wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2023 – 04:10 PM JST

PDB ID	:	4TMC
Title	:	CRYSTAL STRUCTURE of OLD YELLOW ENZYME from CANDIDA MACEDONIENSIS AKU4588 COMPLEXED with P-HYDROXYBENZALDEHYDE
Authors	:	Horita, S.; Kataoka, M.; Kitamura, N.; Nakagawa, T.; Miyakawa, T.; Ohtsuka, J.; Nagata, K.; Shimizu, S.; Tanokura, M.
Deposited on	:	2014-05-31
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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:

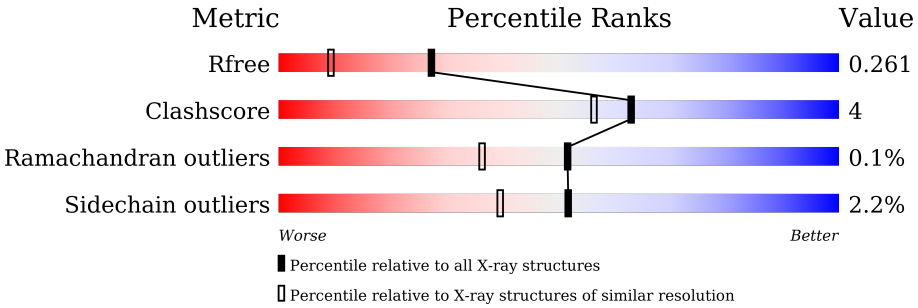
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Mol	Chain	Length	Quality of chain
1	A	403	89% 9% ••
1	B	403	87% 11% •
1	C	403	89% 9% ••
1	D	403	84% 12% • •

2 Entry composition (i)

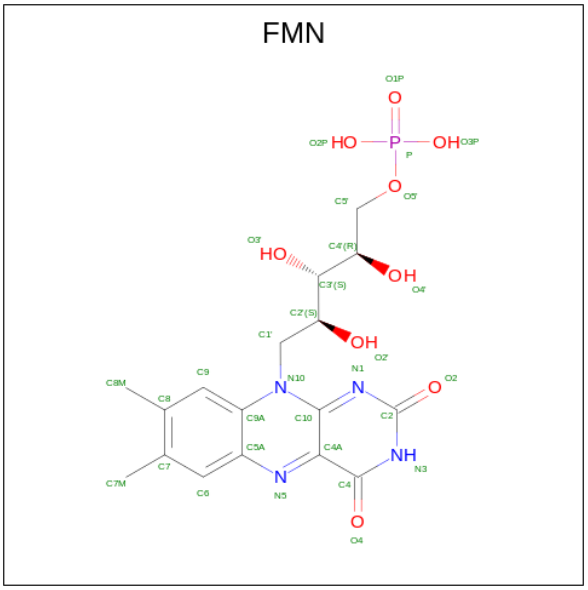
There are 4 unique types of molecules in this entry. The entry contains 14010 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Old yellow enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3209	2055	543	605	6			
1	B	398	Total	C	N	O	S	0	0	0
			3200	2050	542	602	6			
1	C	399	Total	C	N	O	S	0	0	0
			3209	2055	543	605	6			
1	D	396	Total	C	N	O	S	0	0	0
			3182	2038	538	600	6			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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		

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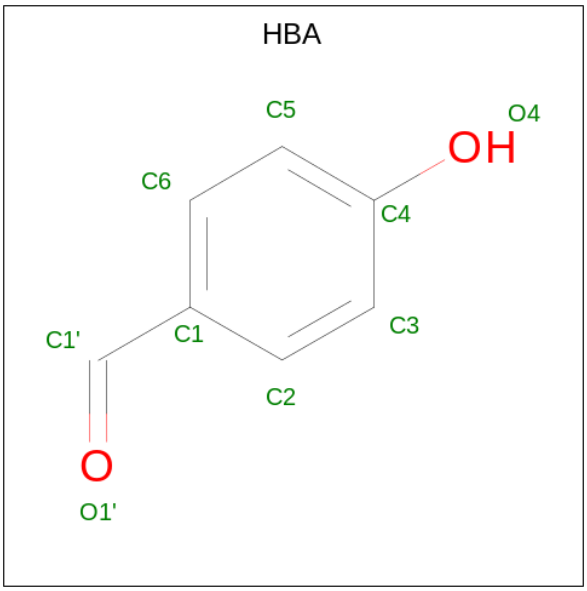
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 31 17 4 9 1	0	0
2	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 3 is P-HYDROXYBENZALDEHYDE (three-letter code: HBA) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0
3	C	1	Total C O 9 7 2	0	0
3	D	1	Total C O 9 7 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	310	Total O 310 310	0	0
4	B	254	Total O 254 254	0	0
4	C	280	Total O 280 280	0	0

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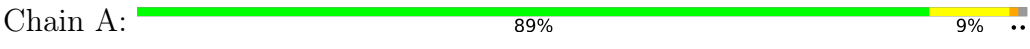
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	206	206	206	0	0

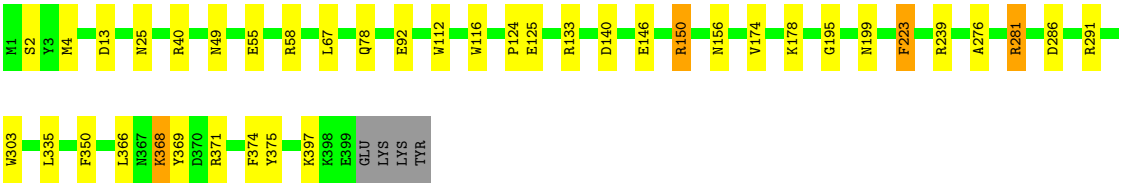
3 Residue-property plots (i)

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. 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. 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: Old yellow enzyme

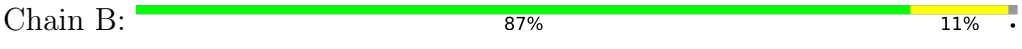
Chain A:

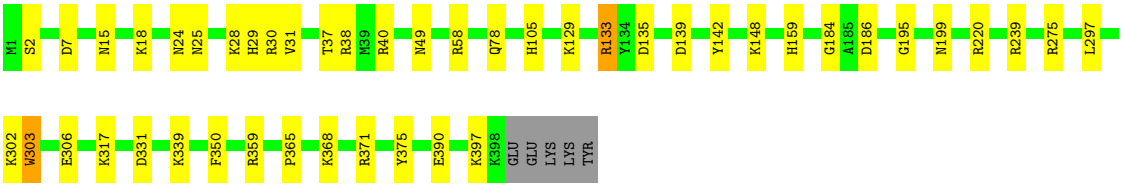




• Molecule 1: Old yellow enzyme

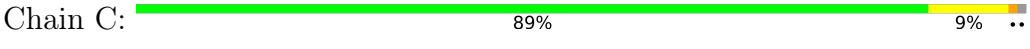
Chain B:

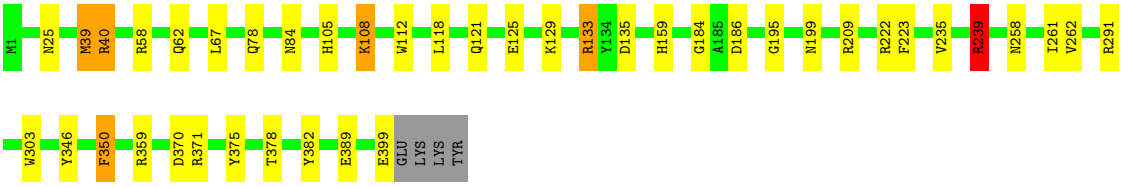




• Molecule 1: Old yellow enzyme

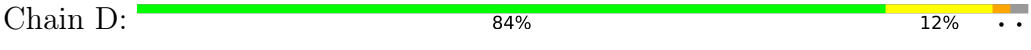
Chain C:

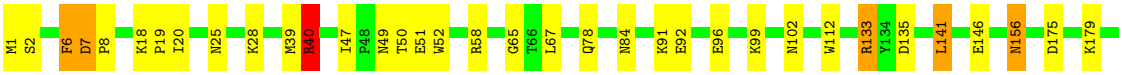


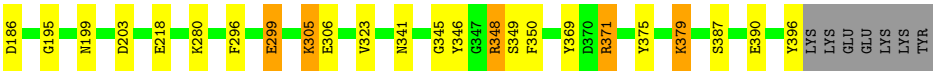


• Molecule 1: Old yellow enzyme

Chain D:






D186
G195
N199
D203
E218
K280
F296
E299
K305
E306
V323
N341
G345
Y346
G347
R348
S349
F350
Y369
D370
R371
Y375
K379
S387
E390
Y396
LYS
LYS
GLU
GLU
LYS
LYS
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.39Å 151.03Å 199.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 1.80 19.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.95-1.80) 99.8 (19.95-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.167 , 0.205 0.240 , 0.261	Depositor DCC
R_{free} test set	7378 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.2	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	0.93	EDS
Total number of atoms	14010	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: HBA, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.97	2/3293 (0.1%)	1.03	9/4463 (0.2%)
1	B	0.97	2/3284 (0.1%)	1.06	19/4451 (0.4%)
1	C	0.95	2/3293 (0.1%)	1.18	21/4463 (0.5%)
1	D	0.89	3/3266 (0.1%)	1.05	13/4429 (0.3%)
All	All	0.94	9/13136 (0.1%)	1.08	62/17806 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	GLU	CD-OE1	9.07	1.35	1.25
1	D	218	GLU	CD-OE1	7.03	1.33	1.25
1	D	218	GLU	CD-OE2	6.57	1.32	1.25
1	B	133	ARG	CD-NE	-6.40	1.35	1.46
1	B	239	ARG	CD-NE	-6.33	1.35	1.46

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	40	ARG	NE-CZ-NH1	24.27	132.43	120.30
1	C	40	ARG	NE-CZ-NH2	-22.28	109.16	120.30
1	B	133	ARG	NE-CZ-NH2	-20.77	109.91	120.30
1	D	40	ARG	NE-CZ-NH2	-18.41	111.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	40	ARG	NE-CZ-NH1	17.81	129.21	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1	MET	Peptide

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	3209	0	3138	27	0
1	B	3200	0	3132	26	0
1	C	3209	0	3138	24	0
1	D	3182	0	3106	35	0
2	A	31	0	19	2	0
2	B	31	0	19	2	0
2	C	31	0	19	0	0
2	D	31	0	19	3	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
3	C	9	0	5	0	0
3	D	9	0	5	0	0
4	A	310	0	0	1	0
4	B	254	0	0	3	0
4	C	280	0	0	1	0
4	D	206	0	0	5	0
All	All	14010	0	12610	111	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 4.

The worst 5 of 111 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:4:MET:HE3	1:A:366:LEU:HB2	1.37	1.07
1:B:368:LYS:HG3	4:B:823:HOH:O	1.52	1.07
1:D:371:ARG:NH2	4:D:641:HOH:O	2.01	0.93
1:A:55:GLU:HG2	4:A:673:HOH:O	1.75	0.87
1:A:4:MET:CE	1:A:366:LEU:HB2	2.06	0.85

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	397/403 (98%)	386 (97%)	11 (3%)	0	100	100
1	B	396/403 (98%)	382 (96%)	14 (4%)	0	100	100
1	C	397/403 (98%)	385 (97%)	12 (3%)	0	100	100
1	D	394/403 (98%)	379 (96%)	14 (4%)	1 (0%)	41	27
All	All	1584/1612 (98%)	1532 (97%)	51 (3%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	6	PHE

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	336/340 (99%)	330 (98%)	6 (2%)	59	48
1	B	335/340 (98%)	328 (98%)	7 (2%)	53	42
1	C	336/340 (99%)	332 (99%)	4 (1%)	71	65
1	D	333/340 (98%)	320 (96%)	13 (4%)	32	17
All	All	1340/1360 (98%)	1310 (98%)	30 (2%)	52	39

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	GLN
1	D	350	PHE
1	D	2	SER
1	D	396	TYR
1	D	156	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	25	ASN
1	C	155	ASN
1	D	332	GLN
1	C	78	GLN
1	C	199	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	HBA	A	502	-	9,9,9	0.69	0	11,11,11	1.42	1 (9%)
2	FMN	B	501	-	33,33,33	1.87	8 (24%)	48,50,50	1.67	12 (25%)
2	FMN	C	501	-	33,33,33	1.16	2 (6%)	48,50,50	1.59	11 (22%)
3	HBA	D	502	-	9,9,9	0.86	0	11,11,11	1.11	1 (9%)
3	HBA	C	502	-	9,9,9	0.95	0	11,11,11	0.99	0
2	FMN	D	501	-	33,33,33	1.65	8 (24%)	48,50,50	1.35	9 (18%)
2	FMN	A	501	-	33,33,33	1.73	7 (21%)	48,50,50	1.64	11 (22%)
3	HBA	B	502	-	9,9,9	0.97	0	11,11,11	1.05	0

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	HBA	A	502	-	-	0/2/2/2	0/1/1/1
2	FMN	B	501	-	-	1/18/18/18	0/3/3/3
2	FMN	C	501	-	-	2/18/18/18	0/3/3/3
3	HBA	D	502	-	-	0/2/2/2	0/1/1/1
3	HBA	C	502	-	-	0/2/2/2	0/1/1/1
2	FMN	D	501	-	-	1/18/18/18	0/3/3/3
2	FMN	A	501	-	-	1/18/18/18	0/3/3/3
3	HBA	B	502	-	-	0/2/2/2	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	FMN	C9A-C5A	5.29	1.50	1.41
2	B	501	FMN	C1'-C2'	4.84	1.59	1.52
2	A	501	FMN	C5'-C4'	4.38	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FMN	C4A-N5	3.89	1.38	1.30
2	B	501	FMN	C8-C7	3.56	1.49	1.40

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	FMN	O2-C2-N1	-5.22	113.18	121.83
2	A	501	FMN	O2'-C2'-C1'	4.02	119.52	109.80
2	A	501	FMN	C9A-C5A-N5	-3.65	118.46	122.43
2	C	501	FMN	C7M-C7-C6	3.50	125.96	119.49
3	A	502	HBA	O1'-C1'-C1	-3.45	113.40	124.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FMN	C4'-C5'-O5'-P
2	D	501	FMN	C4'-C5'-O5'-P
2	C	501	FMN	C2'-C3'-C4'-O4'
2	C	501	FMN	C4'-C5'-O5'-P
2	B	501	FMN	C4'-C5'-O5'-P

There are no ring outliers.

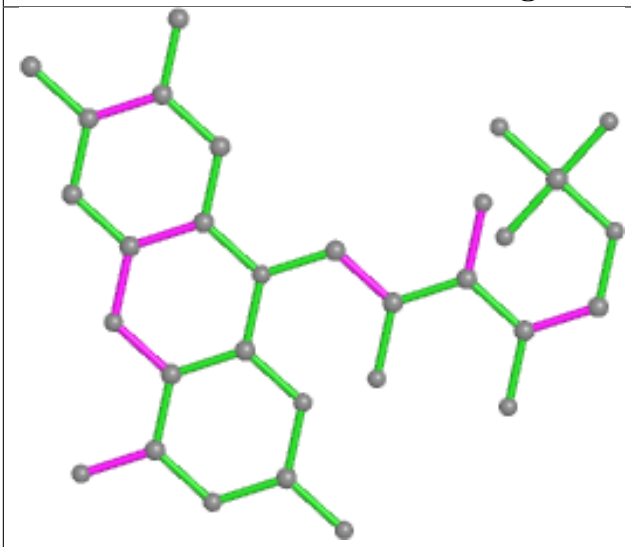
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	FMN	2	0
2	D	501	FMN	3	0
2	A	501	FMN	2	0

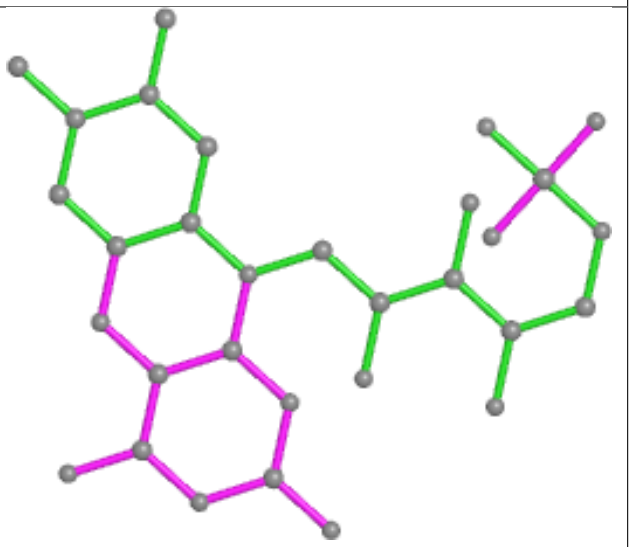
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

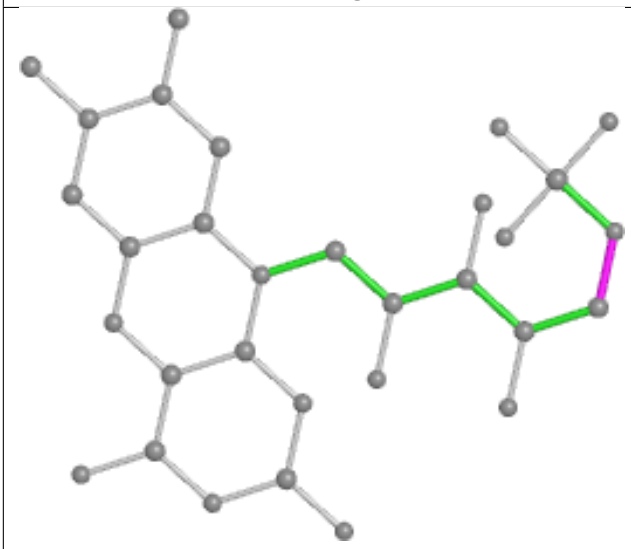
Ligand FMN B 501



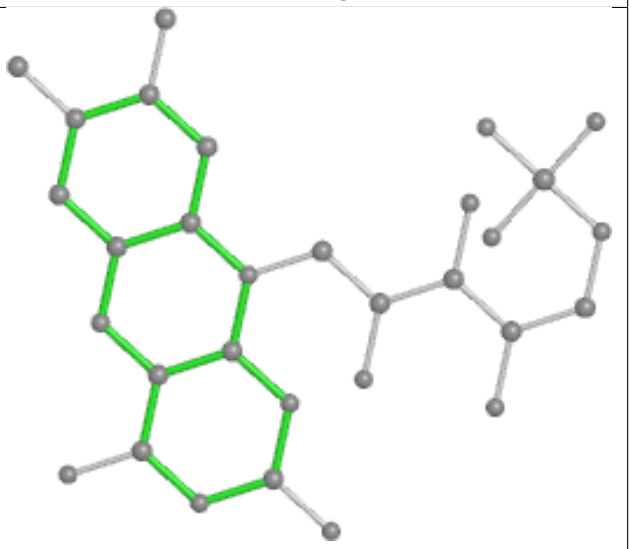
Bond lengths



Bond angles

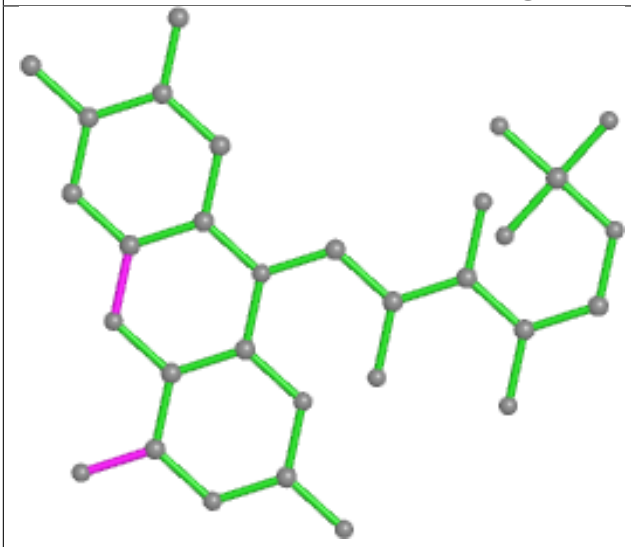


Torsions

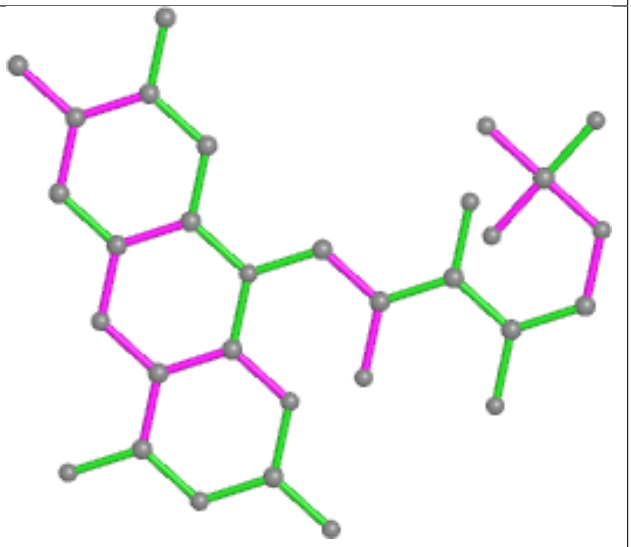


Rings

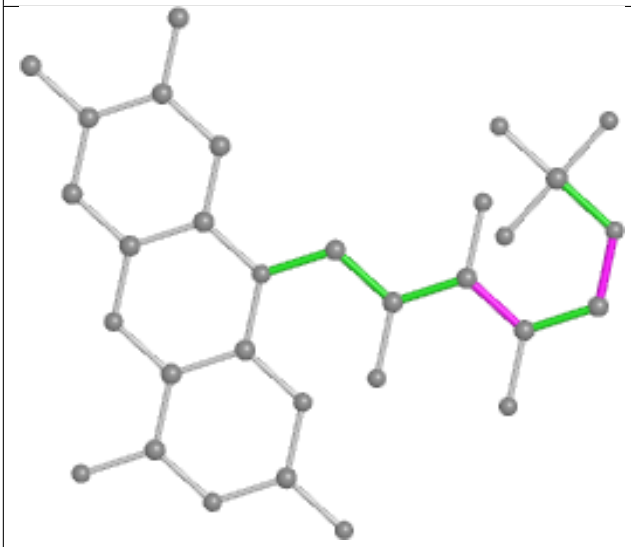
Ligand FMN C 501



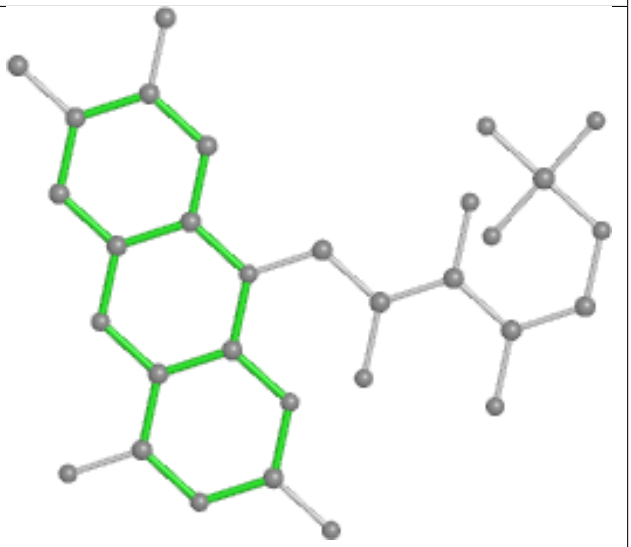
Bond lengths



Bond angles

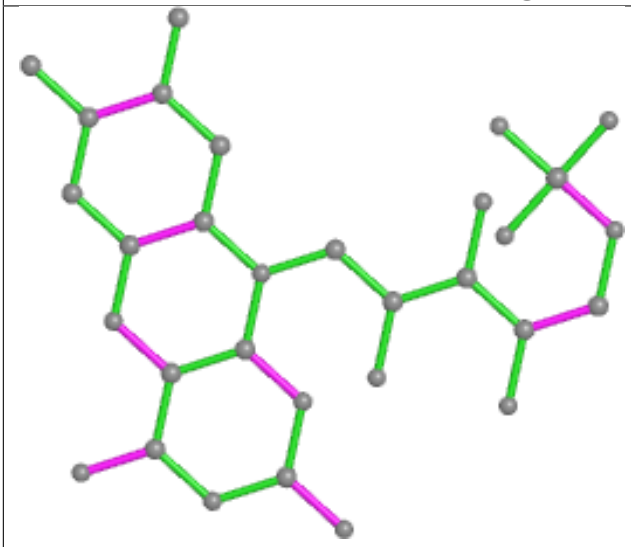


Torsions

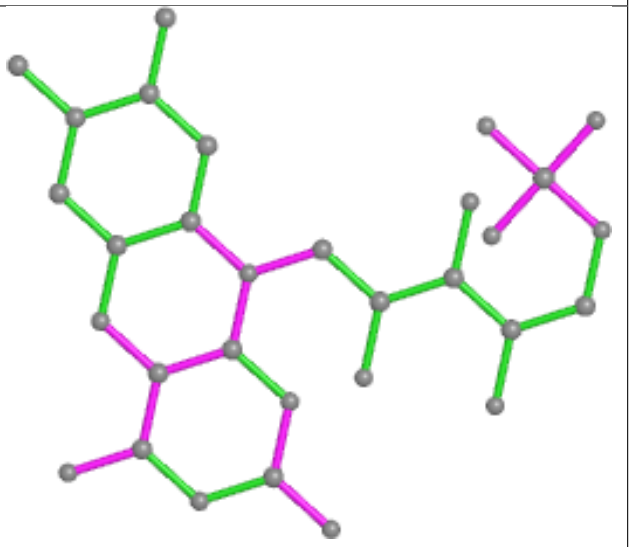


Rings

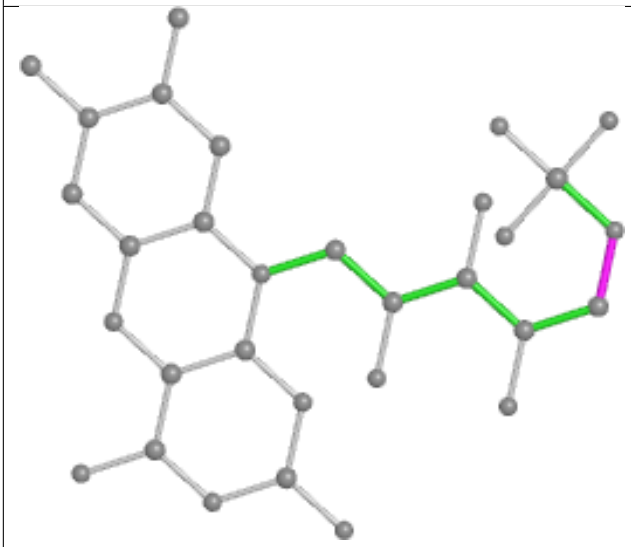
Ligand FMN D 501



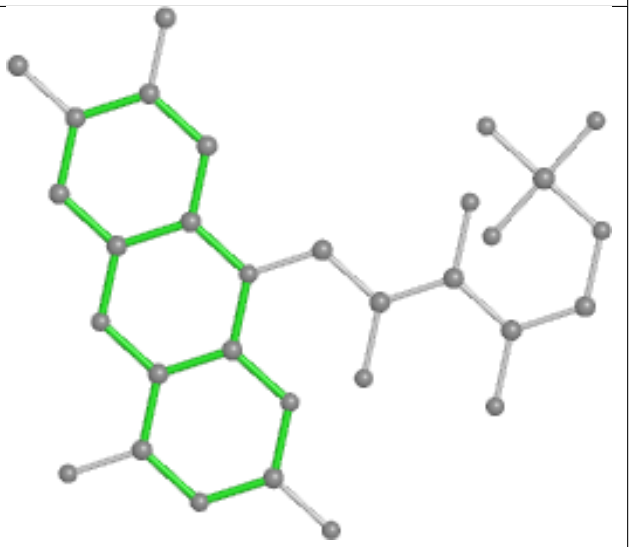
Bond lengths



Bond angles

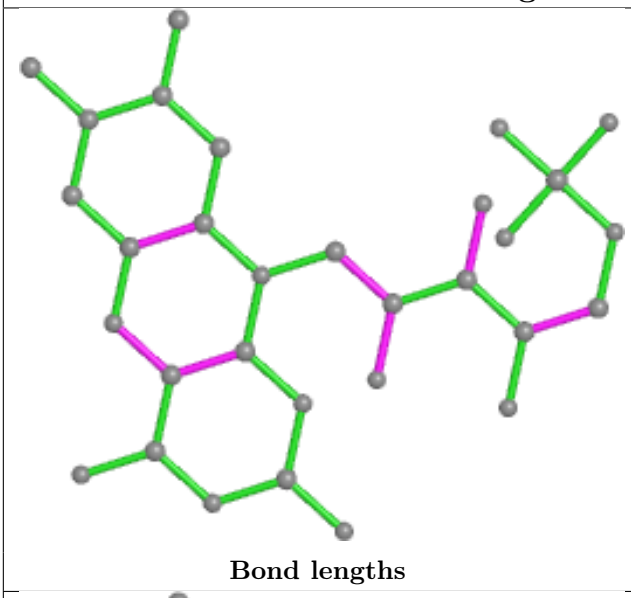


Torsions

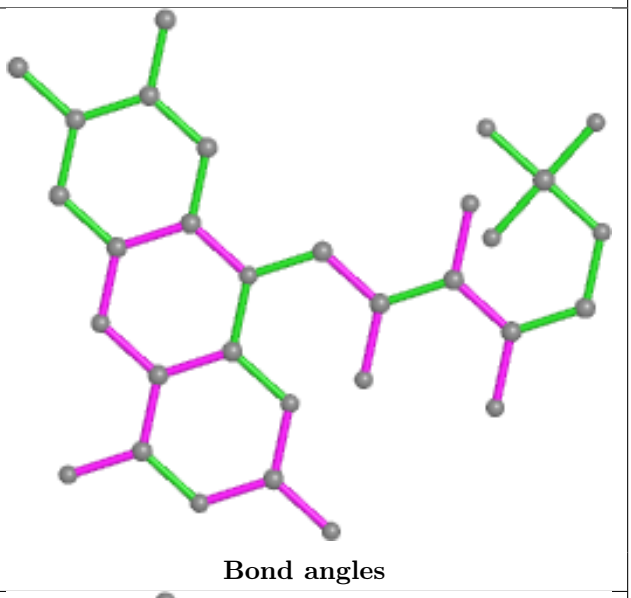


Rings

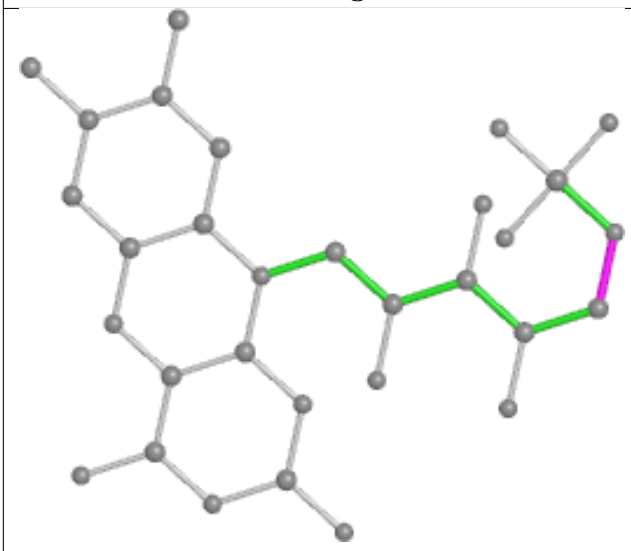
Ligand FMN A 501



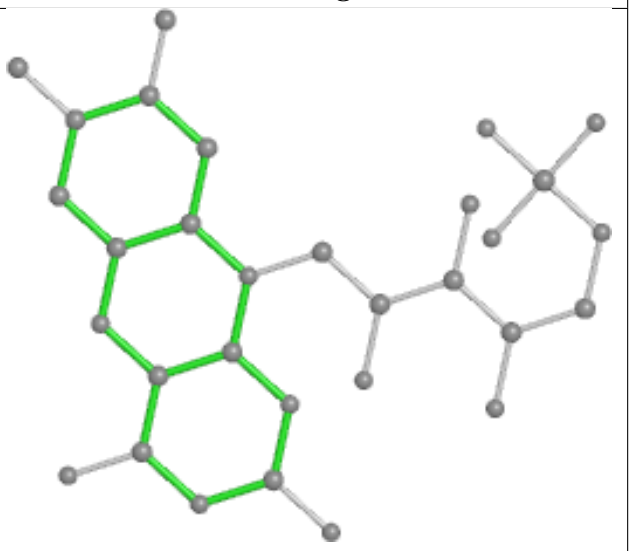
Bond lengths



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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

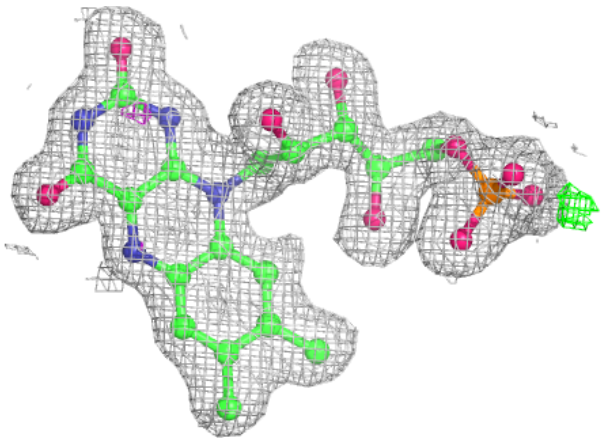
6.4 Ligands

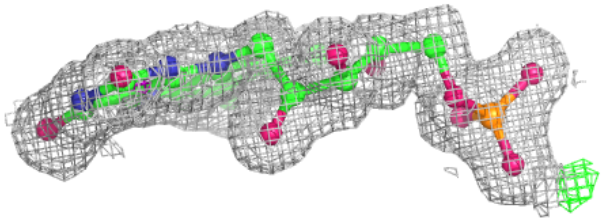
Unable to reproduce the depositors R factor - this section is therefore empty.

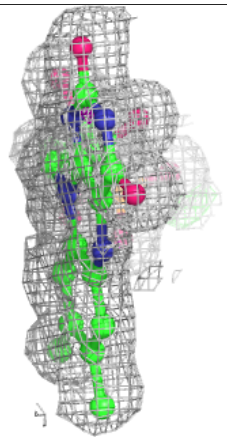
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FMN A 501:

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

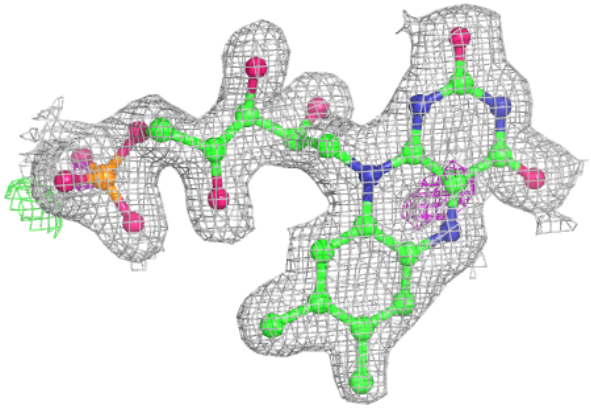


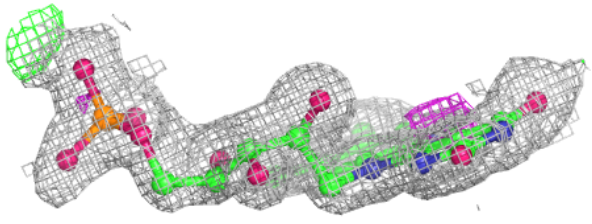


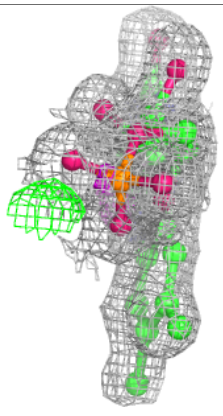


Electron density around FMN B 501:

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

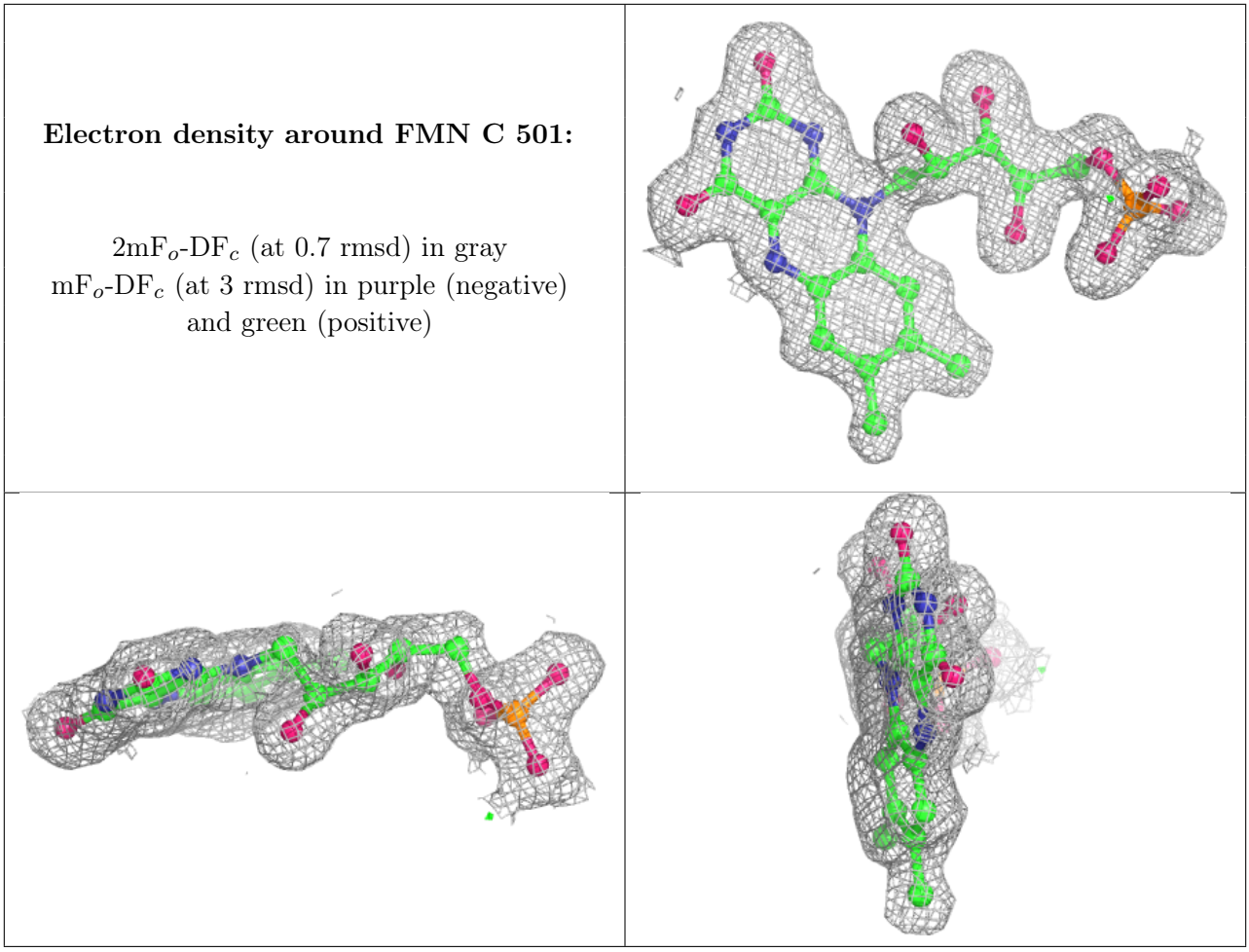






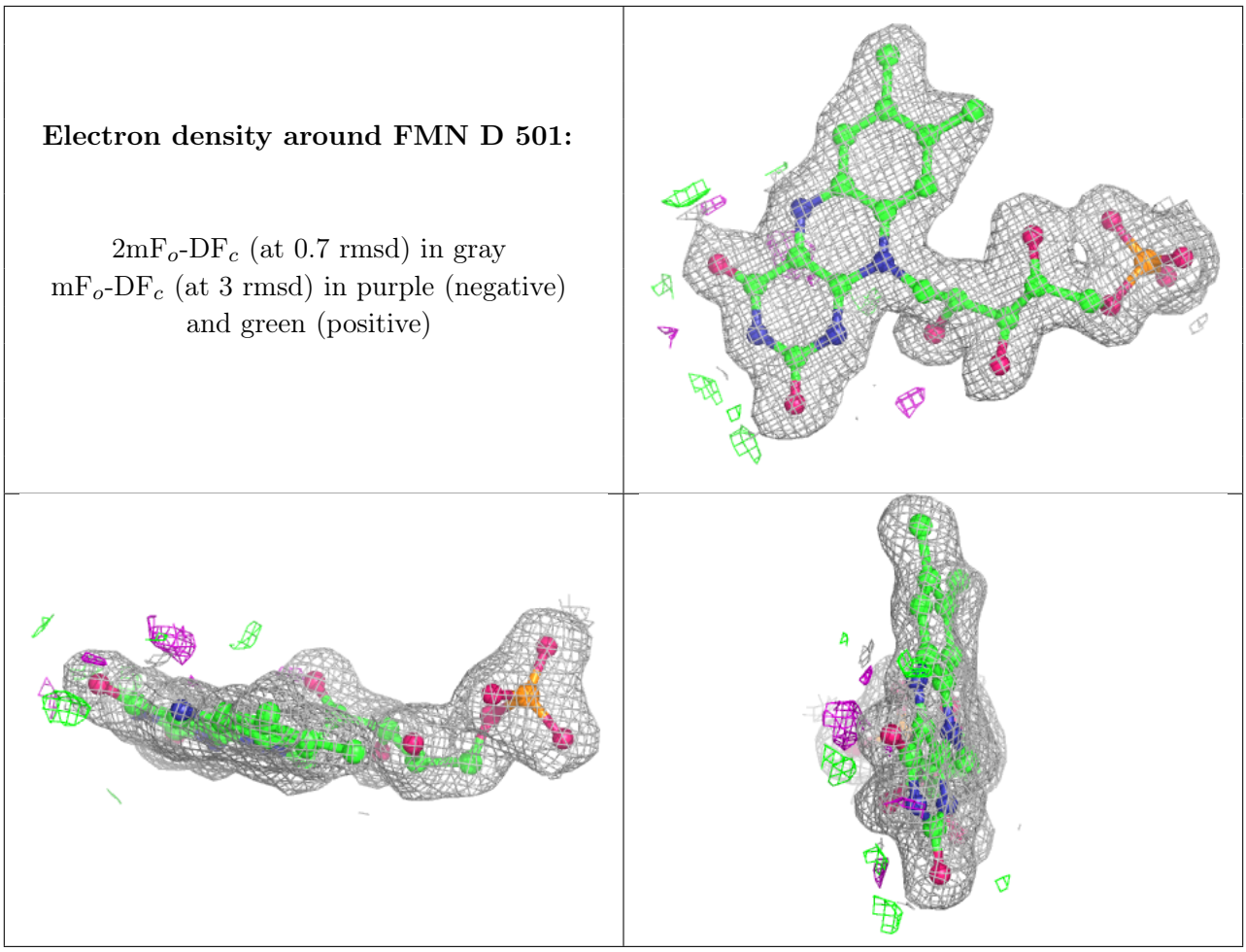
Electron density around FMN C 501:

$2mF_o$-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 501:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.