



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 03:07 AM UTC

PDB ID : 2WET / pdb_00002wet
Title : Crystal structure of tryptophan 5-halogenase (PyrH) complex with FAD (tryptophan)
Authors : De Laurentis, W.; Zhu, X.; Naismith, J.H.
Deposited on : 2009-04-01
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

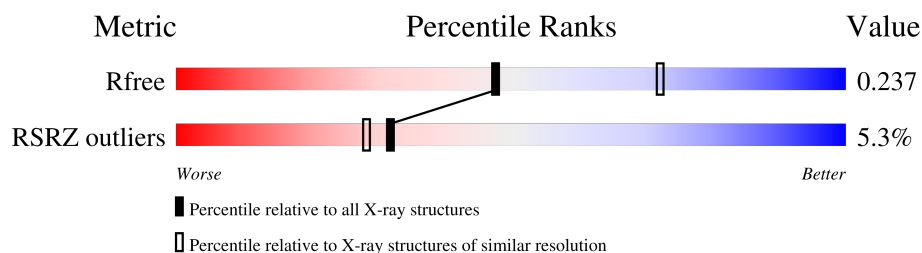
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17003 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.

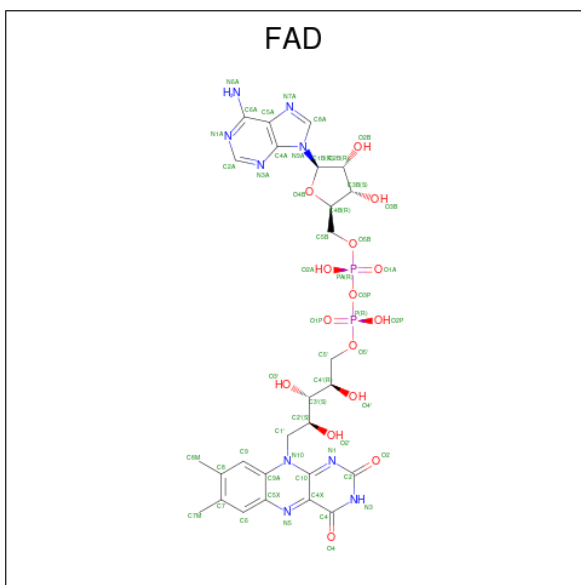
- Molecule 1 is a protein called TRYPTOPHAN 5-HALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	2	0
			4008	2547	708	734	19			
1	B	501	Total	C	N	O	S	0	3	0
			4052	2574	716	743	19			
1	C	494	Total	C	N	O	S	0	1	0
			3983	2533	701	730	19			
1	D	494	Total	C	N	O	S	0	0	0
			3974	2528	699	728	19			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

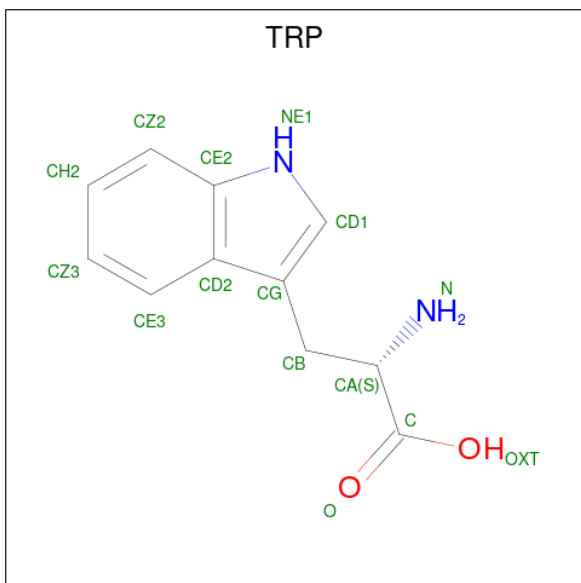
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	2	Total	Cl	0	0
			2	2		
2	C	2	Total	Cl	0	0
			2	2		
2	D	2	Total	Cl	0	0
			2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



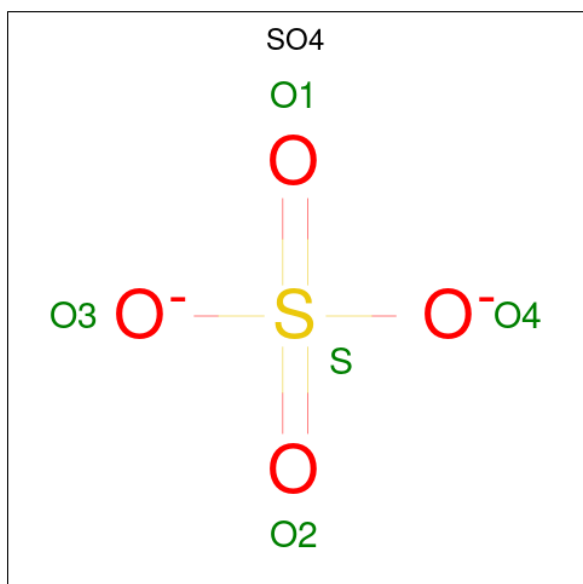
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	251	Total	O	0	0
			251	251		
6	B	207	Total	O	0	0
			207	207		
6	C	183	Total	O	0	0
			183	183		
6	D	105	Total	O	0	0
			105	105		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.53Å 137.53Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.40 48.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.06-2.40) 98.2 (48.06-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.196 , 0.234 0.203 , 0.237	Depositor DCC
R_{free} test set	5779 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17003	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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
5	SO4	C	1514	-	4,4,4	0.52	0	6,6,6	0.68	0
4	TRP	B	650	-	15,16,16	1.19	2 (13%)	18,22,22	1.06	1 (5%)
3	FAD	A	1513	-	58,58,58	1.18	6 (10%)	85,89,89	1.70	16 (18%)
3	FAD	D	1513	-	58,58,58	1.33	7 (12%)	85,89,89	1.56	15 (17%)
3	FAD	B	1652	-	58,58,58	1.40	8 (13%)	85,89,89	1.59	16 (18%)
3	FAD	C	1513	-	58,58,58	1.10	5 (8%)	85,89,89	1.64	16 (18%)

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	TRP	B	650	-	-	2/8/8/8	0/2/2/2
3	FAD	A	1513	-	-	3/34/50/50	0/6/6/6
3	FAD	D	1513	-	-	5/34/50/50	0/6/6/6
3	FAD	B	1652	-	-	4/34/50/50	0/6/6/6
3	FAD	C	1513	-	-	4/34/50/50	0/6/6/6

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1513	FAD	P-O3P	5.08	1.65	1.59
3	B	1652	FAD	P-O3P	4.95	1.64	1.59
3	D	1513	FAD	C4X-N5	4.11	1.39	1.30
3	A	1513	FAD	C4X-N5	3.90	1.39	1.30
3	A	1513	FAD	PA-O3P	3.67	1.63	1.59
3	B	1652	FAD	PA-O3P	3.63	1.63	1.59
3	B	1652	FAD	C4X-N5	3.61	1.38	1.30
3	C	1513	FAD	C4X-N5	3.60	1.38	1.30
4	B	650	TRP	CB-CG	2.83	1.55	1.50
3	D	1513	FAD	PA-O3P	2.81	1.62	1.59
3	B	1652	FAD	C10-N1	2.80	1.38	1.33
3	C	1513	FAD	C10-N1	2.80	1.38	1.33
3	B	1652	FAD	C2A-N1A	2.77	1.38	1.33
3	D	1513	FAD	C10-N1	2.77	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1513	FAD	C2A-N1A	2.61	1.38	1.33
3	B	1652	FAD	C2A-N3A	2.55	1.38	1.33
3	B	1652	FAD	C8A-N7A	2.53	1.36	1.31
3	D	1513	FAD	C2A-N3A	2.48	1.38	1.33
3	C	1513	FAD	C2A-N1A	2.40	1.38	1.33
3	C	1513	FAD	C2A-N3A	2.38	1.38	1.33
3	B	1652	FAD	C5'-C4'	2.37	1.55	1.51
3	D	1513	FAD	C8A-N7A	2.29	1.36	1.31
3	A	1513	FAD	C10-N1	2.28	1.37	1.33
3	A	1513	FAD	C2A-N1A	2.21	1.37	1.33
3	A	1513	FAD	C2A-N3A	2.12	1.37	1.33
3	C	1513	FAD	PA-O3P	2.09	1.61	1.59
4	B	650	TRP	OXT-C	-2.01	1.24	1.30
3	A	1513	FAD	C5A-N7A	-2.01	1.35	1.39

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1513	FAD	N3A-C2A-N1A	-6.55	118.67	128.58
3	C	1513	FAD	N3A-C2A-N1A	-6.37	118.94	128.58
3	B	1652	FAD	N3A-C2A-N1A	-5.75	119.88	128.58
3	D	1513	FAD	N3A-C2A-N1A	-5.66	120.01	128.58
3	A	1513	FAD	N9A-C8A-N7A	-5.01	106.82	113.94
3	B	1652	FAD	C5A-C4A-N3A	-4.50	120.52	126.72
3	C	1513	FAD	N9A-C8A-N7A	-4.46	107.61	113.94
3	D	1513	FAD	N9A-C8A-N7A	-4.43	107.65	113.94
3	A	1513	FAD	C5A-N7A-C8A	4.21	110.07	103.45
3	D	1513	FAD	C5A-C4A-N3A	-4.14	121.02	126.72
3	C	1513	FAD	C5A-C4A-N3A	-4.07	121.11	126.72
3	C	1513	FAD	C5A-N7A-C8A	4.03	109.79	103.45
3	A	1513	FAD	C5A-C4A-N3A	-3.98	121.24	126.72
4	B	650	TRP	OXT-C-O	-3.97	115.08	124.08
3	B	1652	FAD	N9A-C8A-N7A	-3.93	108.36	113.94
3	D	1513	FAD	C5A-N7A-C8A	3.89	109.56	103.45
3	B	1652	FAD	C2A-N3A-C4A	3.66	120.78	111.83
3	A	1513	FAD	C2A-N3A-C4A	3.54	120.48	111.83
3	C	1513	FAD	C2A-N3A-C4A	3.47	120.31	111.83
3	B	1652	FAD	C5A-N7A-C8A	3.37	108.74	103.45
3	D	1513	FAD	C2A-N3A-C4A	3.23	119.71	111.83
3	B	1652	FAD	C4X-C10-N10	3.08	120.90	116.48
3	A	1513	FAD	C4X-C10-N10	3.06	120.86	116.48
3	D	1513	FAD	C4-N3-C2	-3.03	120.26	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1513	FAD	C4A-C5A-N7A	-2.98	107.17	110.58
3	D	1513	FAD	C4X-C10-N10	2.98	120.75	116.48
3	B	1652	FAD	C10-C4X-N5	-2.97	118.74	124.81
3	A	1513	FAD	C4A-N9A-C8A	2.87	108.75	105.74
3	A	1513	FAD	C4-C4X-N5	2.86	122.16	118.21
3	C	1513	FAD	N3A-C4A-N9A	2.81	131.95	127.17
3	C	1513	FAD	C4A-C5A-N7A	-2.81	107.37	110.58
3	A	1513	FAD	C4X-C4-N3	2.80	120.39	113.25
3	B	1652	FAD	N3A-C4A-N9A	2.79	131.92	127.17
3	C	1513	FAD	C4-N3-C2	-2.78	120.71	125.64
3	B	1652	FAD	O2A-PA-O3P	2.77	114.77	107.27
3	A	1513	FAD	C4-N3-C2	-2.77	120.73	125.64
3	A	1513	FAD	C4A-C5A-N7A	-2.76	107.43	110.58
3	A	1513	FAD	N3A-C4A-N9A	2.74	131.83	127.17
3	D	1513	FAD	N3A-C4A-N9A	2.73	131.80	127.17
3	C	1513	FAD	C10-C4X-N5	-2.72	119.26	124.81
3	C	1513	FAD	C4X-C10-N10	2.70	120.35	116.48
3	B	1652	FAD	C4-C4X-N5	2.68	121.91	118.21
3	D	1513	FAD	C10-C4X-N5	-2.64	119.42	124.81
3	A	1513	FAD	O4B-C1B-N9A	2.62	113.13	108.09
3	D	1513	FAD	C4X-C4-N3	2.60	119.86	113.25
3	B	1652	FAD	C4A-C5A-N7A	-2.58	107.63	110.58
3	C	1513	FAD	C4X-C4-N3	2.58	119.81	113.25
3	D	1513	FAD	C4A-N9A-C8A	2.57	108.44	105.74
3	A	1513	FAD	C10-C4X-N5	-2.53	119.64	124.81
3	C	1513	FAD	O3B-C3B-C4B	-2.53	103.81	111.08
3	C	1513	FAD	C4-C4X-N5	2.46	121.61	118.21
3	C	1513	FAD	C4A-N9A-C8A	2.43	108.28	105.74
3	B	1652	FAD	C4X-C4-N3	2.40	119.36	113.25
3	A	1513	FAD	C9A-C5X-N5	-2.32	119.99	122.45
3	D	1513	FAD	C4-C4X-N5	2.26	121.33	118.21
3	A	1513	FAD	O2A-PA-O3P	2.20	113.23	107.27
3	C	1513	FAD	C9A-C5X-N5	-2.19	120.13	122.45
3	B	1652	FAD	C10-N1-C2	2.18	121.56	116.85
3	D	1513	FAD	C9A-C5X-N5	-2.15	120.17	122.45
3	C	1513	FAD	O4B-C1B-N9A	2.07	112.06	108.09
3	B	1652	FAD	C4X-C10-N1	-2.06	119.55	124.59
3	B	1652	FAD	C4-N3-C2	-2.05	122.00	125.64
3	D	1513	FAD	C6A-C5A-C4A	2.03	119.94	117.18
3	B	1652	FAD	C9A-C5X-N5	-2.02	120.31	122.45

There are no chirality outliers.

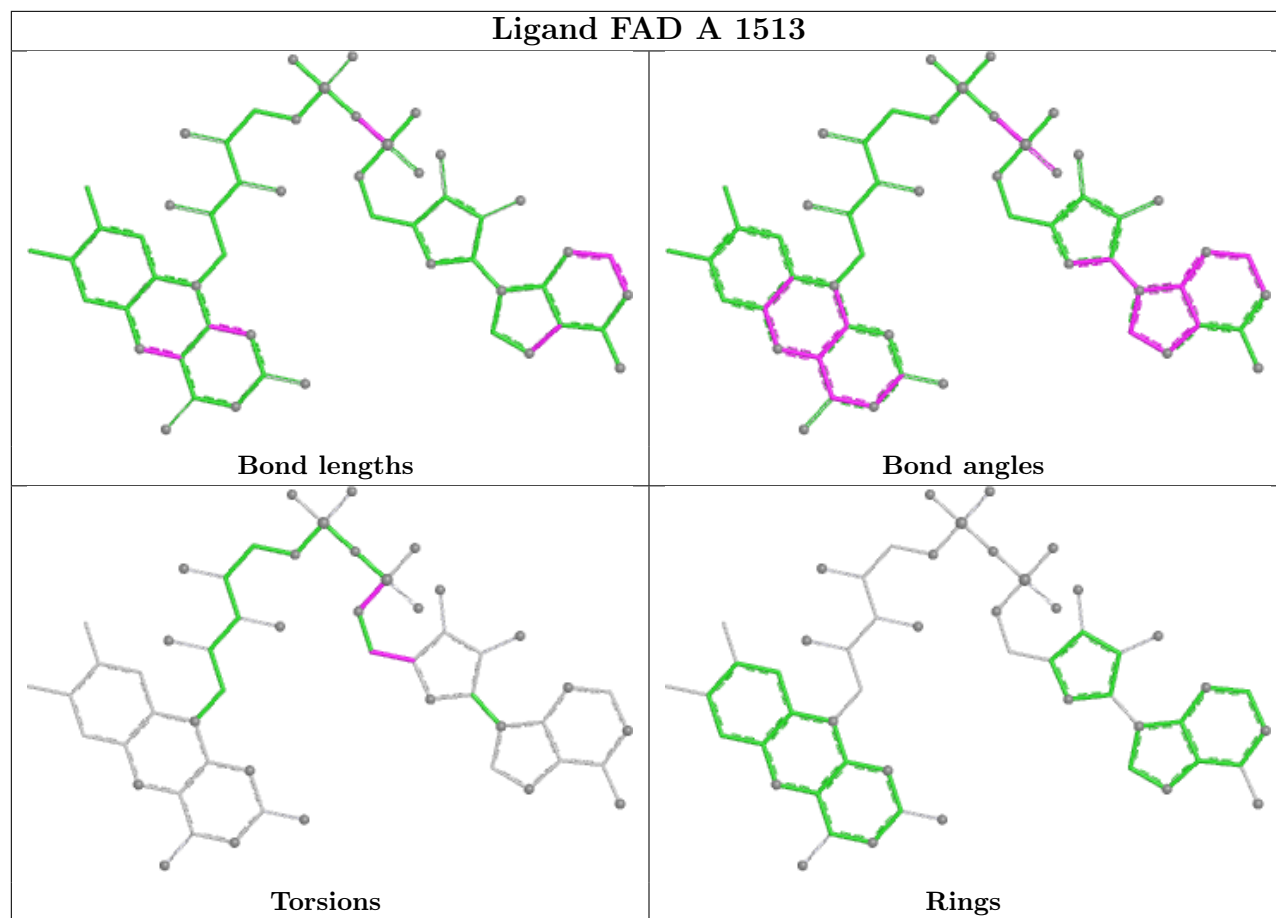
All (18) torsion outliers are listed below:

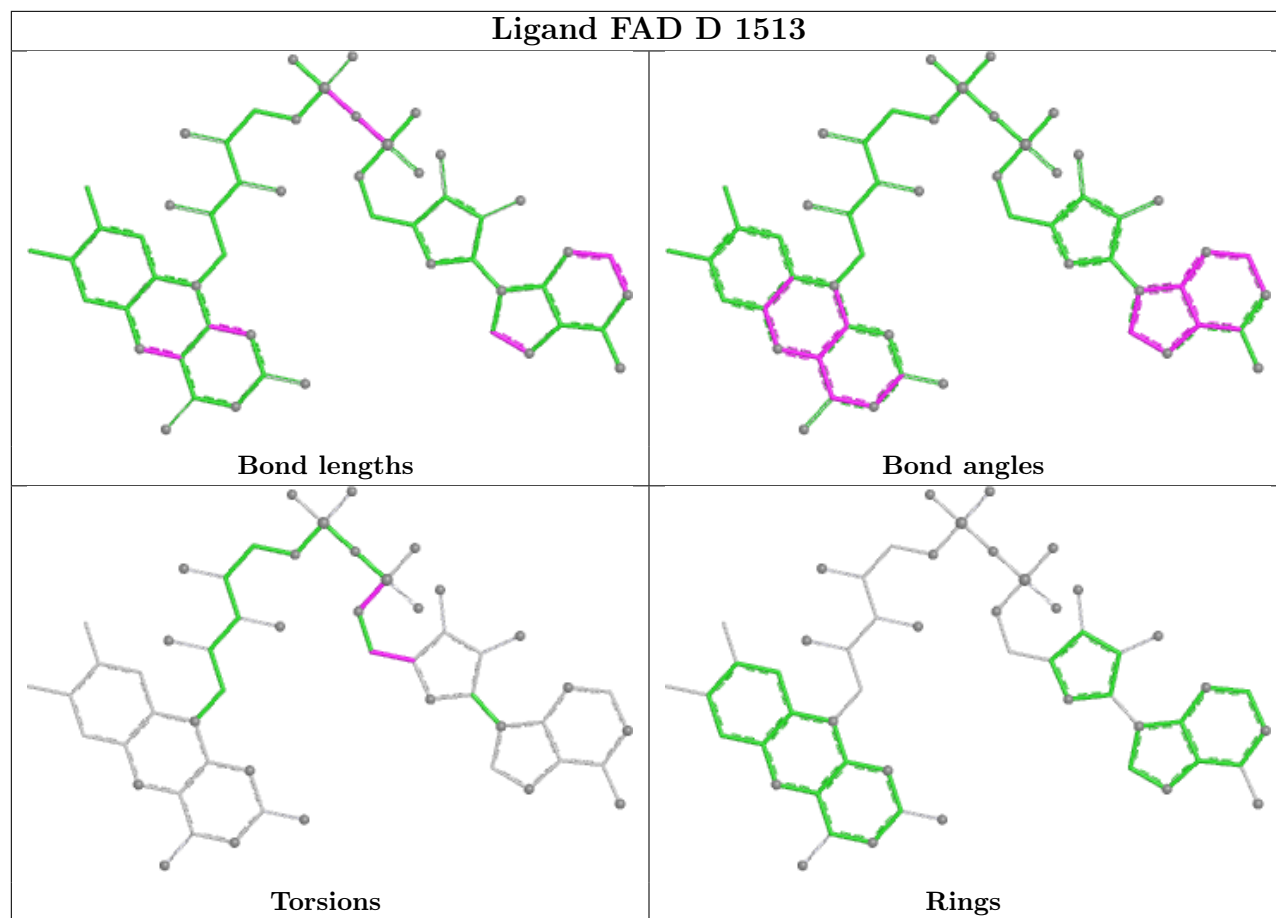
Mol	Chain	Res	Type	Atoms
3	B	1652	FAD	C5B-O5B-PA-O1A
3	C	1513	FAD	C5B-O5B-PA-O1A
3	D	1513	FAD	C5B-O5B-PA-O1A
3	B	1652	FAD	O4B-C4B-C5B-O5B
3	B	1652	FAD	C3B-C4B-C5B-O5B
3	D	1513	FAD	O4B-C4B-C5B-O5B
3	D	1513	FAD	C3B-C4B-C5B-O5B
3	A	1513	FAD	C5B-O5B-PA-O1A
3	A	1513	FAD	C5B-O5B-PA-O2A
3	B	1652	FAD	C5B-O5B-PA-O2A
3	C	1513	FAD	C5B-O5B-PA-O2A
3	D	1513	FAD	C5B-O5B-PA-O2A
3	D	1513	FAD	C5B-O5B-PA-O3P
4	B	650	TRP	O-C-CA-CB
4	B	650	TRP	OXT-C-CA-CB
3	C	1513	FAD	O4B-C4B-C5B-O5B
3	A	1513	FAD	O4B-C4B-C5B-O5B
3	C	1513	FAD	C3B-C4B-C5B-O5B

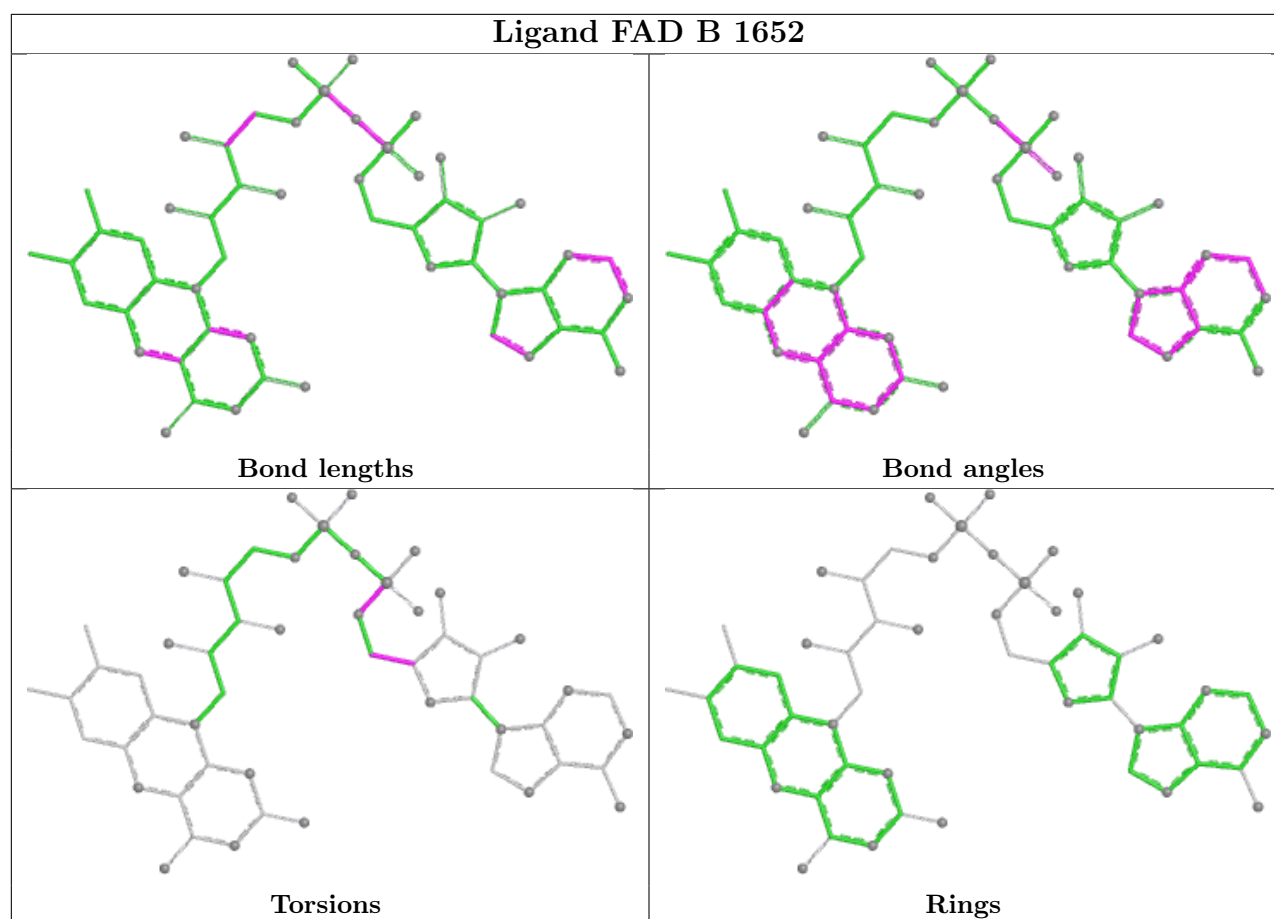
There are no ring outliers.

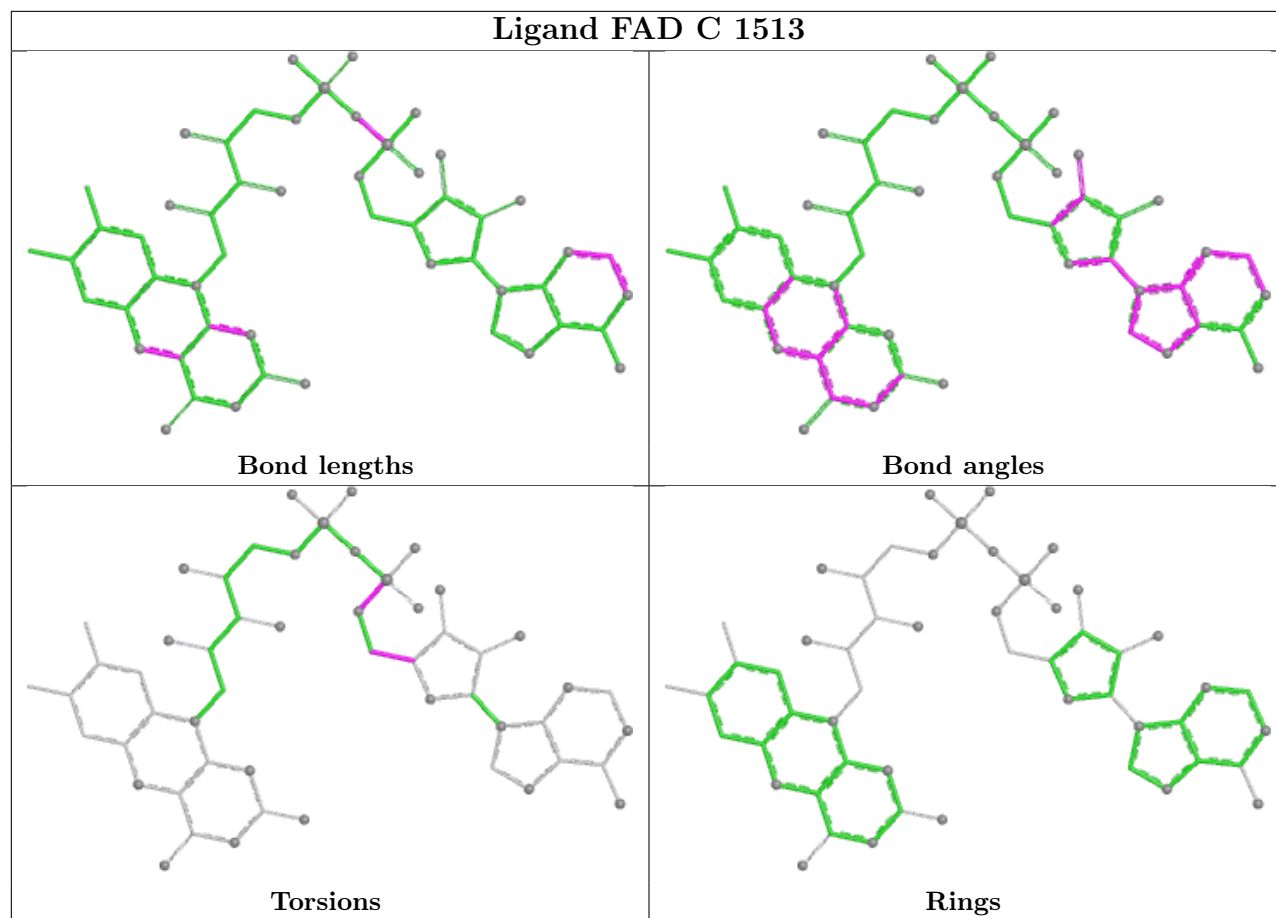
No monomer is involved in short contacts.

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.









4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	496/511 (97%)	-0.36	3 (0%) 85 83	10, 19, 26, 32	2 (0%)
1	B	501/511 (98%)	-0.34	10 (1%) 65 60	8, 20, 32, 53	3 (0%)
1	C	494/511 (96%)	0.02	3 (0%) 85 83	11, 19, 25, 33	1 (0%)
1	D	494/511 (96%)	1.25	90 (18%) 3 3	15, 19, 26, 32	0
All	All	1985/2044 (97%)	0.14	106 (5%) 32 28	8, 19, 28, 53	6 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	380	VAL	5.3
1	D	44	VAL	4.3
1	D	73	GLY	3.9
1	B	44	VAL	3.9
1	B	39	VAL	3.8
1	D	377	TRP	3.5
1	D	165	PRO	3.5
1	D	287	LYS	3.5
1	D	447	TYR	3.4
1	B	45	GLY	3.4
1	D	91	TYR	3.3
1	D	126	THR	3.3
1	B	155	SER	3.3
1	D	411	ASP	3.1
1	D	259	PRO	3.1
1	D	170	PHE	3.1
1	D	45	GLY	3.1
1	D	72	GLY	3.0
1	D	383	SER	3.0
1	D	206	ILE	2.9
1	D	408	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	82	ASN	2.9
1	D	432	GLU	2.9
1	D	280	MET	2.9
1	D	144	PHE	2.8
1	D	141	GLY	2.8
1	D	1	MET	2.7
1	D	164	PHE	2.7
1	D	372	PHE	2.7
1	D	264	GLU	2.7
1	B	43	GLY	2.7
1	D	374	GLY	2.7
1	D	384	ALA	2.7
1	C	375	GLU	2.7
1	D	316	GLY	2.7
1	D	444	ILE	2.7
1	D	376	ARG	2.6
1	D	285	LEU	2.6
1	D	238	GLY	2.6
1	D	289	ASP	2.6
1	B	158	ALA	2.6
1	B	41	ARG	2.6
1	D	161	ARG	2.6
1	D	472	PRO	2.6
1	D	204	GLY	2.5
1	D	239	GLY	2.5
1	D	202	GLU	2.5
1	D	504	TYR	2.5
1	D	171	ASP	2.5
1	B	40	ARG	2.5
1	D	43	GLY	2.5
1	D	387	GLU	2.4
1	D	240	ARG	2.4
1	D	118	SER	2.4
1	D	212	LYS	2.4
1	C	163	GLN	2.4
1	D	381	LEU	2.4
1	D	445	TYR	2.4
1	D	218	SER	2.3
1	D	143	LEU	2.3
1	B	38	ASN	2.3
1	D	66	TRP	2.3
1	A	240	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	157	LEU	2.3
1	D	427	LEU	2.3
1	D	128	ARG	2.3
1	D	340	CYS	2.3
1	D	109	TRP	2.3
1	D	136	PRO	2.3
1	D	236	THR	2.2
1	D	42	ILE	2.2
1	D	266	MET	2.2
1	D	286	PHE	2.2
1	C	86	PRO	2.2
1	D	172	ALA	2.2
1	D	348	ALA	2.2
1	A	117	THR	2.2
1	D	2	ILE	2.2
1	D	407	ALA	2.2
1	D	203	ARG	2.2
1	D	332	ASN	2.2
1	D	320	LEU	2.2
1	D	426	GLY	2.2
1	D	331	ARG	2.2
1	D	38	ASN	2.1
1	D	234	ASN	2.1
1	D	235	GLN	2.1
1	D	76	LEU	2.1
1	D	406	GLY	2.1
1	D	448	TYR	2.1
1	D	138	MET	2.1
1	D	198	VAL	2.1
1	D	231	LEU	2.1
1	D	339	ASN	2.1
1	D	267	ARG	2.1
1	D	140	ASP	2.1
1	D	263	ASP	2.1
1	D	130	CYS	2.1
1	D	373	PRO	2.1
1	A	40[A]	ARG	2.0
1	D	390	ALA	2.0
1	D	386	ASN	2.0
1	D	112	VAL	2.0
1	D	341	VAL	2.0
1	D	159	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	215	GLY	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

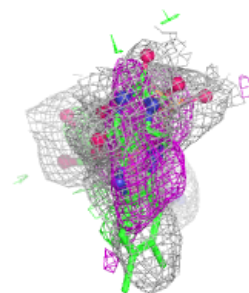
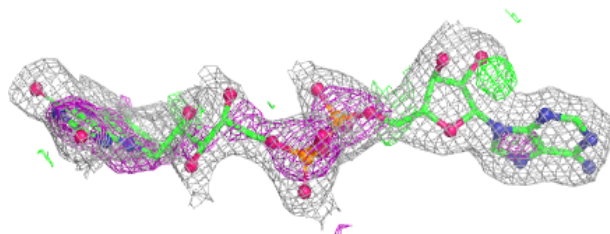
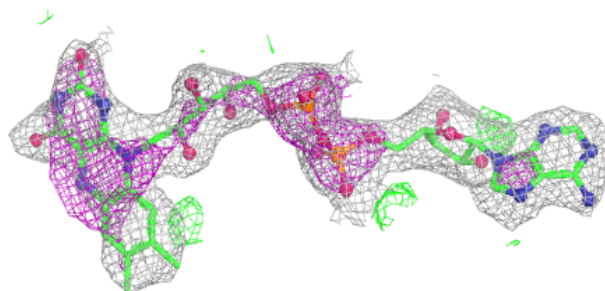
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	B	1652	53/53	0.85	0.12	16,23,27,27	0
3	FAD	D	1513	53/53	0.87	0.10	16,22,27,27	0
5	SO4	C	1514	5/5	0.88	0.16	41,49,51,53	0
4	TRP	B	650	15/15	0.91	0.11	41,44,47,47	0
2	CL	D	1514	1/1	0.92	0.24	49,49,49,49	0
2	CL	D	700	1/1	0.93	0.24	39,39,39,39	0
2	CL	B	700	1/1	0.93	0.15	50,50,50,50	0
2	CL	C	700	1/1	0.93	0.12	37,37,37,37	0
3	FAD	C	1513	53/53	0.95	0.08	15,22,27,27	0
3	FAD	A	1513	53/53	0.97	0.07	15,21,27,27	0
2	CL	B	1653	1/1	0.97	0.13	53,53,53,53	0
2	CL	C	1515	1/1	0.98	0.16	41,41,41,41	0
2	CL	A	1514	1/1	0.98	0.21	50,50,50,50	0
2	CL	A	700	1/1	0.98	0.07	35,35,35,35	0

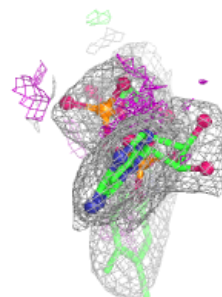
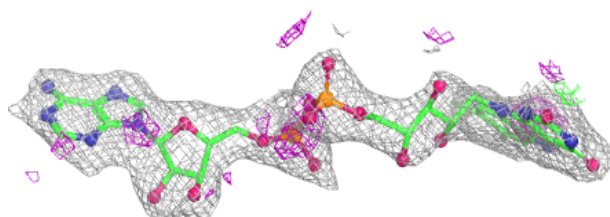
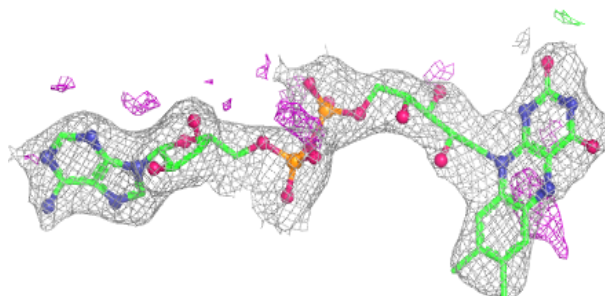
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1652:

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

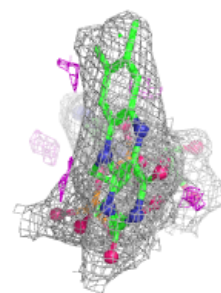
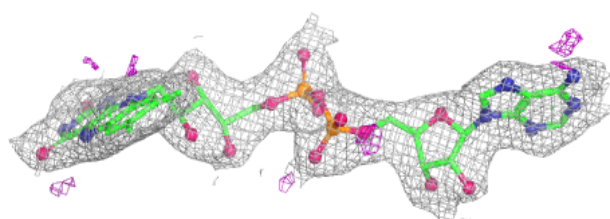
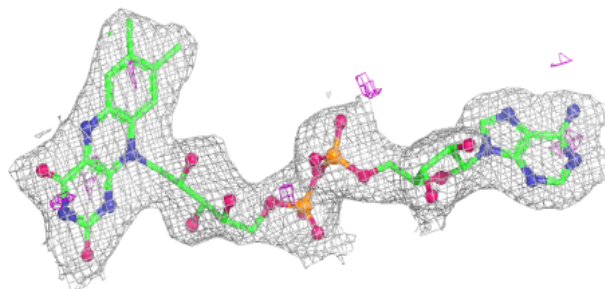
**Electron density around FAD D 1513:**

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

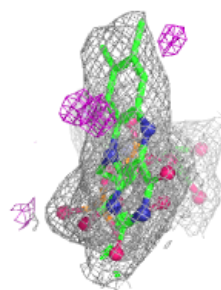
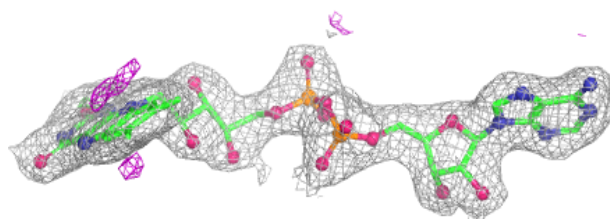
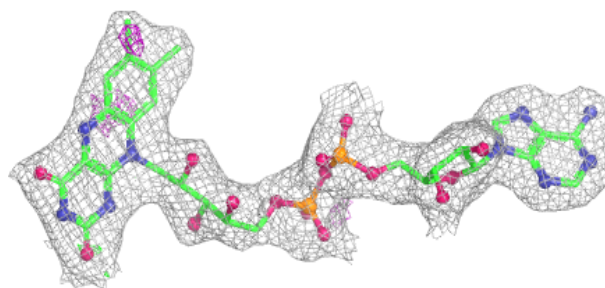


Electron density around FAD C 1513:

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

**Electron density around FAD A 1513:**

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



5.5 Other polymers [i](#)

There are no such residues in this entry.