



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 08:42 pm BST

PDB ID : 2Y6Q
Title : Structure of the TetX monooxygenase in complex with the substrate 7- Iodetracycline
Authors : Volkers, G.; Palm, G.J.; Weiss, M.S.; Wright, G.D.; Hinrichs, W.
Deposited on : 2011-01-25
Resolution : 2.37 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 ⓘ symbol.

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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

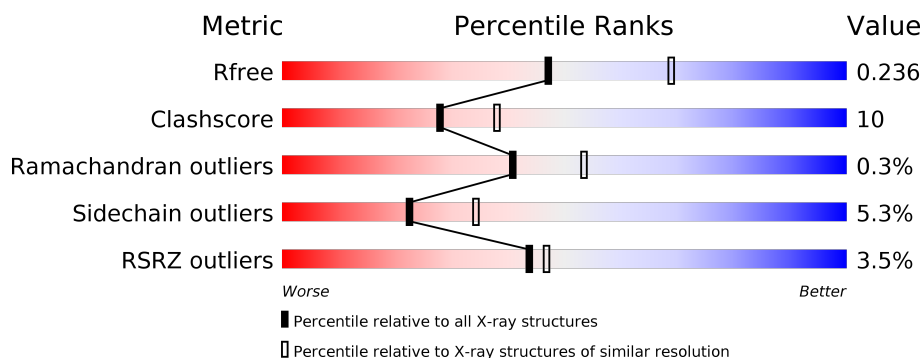
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	398	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>••</div> <div>8%</div> </div> </div>
1	B	398	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	398	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	398	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>••</div> <div>8%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11961 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 TETX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	2	0
			2865	1817	483	553	12			
1	B	368	Total	C	N	O	S	0	2	0
			2863	1816	482	553	12			
1	C	367	Total	C	N	O	S	0	0	0
			2828	1793	476	547	12			
1	D	365	Total	C	N	O	S	0	0	0
			2812	1782	473	545	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q93L51
A	-8	GLY	-	expression tag	UNP Q93L51
A	-7	SER	-	expression tag	UNP Q93L51
A	-6	SER	-	expression tag	UNP Q93L51
A	-5	HIS	-	expression tag	UNP Q93L51
A	-4	HIS	-	expression tag	UNP Q93L51
A	-3	HIS	-	expression tag	UNP Q93L51
A	-2	HIS	-	expression tag	UNP Q93L51
A	-1	HIS	-	expression tag	UNP Q93L51
A	0	HIS	-	expression tag	UNP Q93L51
A	1	SER	-	expression tag	UNP Q93L51
A	2	SER	-	expression tag	UNP Q93L51
A	3	GLY	-	expression tag	UNP Q93L51
A	4	LEU	-	expression tag	UNP Q93L51
A	5	VAL	-	expression tag	UNP Q93L51
A	6	PRO	-	expression tag	UNP Q93L51
A	7	ARG	-	expression tag	UNP Q93L51
A	8	GLY	-	expression tag	UNP Q93L51
A	9	SER	-	expression tag	UNP Q93L51
A	10	HIS	-	expression tag	UNP Q93L51
B	-9	MET	-	expression tag	UNP Q93L51

Continued on next page...

Continued from previous page...

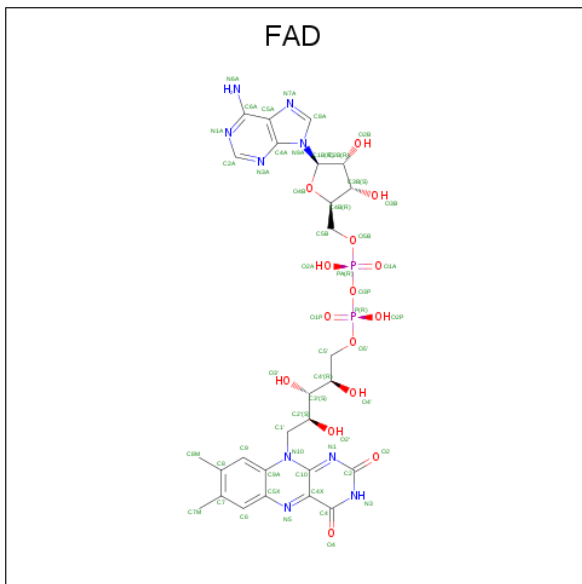
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q93L51
B	-7	SER	-	expression tag	UNP Q93L51
B	-6	SER	-	expression tag	UNP Q93L51
B	-5	HIS	-	expression tag	UNP Q93L51
B	-4	HIS	-	expression tag	UNP Q93L51
B	-3	HIS	-	expression tag	UNP Q93L51
B	-2	HIS	-	expression tag	UNP Q93L51
B	-1	HIS	-	expression tag	UNP Q93L51
B	0	HIS	-	expression tag	UNP Q93L51
B	1	SER	-	expression tag	UNP Q93L51
B	2	SER	-	expression tag	UNP Q93L51
B	3	GLY	-	expression tag	UNP Q93L51
B	4	LEU	-	expression tag	UNP Q93L51
B	5	VAL	-	expression tag	UNP Q93L51
B	6	PRO	-	expression tag	UNP Q93L51
B	7	ARG	-	expression tag	UNP Q93L51
B	8	GLY	-	expression tag	UNP Q93L51
B	9	SER	-	expression tag	UNP Q93L51
B	10	HIS	-	expression tag	UNP Q93L51
C	-9	MET	-	expression tag	UNP Q93L51
C	-8	GLY	-	expression tag	UNP Q93L51
C	-7	SER	-	expression tag	UNP Q93L51
C	-6	SER	-	expression tag	UNP Q93L51
C	-5	HIS	-	expression tag	UNP Q93L51
C	-4	HIS	-	expression tag	UNP Q93L51
C	-3	HIS	-	expression tag	UNP Q93L51
C	-2	HIS	-	expression tag	UNP Q93L51
C	-1	HIS	-	expression tag	UNP Q93L51
C	0	HIS	-	expression tag	UNP Q93L51
C	1	SER	-	expression tag	UNP Q93L51
C	2	SER	-	expression tag	UNP Q93L51
C	3	GLY	-	expression tag	UNP Q93L51
C	4	LEU	-	expression tag	UNP Q93L51
C	5	VAL	-	expression tag	UNP Q93L51
C	6	PRO	-	expression tag	UNP Q93L51
C	7	ARG	-	expression tag	UNP Q93L51
C	8	GLY	-	expression tag	UNP Q93L51
C	9	SER	-	expression tag	UNP Q93L51
C	10	HIS	-	expression tag	UNP Q93L51
D	-9	MET	-	expression tag	UNP Q93L51
D	-8	GLY	-	expression tag	UNP Q93L51
D	-7	SER	-	expression tag	UNP Q93L51

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP Q93L51
D	-5	HIS	-	expression tag	UNP Q93L51
D	-4	HIS	-	expression tag	UNP Q93L51
D	-3	HIS	-	expression tag	UNP Q93L51
D	-2	HIS	-	expression tag	UNP Q93L51
D	-1	HIS	-	expression tag	UNP Q93L51
D	0	HIS	-	expression tag	UNP Q93L51
D	1	SER	-	expression tag	UNP Q93L51
D	2	SER	-	expression tag	UNP Q93L51
D	3	GLY	-	expression tag	UNP Q93L51
D	4	LEU	-	expression tag	UNP Q93L51
D	5	VAL	-	expression tag	UNP Q93L51
D	6	PRO	-	expression tag	UNP Q93L51
D	7	ARG	-	expression tag	UNP Q93L51
D	8	GLY	-	expression tag	UNP Q93L51
D	9	SER	-	expression tag	UNP Q93L51
D	10	HIS	-	expression tag	UNP Q93L51

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



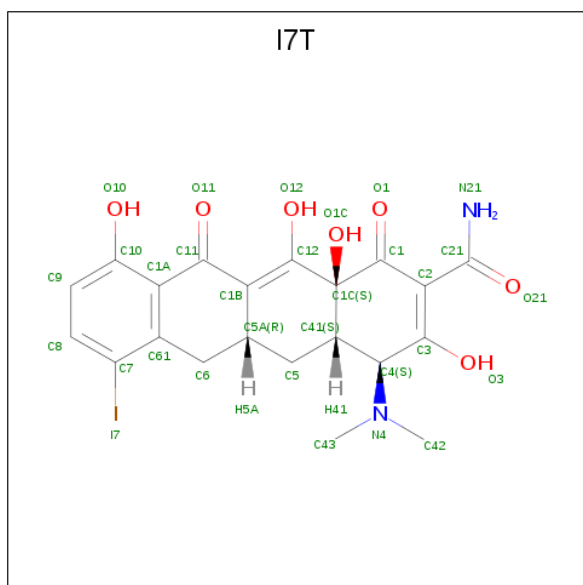
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 7-iodotetracycline (three-letter code: I7T) (formula: $C_{21}H_{21}IN_2O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	0	0
			31	21	1	2	7		
3	B	1	Total	C	I	N	O	0	0
			31	21	1	2	7		
3	C	1	Total	C	I	N	O	0	0
			31	21	1	2	7		
3	D	1	Total	C	I	N	O	0	0
			31	21	1	2	7		

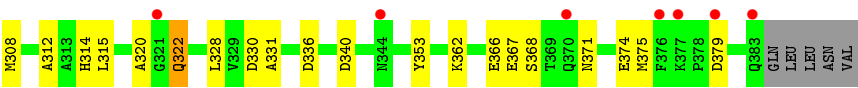
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



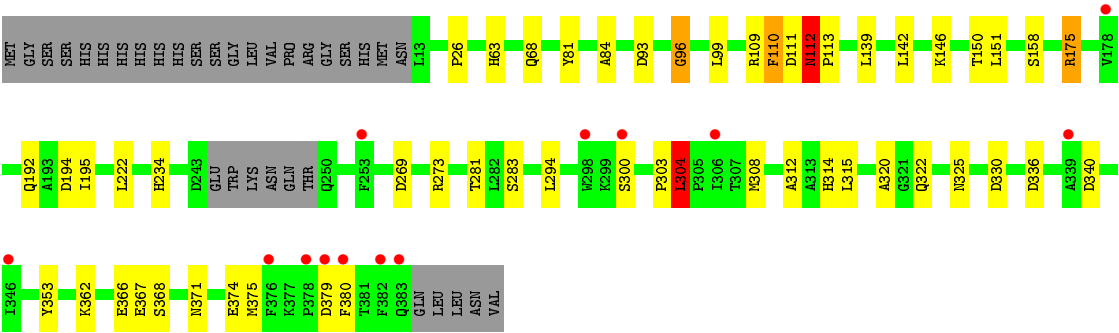
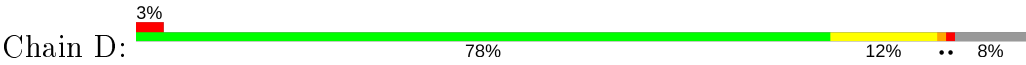
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total 61	O 61	0	0
5	B	55	Total 55	O 55	0	0
5	C	47	Total 47	O 47	0	0
5	D	34	Total 34	O 34	0	0



● Molecule 1: TETX2 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.70 Å 79.96 Å 88.00 Å 111.10° 90.41° 92.96°	Depositor
Resolution (Å)	51.98 – 2.37 51.92 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.5 (51.98-2.37) 74.7 (51.92-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.37 Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.218 , 0.238 0.218 , 0.236	Depositor DCC
R_{free} test set	2623 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11961	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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: I7T, SO4, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.06	4/2929 (0.1%)	0.92	3/3973 (0.1%)
1	B	1.02	3/2927 (0.1%)	0.89	5/3971 (0.1%)
1	C	0.87	3/2886 (0.1%)	0.85	5/3919 (0.1%)
1	D	0.85	1/2868 (0.0%)	0.84	3/3893 (0.1%)
All	All	0.96	11/11610 (0.1%)	0.88	16/15756 (0.1%)

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	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	9

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	GLY	N-CA	5.69	1.54	1.46
1	B	322[A]	GLN	C-O	5.68	1.34	1.23
1	B	322[B]	GLN	C-O	5.68	1.34	1.23
1	A	363	GLU	CG-CD	5.61	1.60	1.51
1	D	96	GLY	N-CA	5.60	1.54	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	D	304	LEU	CB-CG-CD1	7.27	123.36	111.00
1	D	175	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	175	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	121	ARG	NE-CZ-NH2	-6.67	116.96	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ASN	Peptide
1	A	94	GLU	Peptide
1	B	109	ARG	Peptide
1	B	112	ASN	Peptide
1	B	94	GLU	Peptide

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	2865	0	2752	90	0
1	B	2863	0	2745	60	0
1	C	2828	0	2688	48	0
1	D	2812	0	2685	36	0
2	A	53	0	31	5	0
2	B	53	0	30	2	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	31	0	18	4	0
3	B	31	0	18	4	0
3	C	31	0	18	2	0
3	D	31	0	18	1	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	61	0	0	15	0
5	B	55	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	47	0	0	6	0
5	D	34	0	0	1	0
All	All	11961	0	11065	227	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 10.

The worst 5 of 227 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:309:ILE:CG1	1:A:309:ILE:CD1	1.75	1.57
1:A:98:ILE:CG2	1:B:359:ILE:HG23	1.62	1.29
1:A:383:GLN:CB	1:B:359:ILE:HD12	1.67	1.24
1:A:383:GLN:CB	1:B:359:ILE:CD1	2.16	1.22
1:B:96:GLY:HA2	5:B:2014:HOH:O	1.38	1.21

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	366/398 (92%)	345 (94%)	19 (5%)	2 (0%)	29	39
1	B	366/398 (92%)	347 (95%)	18 (5%)	1 (0%)	41	53
1	C	363/398 (91%)	343 (94%)	19 (5%)	1 (0%)	41	53
1	D	361/398 (91%)	344 (95%)	16 (4%)	1 (0%)	41	53
All	All	1456/1592 (92%)	1379 (95%)	72 (5%)	5 (0%)	41	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	B	112	ASN
1	C	112	ASN
1	D	112	ASN
1	A	321	GLY

5.3.2 Protein sidechains ⓘ

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	304/345 (88%)	288 (95%)	16 (5%)	22	34
1	B	303/345 (88%)	288 (95%)	15 (5%)	24	37
1	C	296/345 (86%)	281 (95%)	15 (5%)	24	36
1	D	296/345 (86%)	279 (94%)	17 (6%)	20	30
All	All	1199/1380 (87%)	1136 (95%)	63 (5%)	22	34

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	371	ASN
1	C	269	ASP
1	D	353	TYR
1	B	374	GLU
1	C	110	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	250	GLN
1	C	190	ASN
1	D	234	HIS
1	B	370	GLN
1	B	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

20 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	I7T	D	1385	-	33,34,34	1.65	3 (9%)	37,55,55	1.94	13 (35%)
4	SO4	A	1386	-	4,4,4	0.25	0	6,6,6	0.55	0
4	SO4	B	1386	-	4,4,4	0.22	0	6,6,6	0.33	0
2	FAD	B	1384	-	51,58,58	1.74	12 (23%)	60,89,89	2.25	10 (16%)
3	I7T	A	1385	-	33,34,34	1.85	4 (12%)	37,55,55	2.02	12 (32%)
4	SO4	D	1386	-	4,4,4	0.21	0	6,6,6	0.40	0
2	FAD	D	1384	-	51,58,58	1.75	12 (23%)	60,89,89	2.35	15 (25%)
4	SO4	D	1388	-	4,4,4	0.25	0	6,6,6	0.45	0
4	SO4	C	1388	-	4,4,4	0.22	0	6,6,6	0.55	0
4	SO4	A	1387	-	4,4,4	0.20	0	6,6,6	0.40	0
4	SO4	B	1387	-	4,4,4	0.22	0	6,6,6	0.35	0
3	I7T	C	1385	-	33,34,34	1.74	4 (12%)	37,55,55	2.03	12 (32%)
2	FAD	C	1384	-	51,58,58	1.66	10 (19%)	60,89,89	2.28	17 (28%)
4	SO4	C	1387	-	4,4,4	0.14	0	6,6,6	0.32	0
2	FAD	A	1384	-	51,58,58	1.56	9 (17%)	60,89,89	2.25	18 (30%)
3	I7T	B	1385	-	33,34,34	1.89	3 (9%)	37,55,55	1.62	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	1388	-	4,4,4	0.15	0	6,6,6	0.26	0
4	SO4	D	1387	-	4,4,4	0.11	0	6,6,6	0.30	0
4	SO4	C	1386	-	4,4,4	0.13	0	6,6,6	0.30	0
4	SO4	A	1388	-	4,4,4	0.11	0	6,6,6	0.24	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
2	FAD	C	1384	-	-	2/30/50/50	0/6/6/6
2	FAD	B	1384	-	-	8/30/50/50	0/6/6/6
2	FAD	D	1384	-	-	5/30/50/50	0/6/6/6
3	I7T	D	1385	-	-	5/8/66/66	0/4/4/4
3	I7T	C	1385	-	-	1/8/66/66	0/4/4/4
3	I7T	A	1385	-	-	2/8/66/66	0/4/4/4
2	FAD	A	1384	-	-	1/30/50/50	0/6/6/6
3	I7T	B	1385	-	-	3/8/66/66	0/4/4/4

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1385	I7T	C7-I7	-9.04	1.89	2.10
3	A	1385	I7T	C7-I7	-8.45	1.91	2.10
3	C	1385	I7T	C7-I7	-7.80	1.92	2.10
3	D	1385	I7T	C7-I7	-7.52	1.93	2.10
2	A	1384	FAD	C4X-N5	5.79	1.41	1.33

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1384	FAD	C1'-N10-C9A	9.13	125.48	118.29
2	D	1384	FAD	C5'-C4'-C3'	-8.88	95.05	112.20
2	D	1384	FAD	C1'-N10-C9A	8.77	125.19	118.29
2	C	1384	FAD	C5'-C4'-C3'	-8.39	96.00	112.20
2	B	1384	FAD	C4-N3-C2	7.04	121.09	115.14

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1384	FAD	C2'-C3'-C4'-C5'
2	B	1384	FAD	C5'-O5'-P-O2P
2	B	1384	FAD	C5'-O5'-P-O3P
2	D	1384	FAD	C5B-O5B-PA-O1A
3	D	1385	I7T	C41-C4-N4-C43

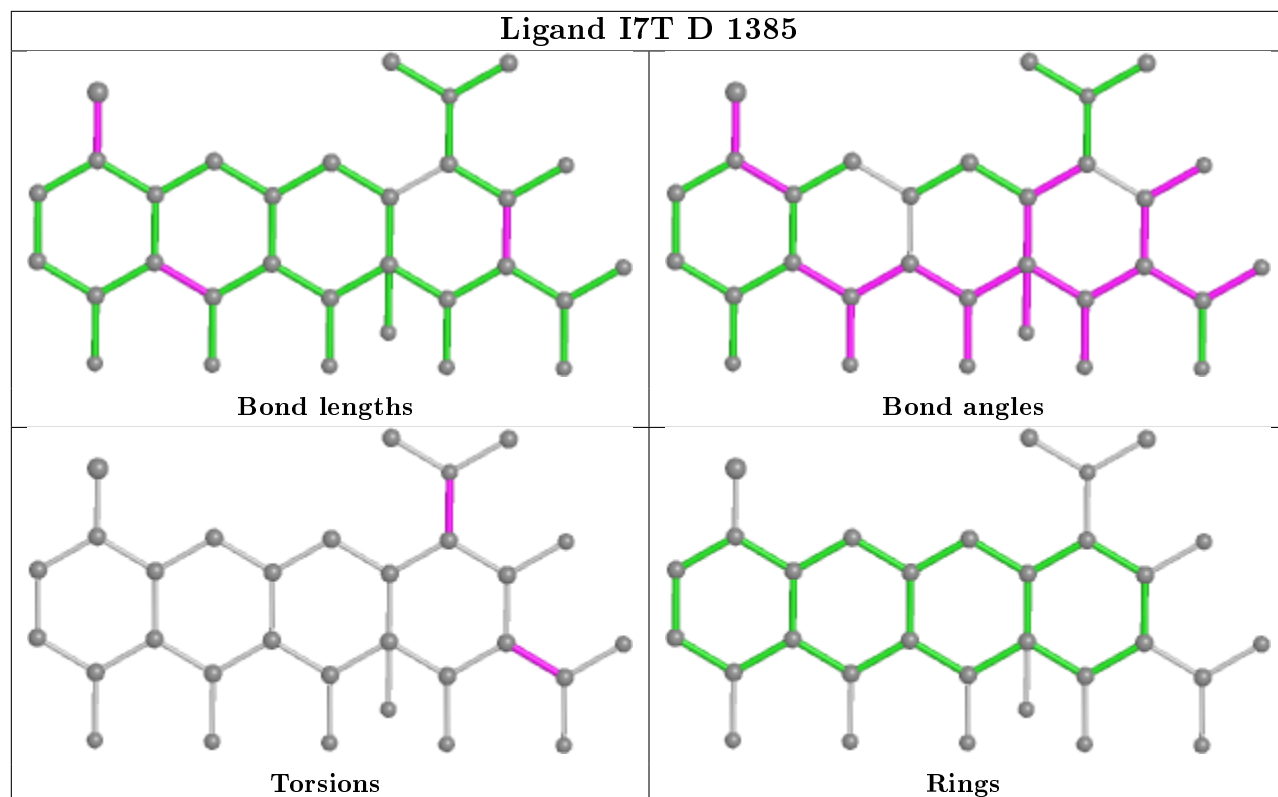
There are no ring outliers.

9 monomers are involved in 16 short contacts:

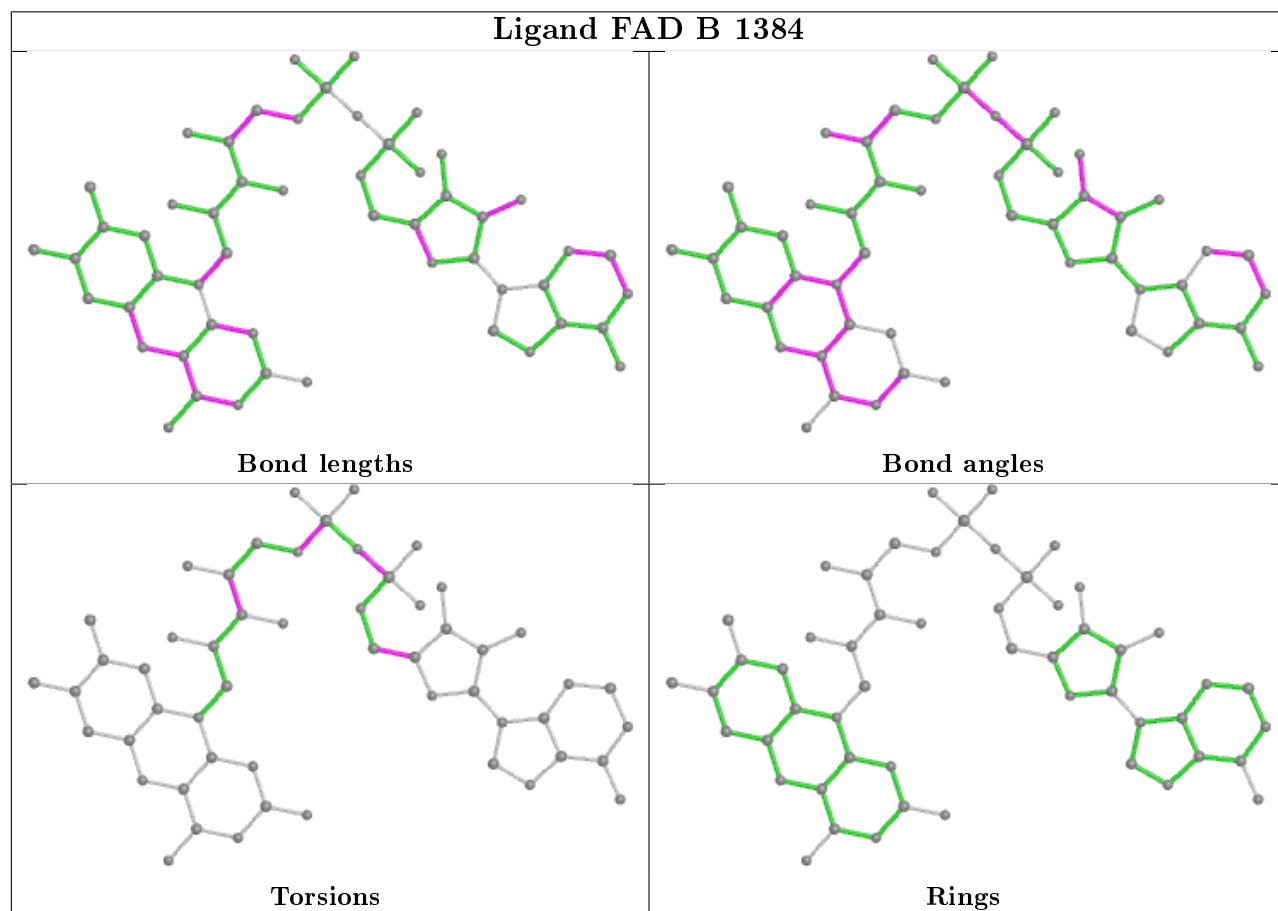
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1385	I7T	1	0
4	A	1386	SO4	1	0
2	B	1384	FAD	2	0
3	A	1385	I7T	4	0
2	D	1384	FAD	1	0
3	C	1385	I7T	2	0
2	C	1384	FAD	1	0
2	A	1384	FAD	5	0
3	B	1385	I7T	4	0

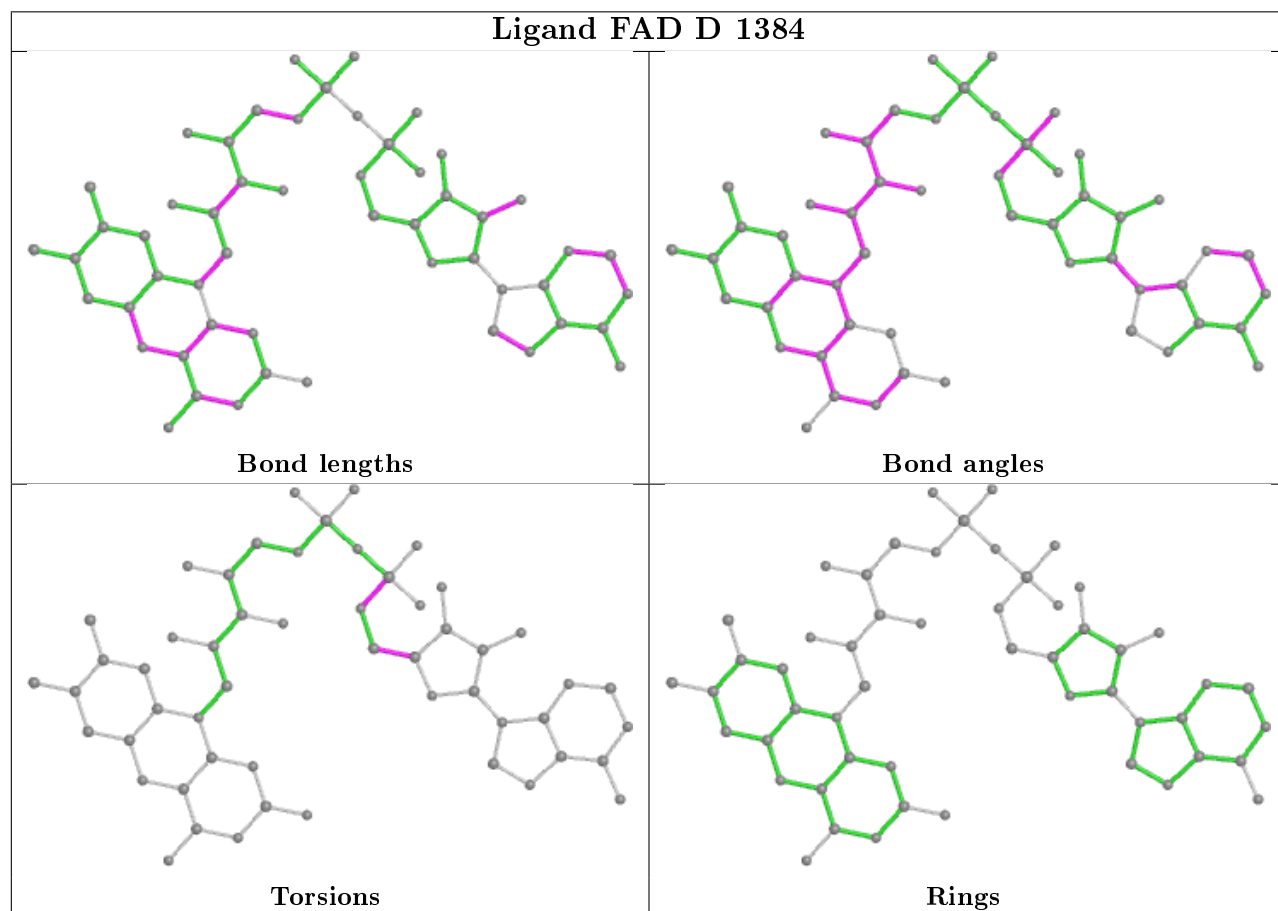
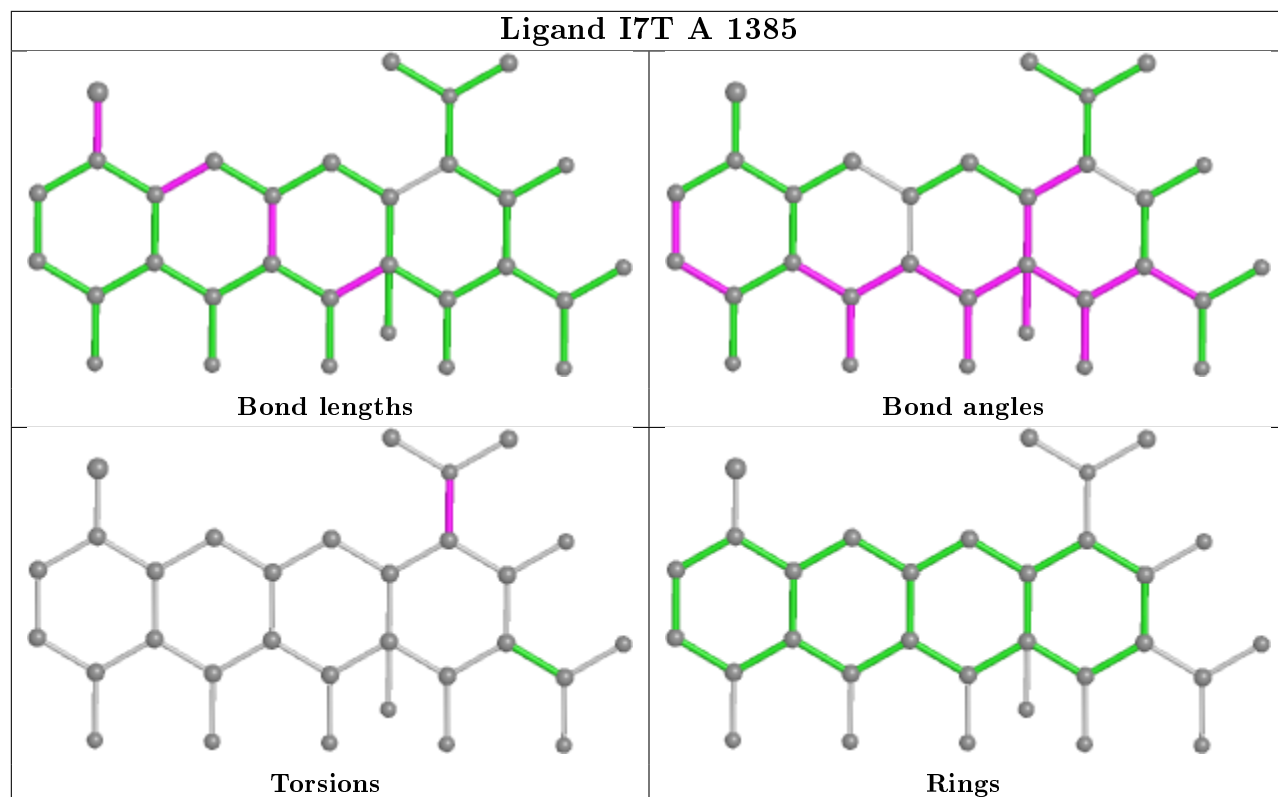
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand I7T D 1385

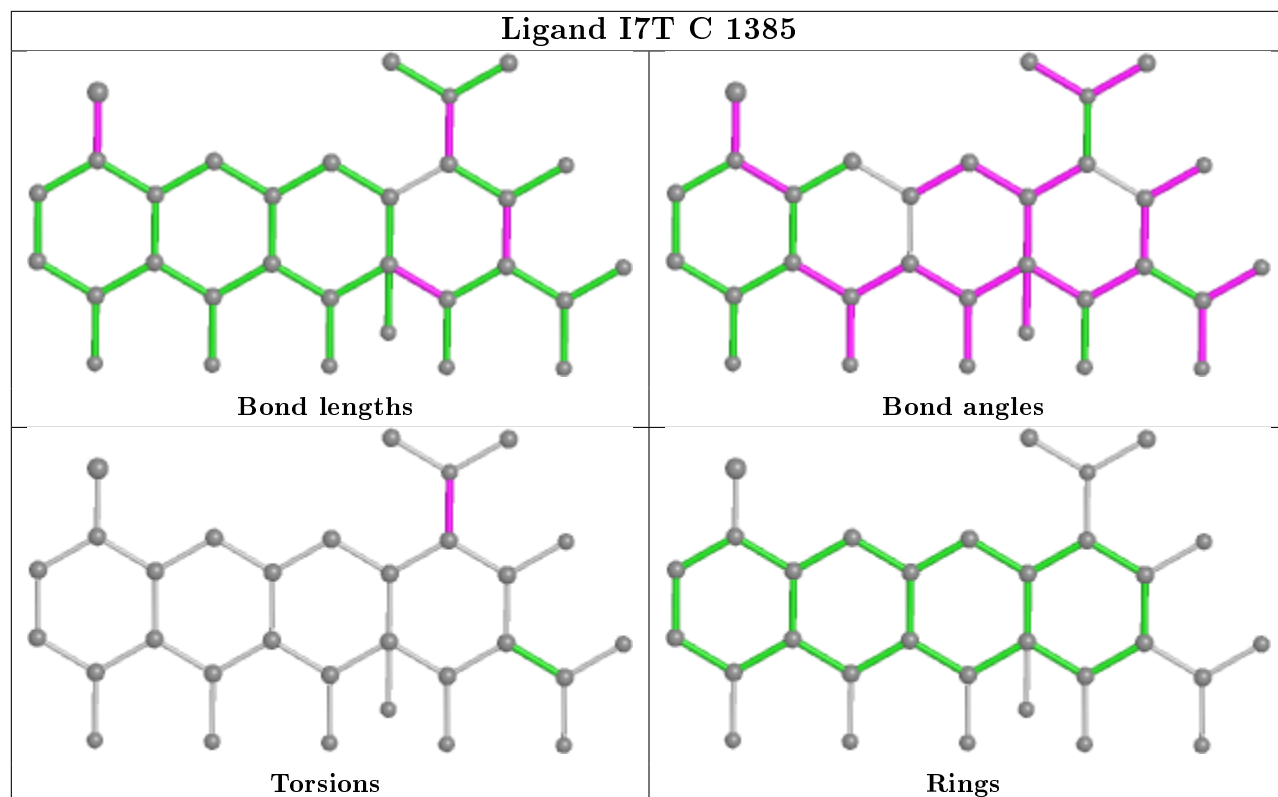


Ligand FAD B 1384

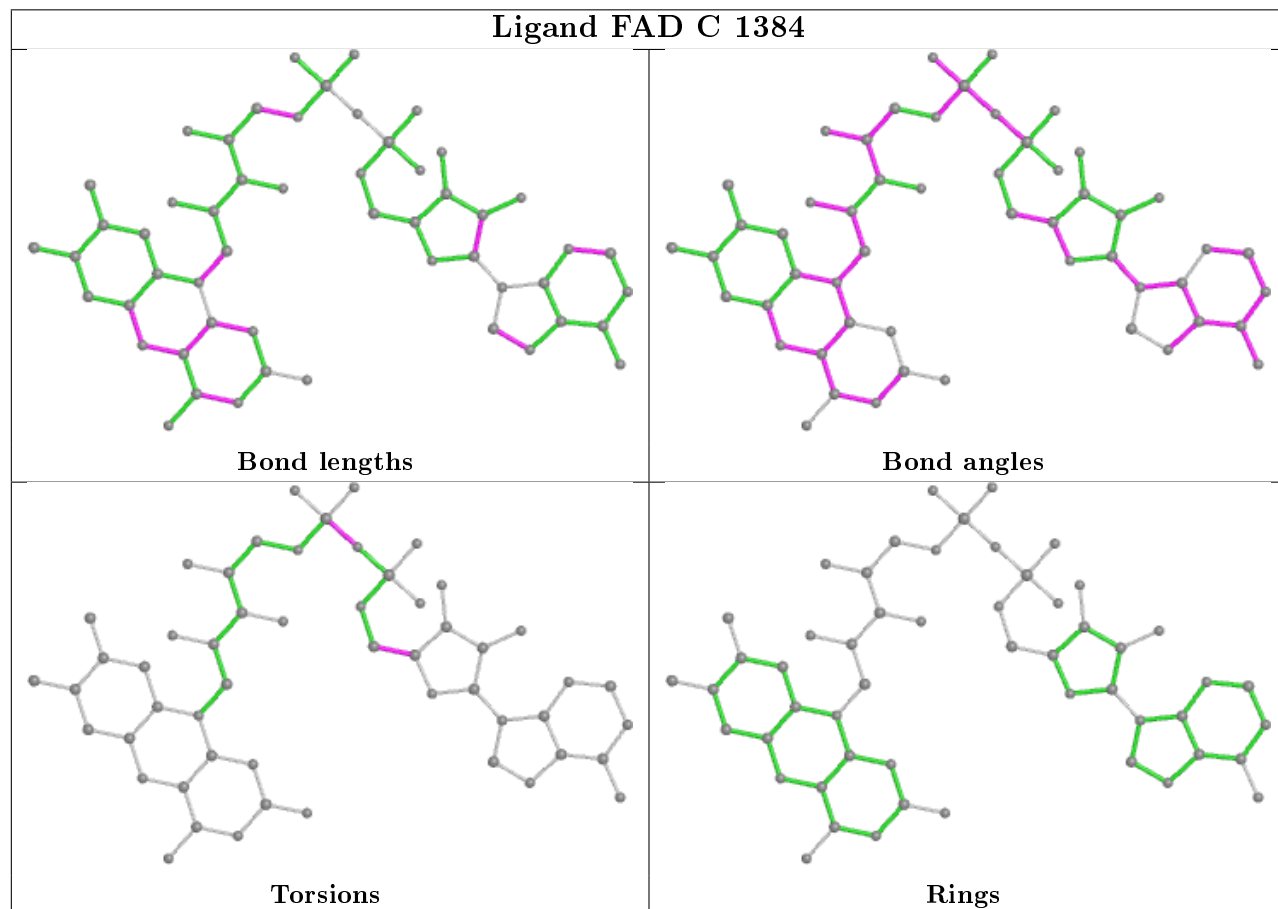




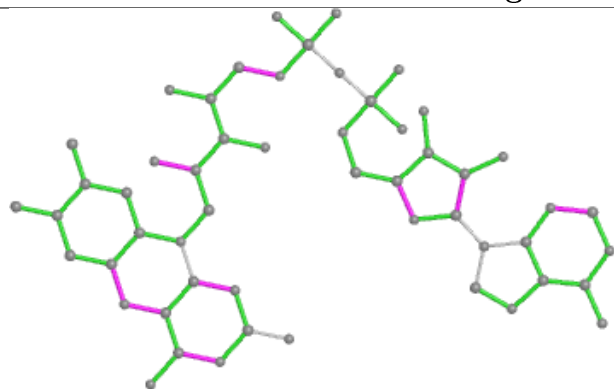
Ligand I7T C 1385



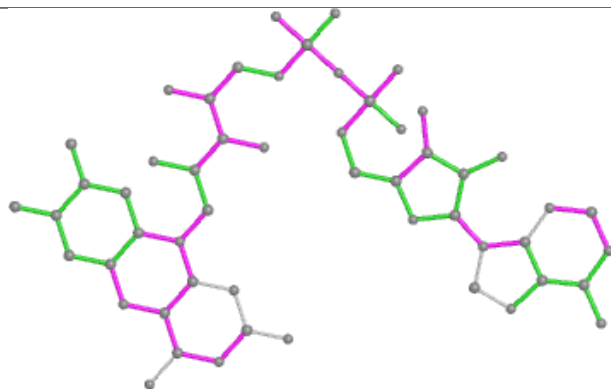
Ligand FAD C 1384



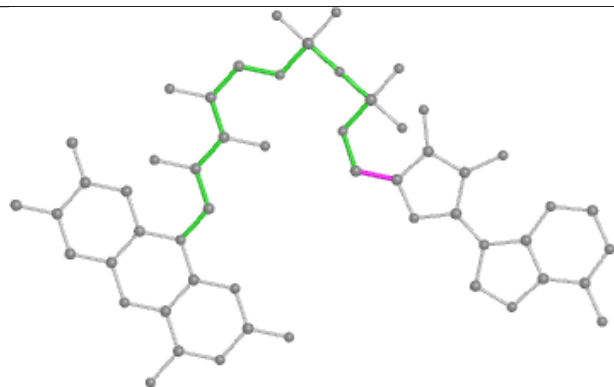
Ligand FAD A 1384



Bond lengths



Bond angles



Torsions



Rings

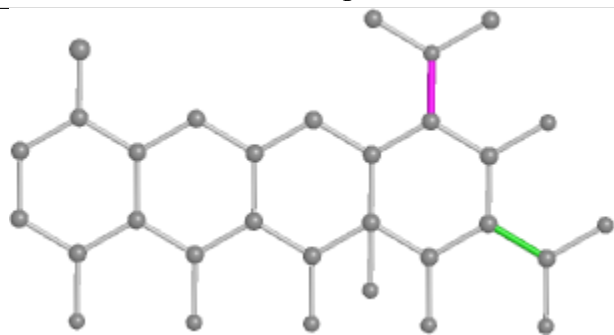
Ligand I7T B 1385



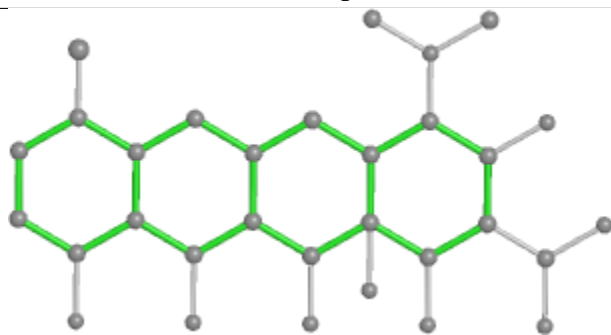
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/398 (92%)	0.18	11 (2%) 50 53	23, 43, 75, 101	0
1	B	368/398 (92%)	0.21	9 (2%) 59 60	24, 45, 80, 105	0
1	C	367/398 (92%)	0.43	19 (5%) 27 30	31, 57, 95, 133	0
1	D	365/398 (91%)	0.36	13 (3%) 42 46	32, 58, 97, 126	0
All	All	1468/1592 (92%)	0.29	52 (3%) 44 47	23, 51, 89, 133	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	PRO	9.6
1	B	378	PRO	5.4
1	C	379	ASP	4.9
1	C	321	GLY	4.9
1	D	379	ASP	4.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

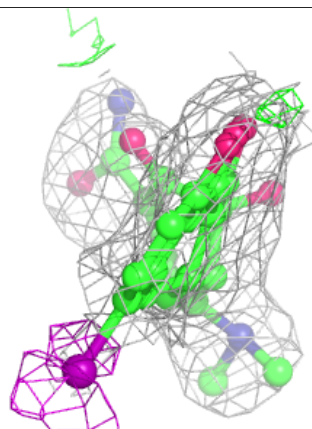
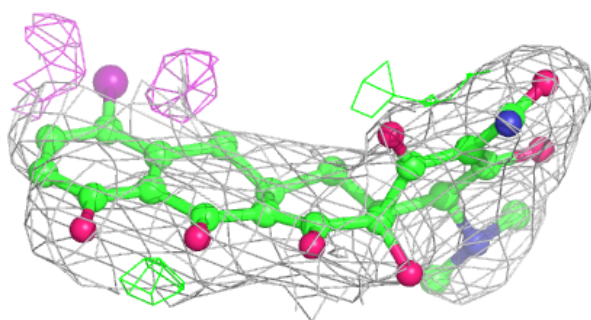
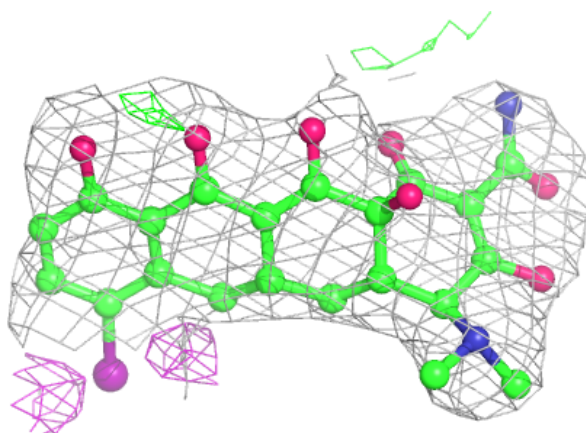
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	C	1387	5/5	0.84	0.16	120,121,121,121	0
4	SO4	B	1387	5/5	0.89	0.11	106,106,107,107	0
4	SO4	A	1387	5/5	0.90	0.17	100,100,102,102	0
4	SO4	B	1388	5/5	0.91	0.12	92,92,93,93	0
4	SO4	D	1387	5/5	0.91	0.21	109,109,110,111	0
3	I7T	D	1385	31/31	0.94	0.16	64,72,85,101	0
3	I7T	B	1385	31/31	0.94	0.16	37,56,75,91	0
3	I7T	C	1385	31/31	0.94	0.12	57,71,86,99	0
4	SO4	B	1386	5/5	0.95	0.14	76,80,80,80	0
4	SO4	D	1388	5/5	0.96	0.15	77,78,79,81	0
4	SO4	A	1388	5/5	0.96	0.13	97,97,98,98	0
4	SO4	A	1386	5/5	0.96	0.11	79,80,82,84	0
4	SO4	C	1388	5/5	0.96	0.08	75,77,79,81	0
4	SO4	D	1386	5/5	0.96	0.11	76,76,77,77	0
2	FAD	C	1384	53/53	0.97	0.13	26,36,57,61	0
3	I7T	A	1385	31/31	0.97	0.14	32,49,64,76	0
2	FAD	D	1384	53/53	0.97	0.13	27,39,58,63	0
2	FAD	A	1384	53/53	0.98	0.14	20,31,55,58	0
2	FAD	B	1384	53/53	0.98	0.14	19,33,50,53	0
4	SO4	C	1386	5/5	0.98	0.07	73,74,77,77	0

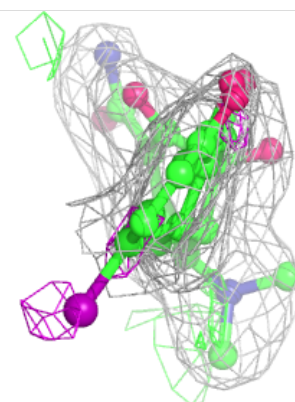
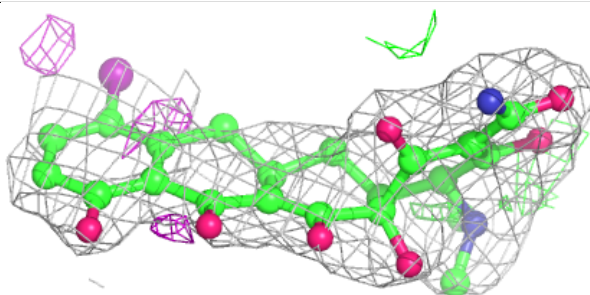
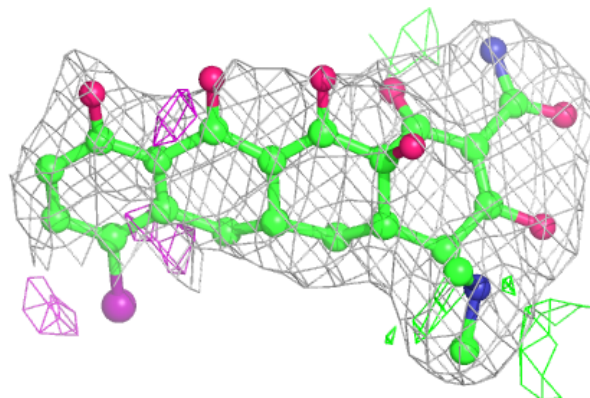
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I7T D 1385:

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

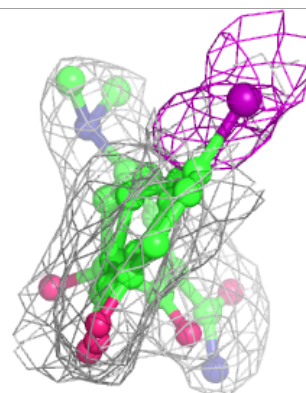
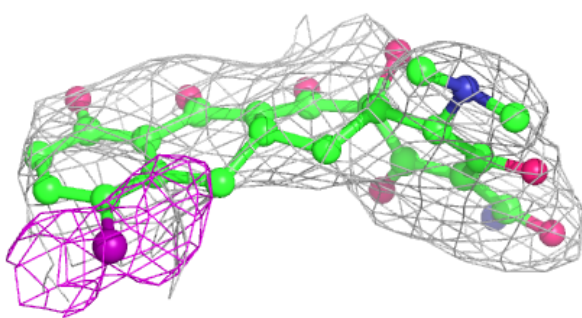
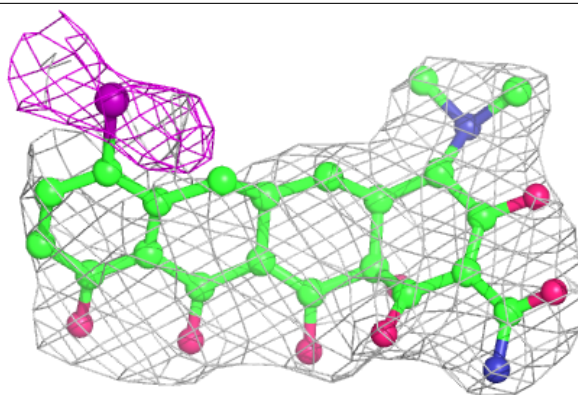
**Electron density around I7T B 1385:**

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

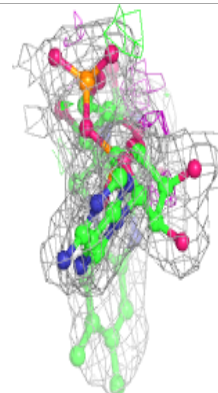
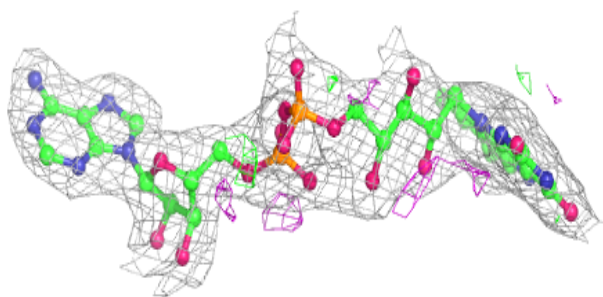
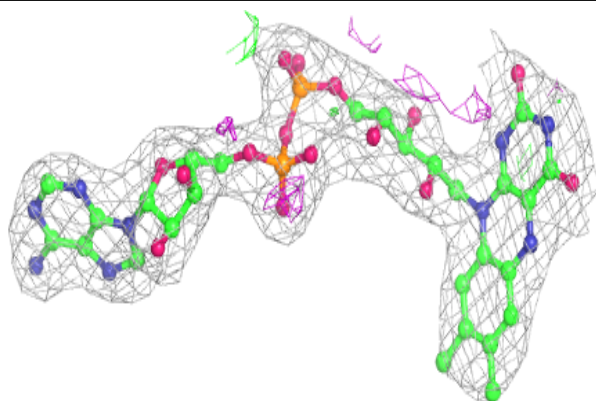


Electron density around I7T C 1385:

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

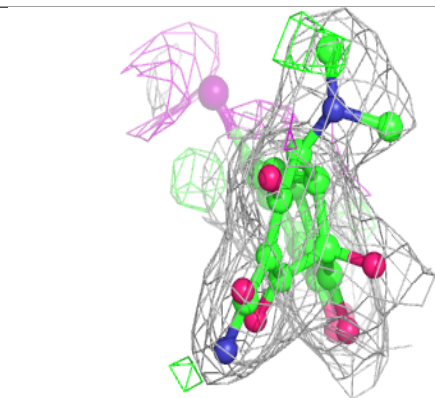
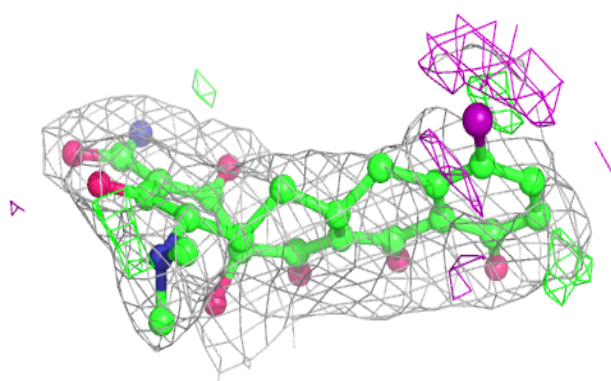
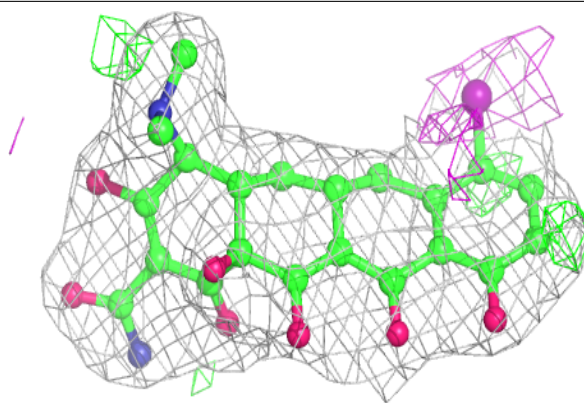
**Electron density around FAD C 1384:**

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

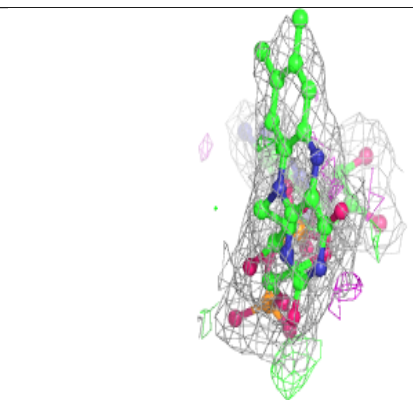
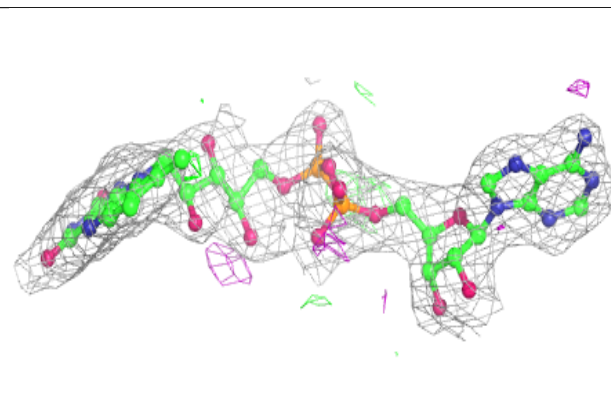
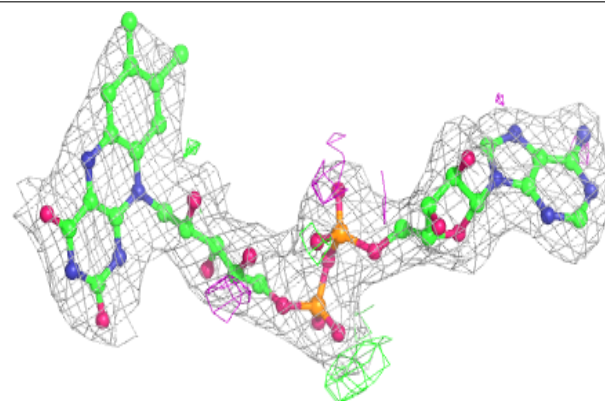


Electron density around I7T A 1385:

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

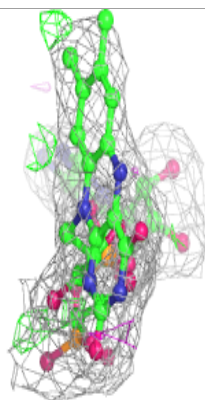
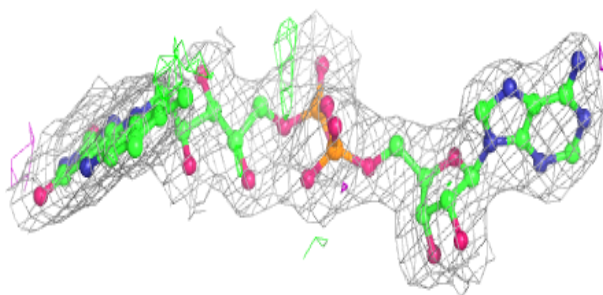
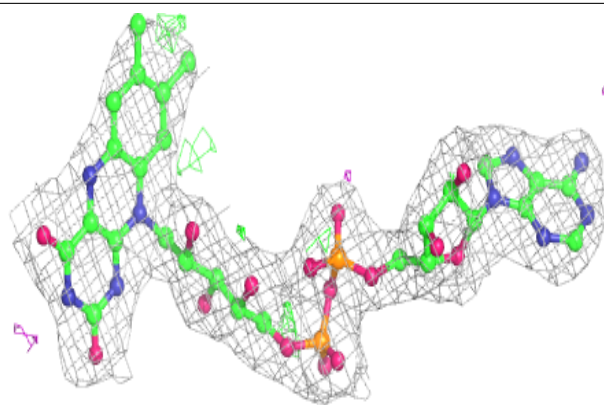
**Electron density around FAD D 1384:**

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

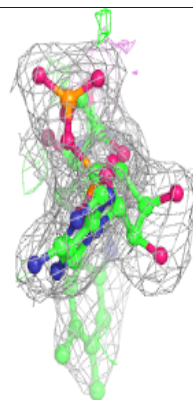
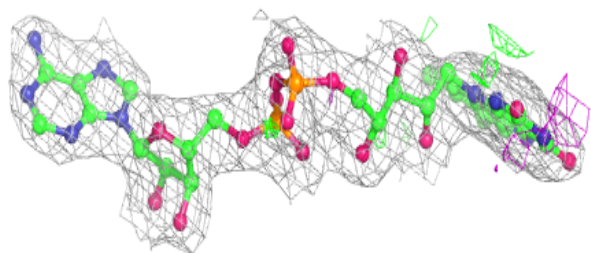
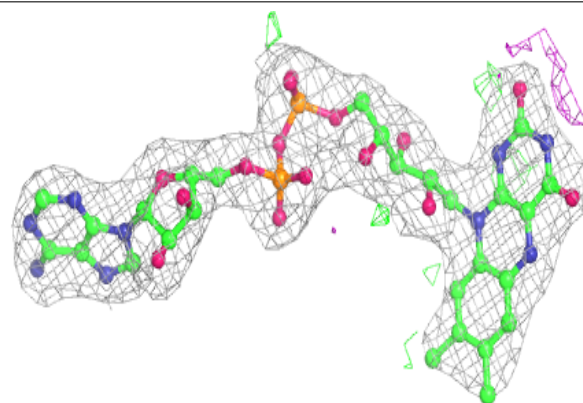


Electron density around FAD A 1384:

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

**Electron density around FAD B 1384:**

$2mF_o-DF_c$ (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.