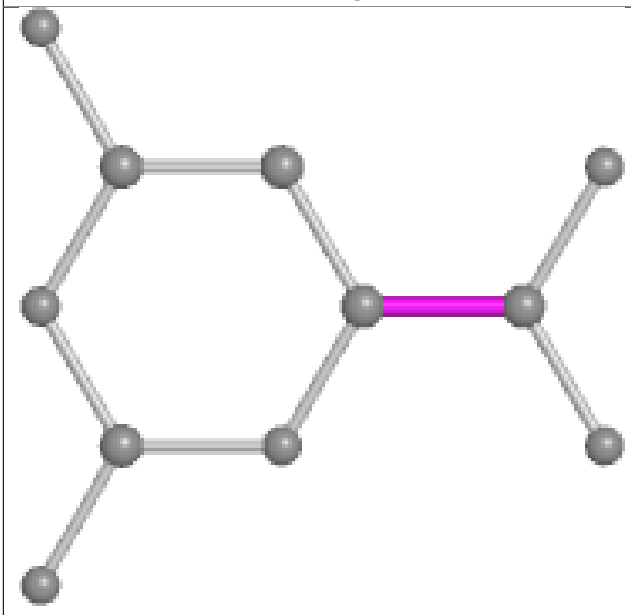
Ligand ORO A 1003



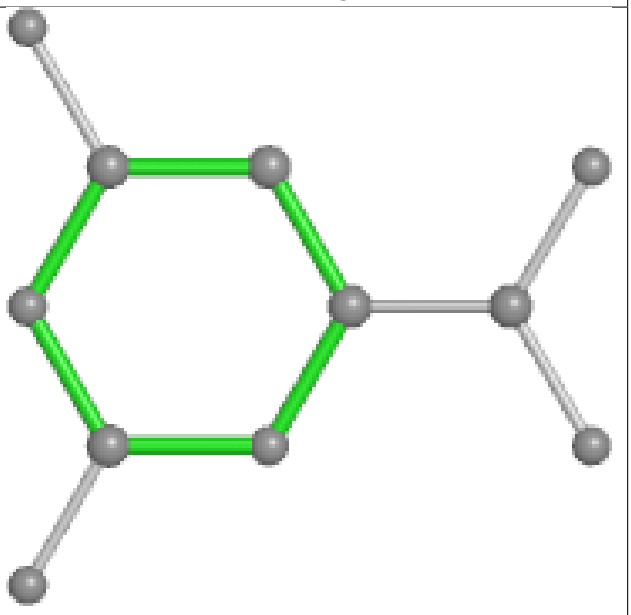
Bond lengths



Bond angles

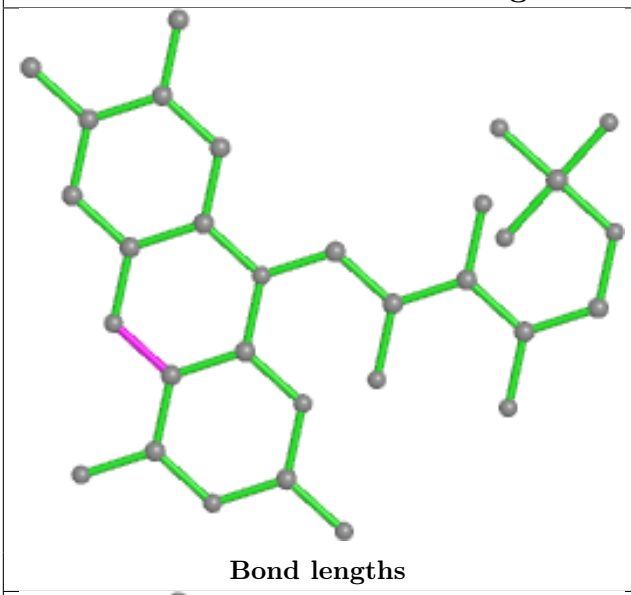


Torsions

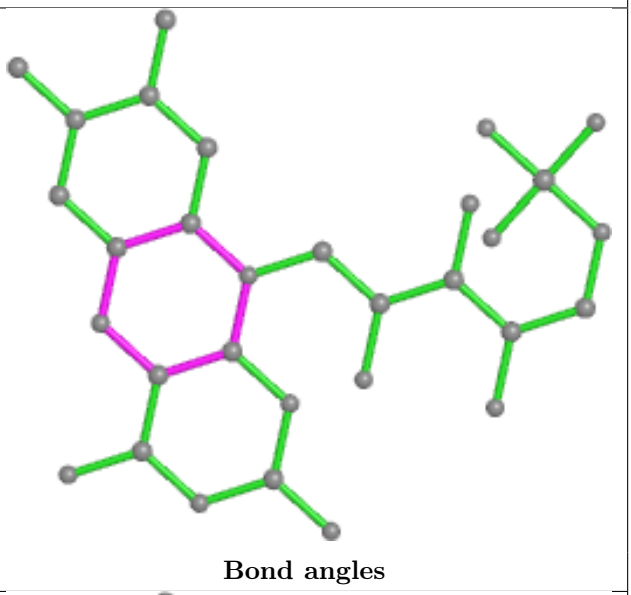


Rings

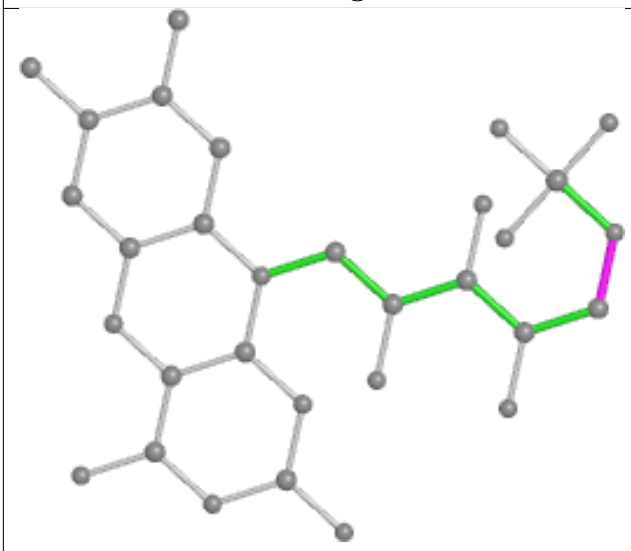
Ligand FMN A 1002



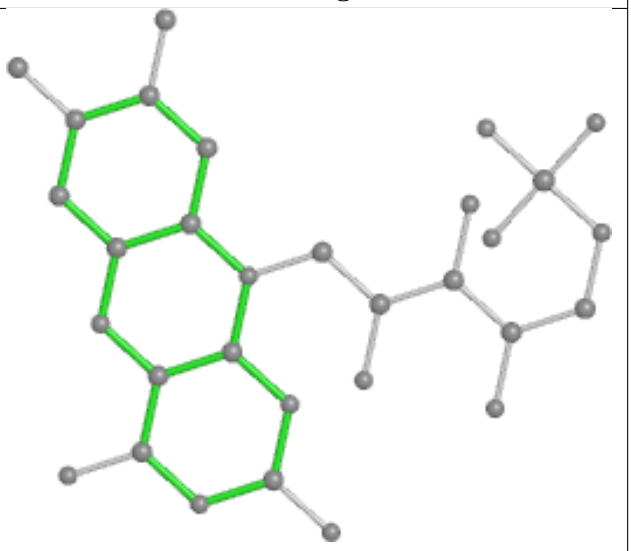
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	372/401 (92%)	0.01	15 (4%)	38	35	5, 17, 36, 63	0
1	B	385/401 (96%)	0.00	25 (6%)	18	17	5, 17, 41, 55	0
All	All	757/802 (94%)	0.01	40 (5%)	26	24	5, 17, 38, 63	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	PHE	8.7
1	A	161	TYR	7.6
1	B	161	TYR	6.1
1	A	377	ASN	6.0
1	B	201	THR	6.0
1	B	471	ASN	5.6
1	A	201	THR	4.0
1	B	-7	HIS	3.9
1	A	376	LYS	3.8
1	B	467	LYS	3.4
1	A	415	LEU	3.4
1	B	464	ASN	3.4
1	B	-6	HIS	3.2
1	B	159	GLU	3.1
1	B	414	PHE	3.1
1	B	203	ASN	3.0
1	A	464	ASN	3.0
1	A	202	SER	3.0
1	A	302	LEU	2.8
1	B	470	GLU	2.8
1	B	465	ASP	2.8
1	B	301	LYS	2.7
1	A	467	LYS	2.6
1	B	302	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	466	ILE	2.5
1	B	556	TYR	2.5
1	B	567	SER	2.3
1	B	194	TYR	2.3
1	B	202	SER	2.2
1	B	382	ASP	2.2
1	A	178	TYR	2.2
1	B	199	TYR	2.2
1	A	165	PHE	2.1
1	A	203	ASN	2.1
1	B	178	TYR	2.1
1	B	264	PHE	2.1
1	B	261	PRO	2.1
1	A	301	LYS	2.1
1	B	206	ILE	2.1
1	A	159	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

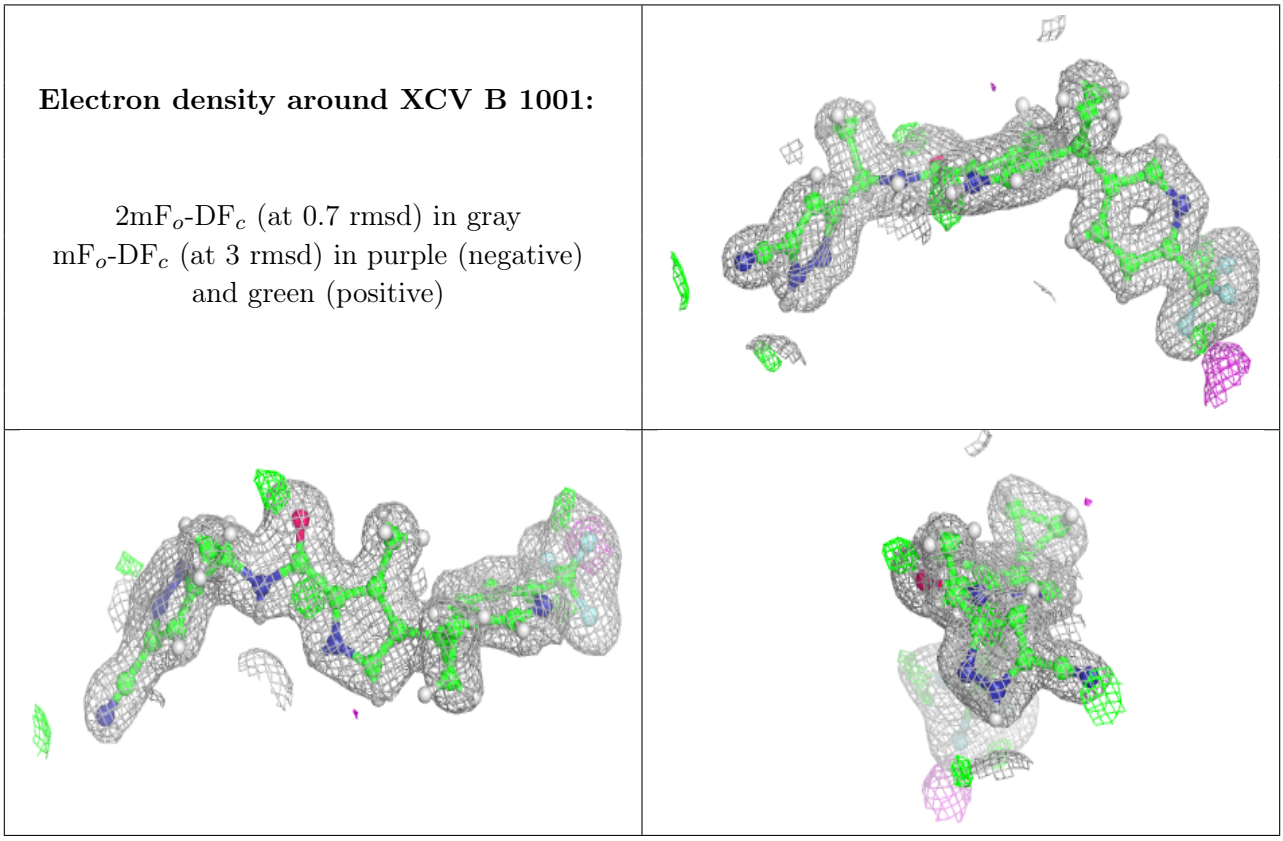
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	XCV	B	1001	31/31	0.94	0.09	16,20,25,26	0
4	ORO	A	1003	11/11	0.95	0.08	10,16,18,19	0
4	ORO	B	1003	11/11	0.95	0.08	9,15,18,19	0
2	XCV	A	1001	31/31	0.96	0.07	12,17,21,25	0
3	FMN	A	1002	31/31	0.98	0.13	6,9,12,12	0
3	FMN	B	1002	31/31	0.98	0.12	7,10,14,17	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.

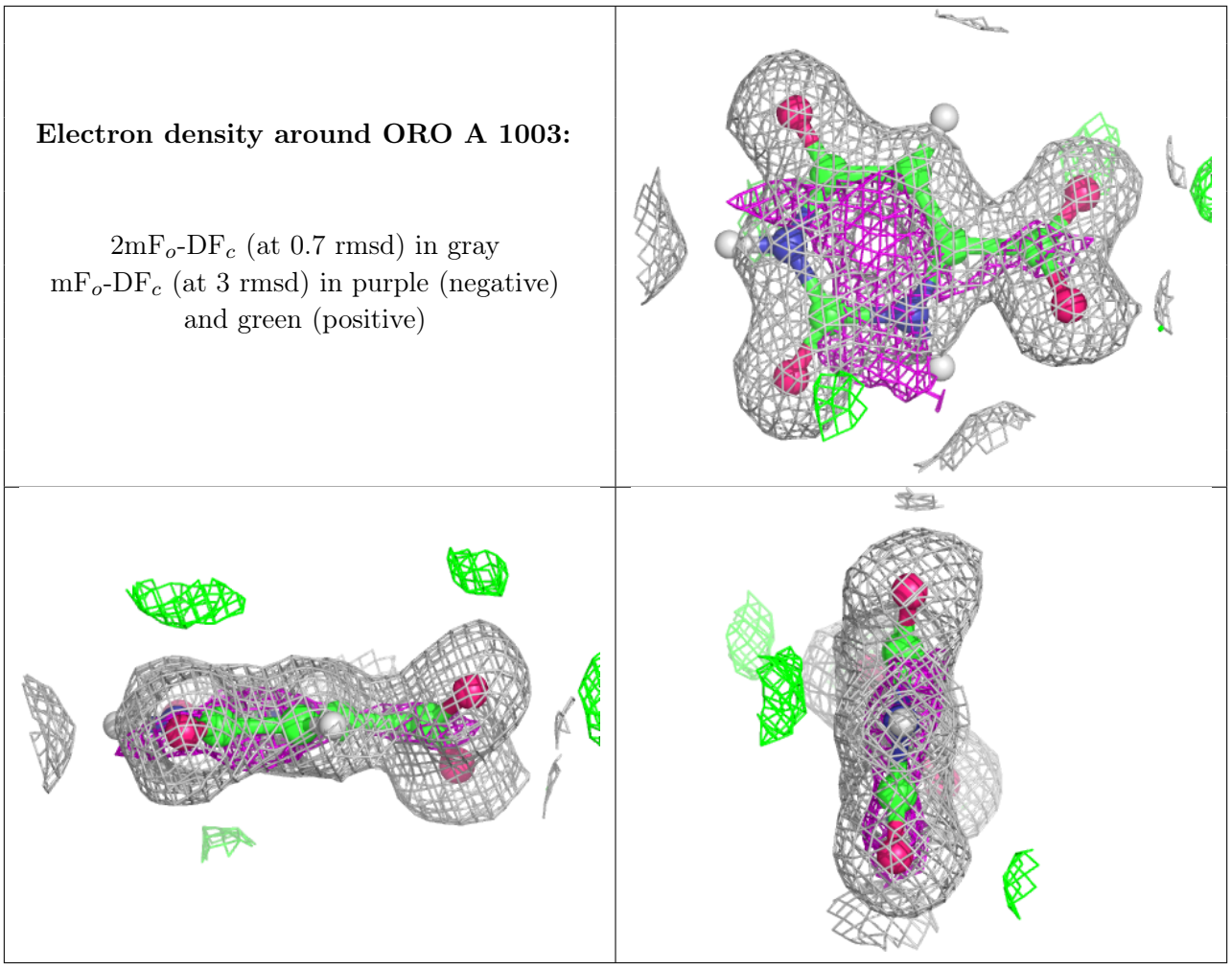
Electron density around XCV B 1001:

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



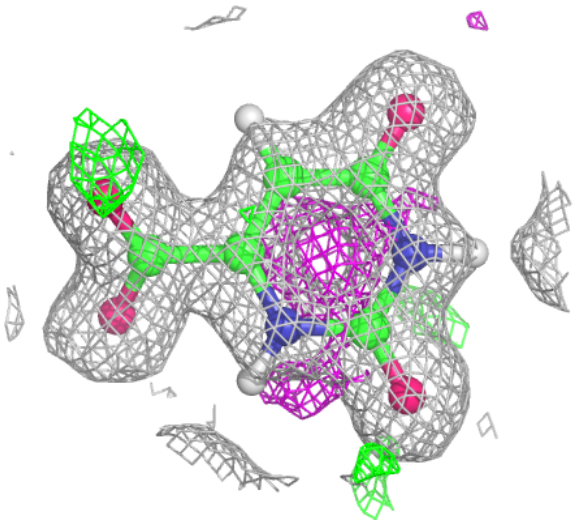
Electron density around ORO A 1003:

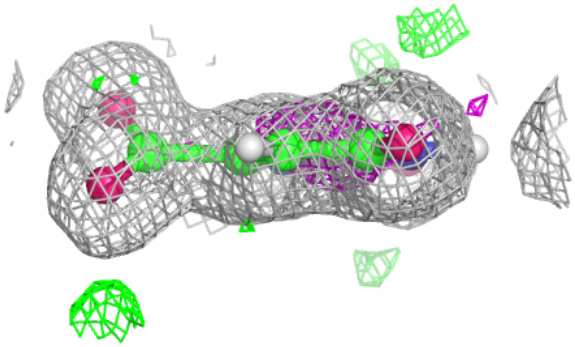
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

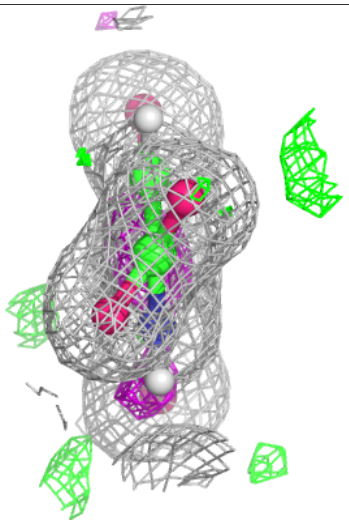


Electron density around ORO B 1003:

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

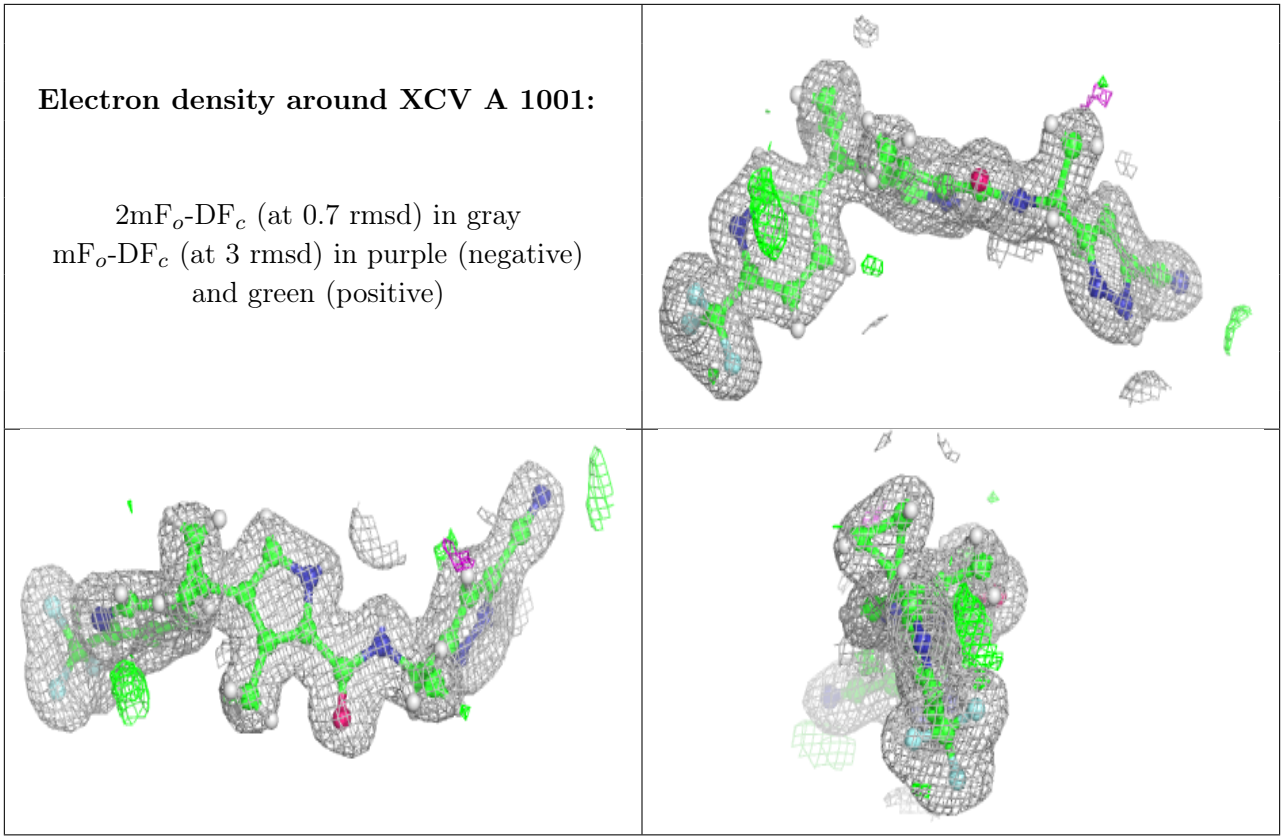






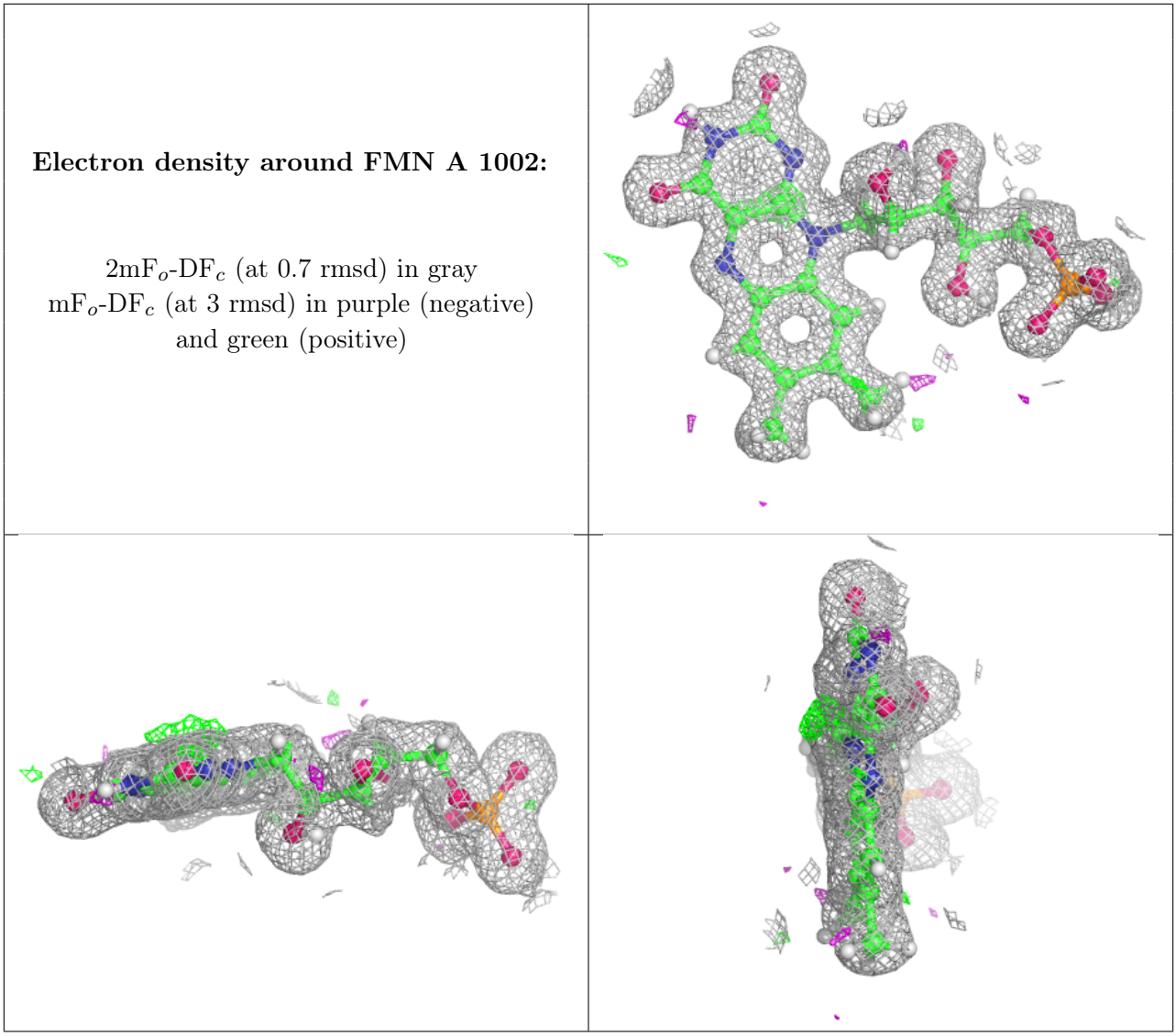
Electron density around XCV A 1001:

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



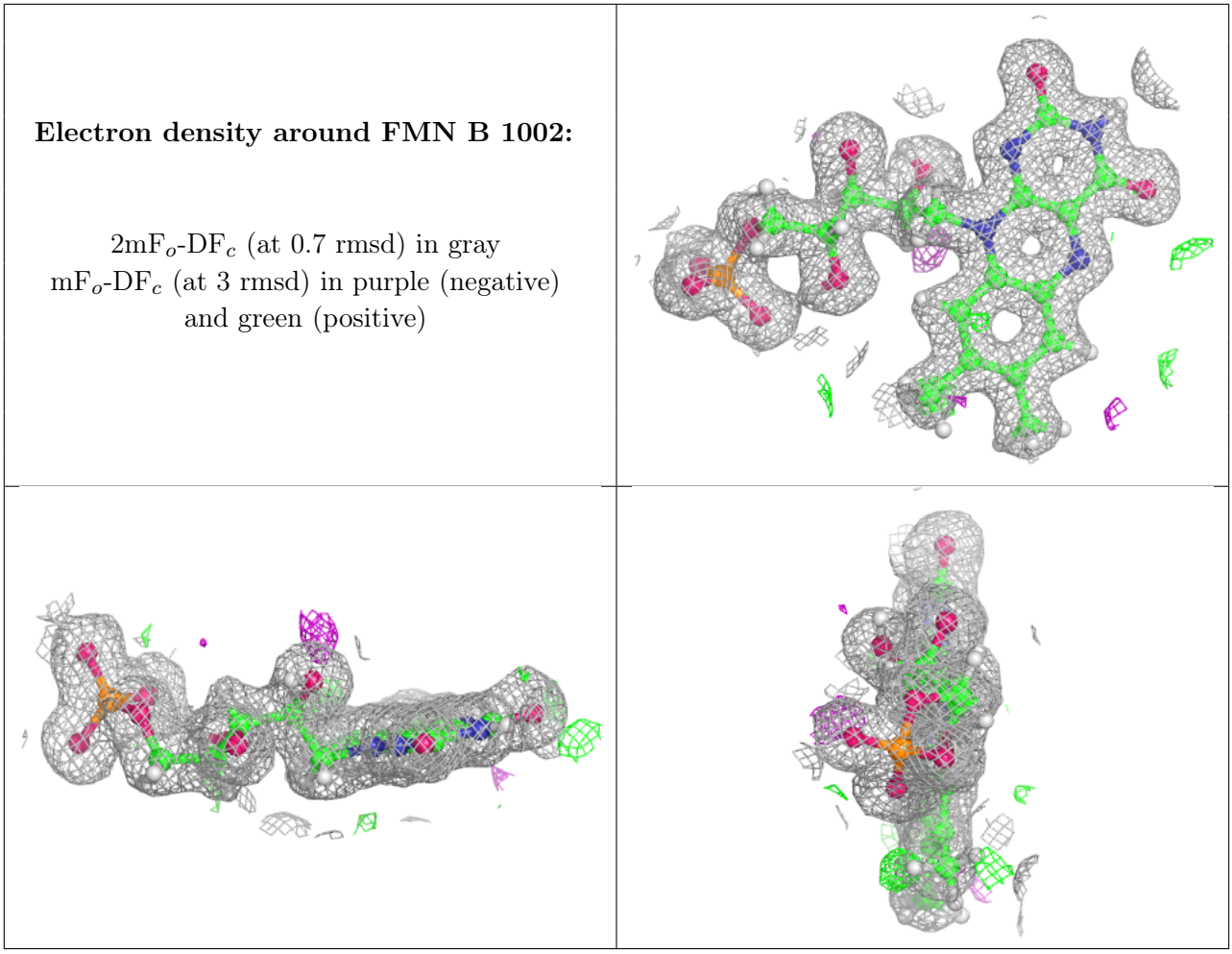
Electron density around FMN A 1002:

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



Electron density around 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

There are no such residues in this entry.