



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 11:13 AM UTC

PDB ID : 2WES / pdb_00002wes
Title : Crystal structures of mutant E46Q of tryptophan 5-halogenase (PyrH)
Authors : Zhu, X.; Naismith, J.H.
Deposited on : 2009-04-01
Resolution : 2.50 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

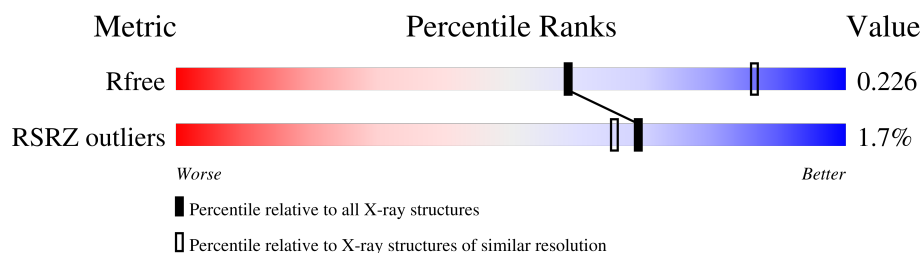
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17104 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.

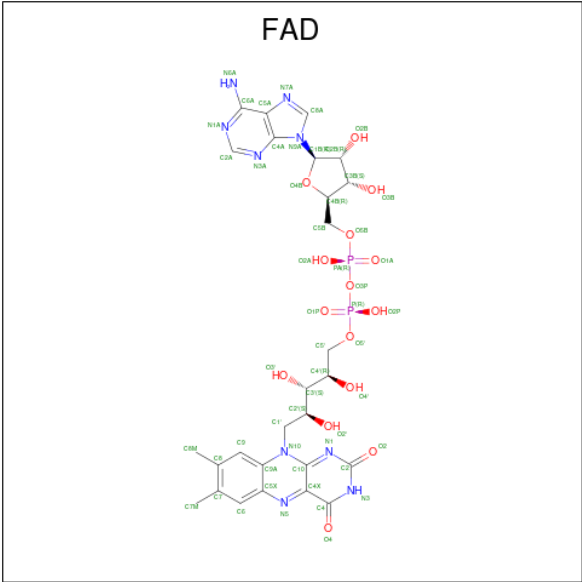
- Molecule 1 is a protein called TRYPTOPHAN 5-HALOGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3987	2535	702	731	19			
1	B	496	Total	C	N	O	S	0	0	0
			3987	2535	702	731	19			
1	C	496	Total	C	N	O	S	0	0	0
			3987	2535	702	731	19			
1	D	496	Total	C	N	O	S	0	0	0
			3987	2535	702	731	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLN	GLU	engineered mutation	UNP A4D0H5
B	46	GLN	GLU	engineered mutation	UNP A4D0H5
C	46	GLN	GLU	engineered mutation	UNP A4D0H5
D	46	GLN	GLU	engineered mutation	UNP A4D0H5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			52	27	9	14	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	304	Total	O	0	0
			304	304		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	239	Total 239	O 239	0	0
4	C	203	Total 203	O 203	0	0
4	D	195	Total 195	O 195	0	0

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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	137.57Å 137.57Å 309.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.50 48.25 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.25-2.50) 99.9 (48.25-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.97 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.193 , 0.230 0.191 , 0.226	Depositor DCC
R_{free} test set	5192 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17104	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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](#)

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

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
2	FAD	B	650	-	58,58,58	1.29	7 (12%)	85,89,89	1.63	14 (16%)
2	FAD	A	650	-	58,58,58	1.15	5 (8%)	85,89,89	1.71	15 (17%)
2	FAD	D	650	-	58,58,58	1.28	7 (12%)	85,89,89	1.50	14 (16%)
2	FAD	C	650	-	53,57,58	1.06	5 (9%)	78,86,89	1.63	14 (17%)

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	B	650	-	-	6/34/50/50	0/6/6/6
2	FAD	A	650	-	-	4/34/50/50	0/6/6/6
2	FAD	D	650	-	-	5/34/50/50	0/6/6/6
2	FAD	C	650	-	-	4/28/48/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	650	FAD	P-O3P	4.54	1.64	1.59
2	D	650	FAD	P-O3P	4.11	1.63	1.59
2	A	650	FAD	C4X-N5	3.94	1.39	1.30
2	B	650	FAD	C4X-N5	3.82	1.39	1.30
2	D	650	FAD	C4X-N5	3.71	1.38	1.30
2	D	650	FAD	PA-O3P	3.62	1.63	1.59
2	B	650	FAD	C2A-N1A	3.30	1.39	1.33
2	C	650	FAD	C4X-N5	3.13	1.37	1.30
2	A	650	FAD	PA-O3P	2.81	1.62	1.59
2	B	650	FAD	C8A-N7A	2.69	1.36	1.31
2	C	650	FAD	C8A-N7A	2.64	1.36	1.31
2	A	650	FAD	C2A-N1A	2.61	1.38	1.33
2	B	650	FAD	C2A-N3A	2.61	1.38	1.33
2	B	650	FAD	PA-O3P	2.58	1.62	1.59
2	D	650	FAD	C8A-N7A	2.54	1.36	1.31
2	D	650	FAD	C2A-N1A	2.47	1.38	1.33
2	D	650	FAD	C10-N1	2.45	1.38	1.33
2	C	650	FAD	C10-N1	2.33	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	650	FAD	C2A-N1A	2.32	1.38	1.33
2	A	650	FAD	C5A-N7A	-2.17	1.35	1.39
2	B	650	FAD	C10-N1	2.15	1.37	1.33
2	A	650	FAD	P-O3P	2.11	1.61	1.59
2	D	650	FAD	C2A-N3A	2.09	1.37	1.33
2	C	650	FAD	C2A-N3A	2.02	1.37	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	650	FAD	N3A-C2A-N1A	-6.58	118.62	128.58
2	C	650	FAD	N3A-C2A-N1A	-6.45	118.82	128.58
2	B	650	FAD	N3A-C2A-N1A	-6.41	118.87	128.58
2	D	650	FAD	N3A-C2A-N1A	-5.28	120.59	128.58
2	A	650	FAD	N9A-C8A-N7A	-4.93	106.94	113.94
2	B	650	FAD	N9A-C8A-N7A	-4.63	107.36	113.94
2	A	650	FAD	C5A-N7A-C8A	4.22	110.09	103.45
2	D	650	FAD	N9A-C8A-N7A	-4.05	108.19	113.94
2	C	650	FAD	N9A-C8A-N7A	-3.97	108.30	113.94
2	C	650	FAD	C5A-C4A-N3A	-3.96	121.26	126.72
2	A	650	FAD	C5A-C4A-N3A	-3.79	121.50	126.72
2	B	650	FAD	C5A-N7A-C8A	3.78	109.38	103.45
2	C	650	FAD	C2A-N3A-C4A	3.71	120.88	111.83
2	B	650	FAD	C5A-C4A-N3A	-3.70	121.62	126.72
2	A	650	FAD	C2A-N3A-C4A	3.63	120.69	111.83
2	D	650	FAD	C5A-C4A-N3A	-3.46	121.95	126.72
2	D	650	FAD	C5A-N7A-C8A	3.45	108.87	103.45
2	B	650	FAD	C2A-N3A-C4A	3.40	120.14	111.83
2	B	650	FAD	C4X-C10-N10	3.39	121.34	116.48
2	C	650	FAD	C4X-C10-N10	3.27	121.17	116.48
2	A	650	FAD	C4X-C10-N10	3.21	121.08	116.48
2	B	650	FAD	C10-C4X-N5	-3.19	118.30	124.81
2	A	650	FAD	C10-C4X-N5	-3.16	118.35	124.81
2	C	650	FAD	C4-N3-C2	-3.15	120.05	125.64
2	D	650	FAD	C4X-C10-N10	3.14	120.98	116.48
2	C	650	FAD	C5A-N7A-C8A	3.12	108.36	103.45
2	D	650	FAD	C10-C4X-N5	-3.06	118.55	124.81
2	C	650	FAD	C10-C4X-N5	-3.03	118.61	124.81
2	A	650	FAD	C4A-N9A-C8A	3.03	108.92	105.74
2	D	650	FAD	C2A-N3A-C4A	2.95	119.03	111.83
2	B	650	FAD	C4A-C5A-N7A	-2.94	107.22	110.58
2	A	650	FAD	C4A-C5A-N7A	-2.92	107.24	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	650	FAD	C4A-N9A-C8A	2.78	108.66	105.74
2	D	650	FAD	C4A-C5A-N7A	-2.71	107.48	110.58
2	A	650	FAD	C4-C4X-N5	2.71	121.95	118.21
2	A	650	FAD	N3A-C4A-N9A	2.66	131.69	127.17
2	C	650	FAD	C4-C4X-N5	2.55	121.73	118.21
2	C	650	FAD	C4X-C4-N3	2.54	119.73	113.25
2	B	650	FAD	C4-C4X-N5	2.53	121.71	118.21
2	A	650	FAD	C10-N1-C2	2.42	122.09	116.85
2	A	650	FAD	C4-N3-C2	-2.41	121.36	125.64
2	D	650	FAD	C4-N3-C2	-2.41	121.36	125.64
2	C	650	FAD	N3A-C4A-N9A	2.41	131.26	127.17
2	A	650	FAD	O4'-C4'-C3'	2.33	114.69	109.25
2	B	650	FAD	N3A-C4A-N9A	2.25	131.00	127.17
2	D	650	FAD	C4-C4X-N5	2.21	121.26	118.21
2	B	650	FAD	O5'-C5'-C4'	2.20	115.23	109.36
2	B	650	FAD	O4'-C4'-C3'	2.18	114.35	109.25
2	D	650	FAD	C4X-C10-N1	-2.17	119.27	124.59
2	C	650	FAD	C4A-C5A-N7A	-2.17	108.10	110.58
2	C	650	FAD	O4'-C4'-C3'	2.15	114.27	109.25
2	C	650	FAD	C4X-C10-N1	-2.14	119.35	124.59
2	D	650	FAD	C4X-C4-N3	2.14	118.69	113.25
2	B	650	FAD	C4-N3-C2	-2.07	121.97	125.64
2	D	650	FAD	C4A-N9A-C8A	2.06	107.90	105.74
2	D	650	FAD	C10-N1-C2	2.04	121.26	116.85
2	A	650	FAD	C4X-C10-N1	-2.03	119.60	124.59

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	650	FAD	C2'-C3'-C4'-O4'
2	A	650	FAD	C2'-C3'-C4'-C5'
2	C	650	FAD	O3'-C3'-C4'-O4'
2	A	650	FAD	C2'-C3'-C4'-O4'
2	B	650	FAD	C2'-C3'-C4'-O4'
2	D	650	FAD	C2'-C3'-C4'-O4'
2	B	650	FAD	O3'-C3'-C4'-O4'
2	A	650	FAD	O3'-C3'-C4'-C5'
2	B	650	FAD	O3'-C3'-C4'-C5'
2	C	650	FAD	O3'-C3'-C4'-C5'
2	D	650	FAD	O3'-C3'-C4'-O4'
2	D	650	FAD	O3'-C3'-C4'-C5'

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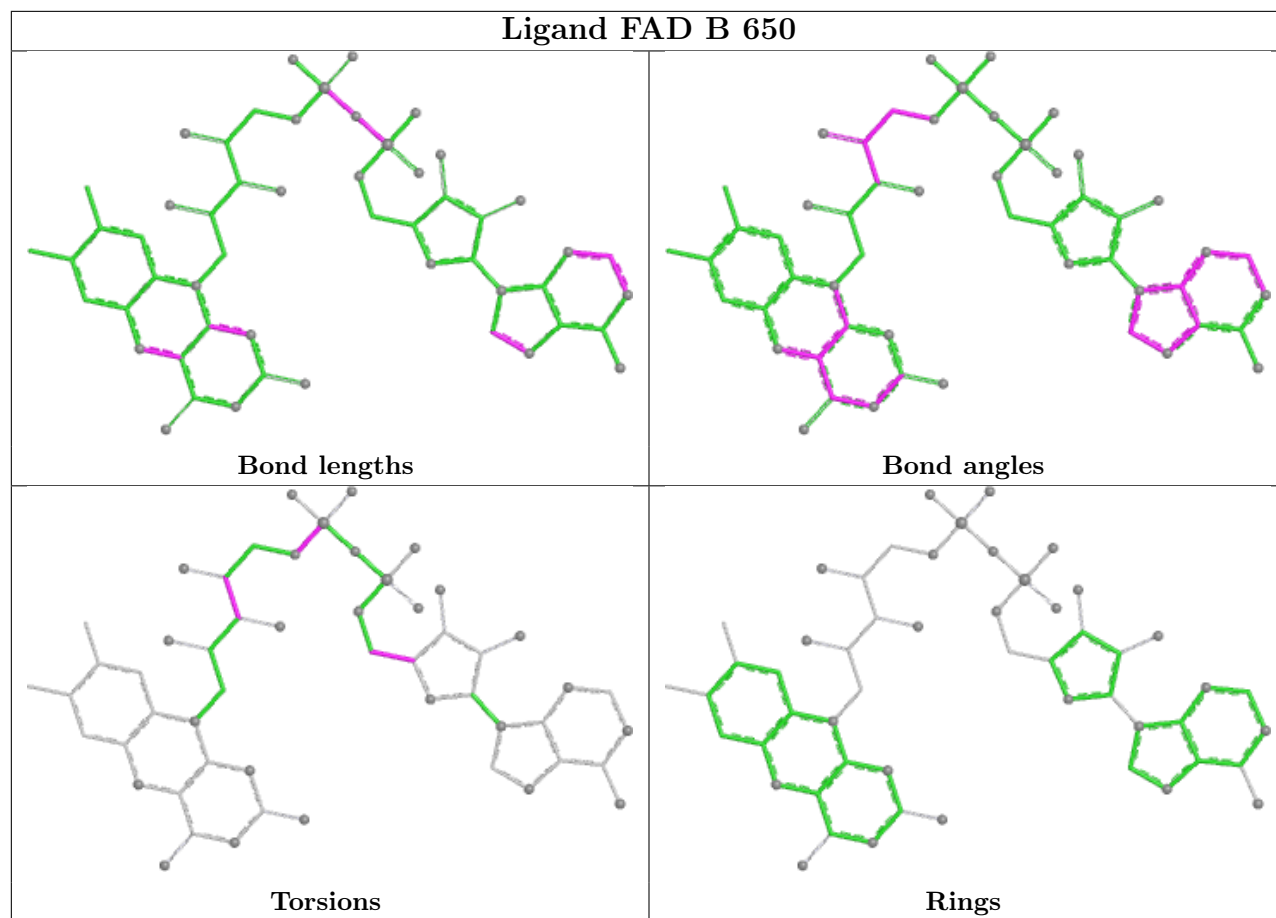
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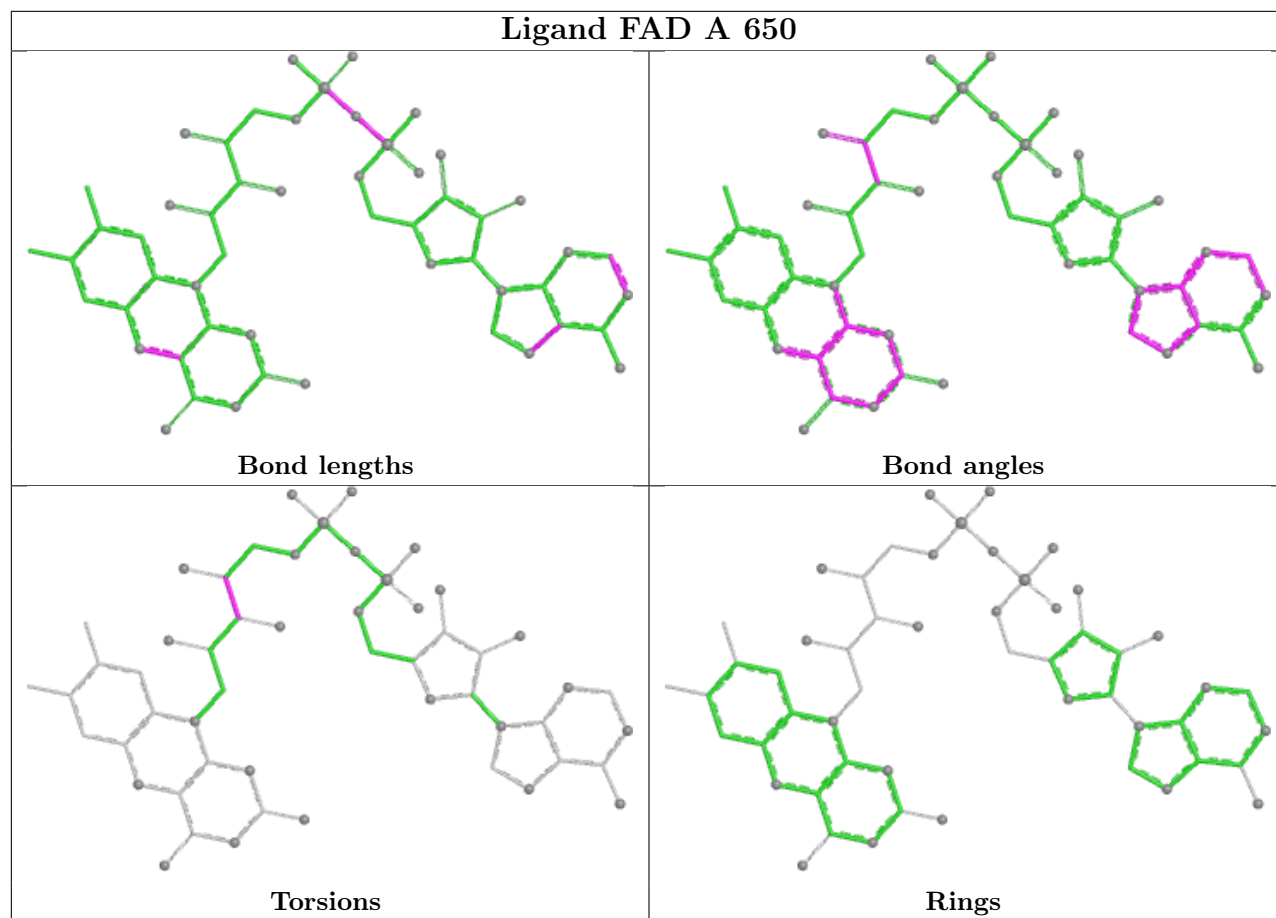
Mol	Chain	Res	Type	Atoms
2	B	650	FAD	C2'-C3'-C4'-C5'
2	C	650	FAD	C2'-C3'-C4'-C5'
2	A	650	FAD	O3'-C3'-C4'-O4'
2	D	650	FAD	C2'-C3'-C4'-C5'
2	B	650	FAD	C5'-O5'-P-O2P
2	B	650	FAD	O4B-C4B-C5B-O5B
2	D	650	FAD	O4B-C4B-C5B-O5B

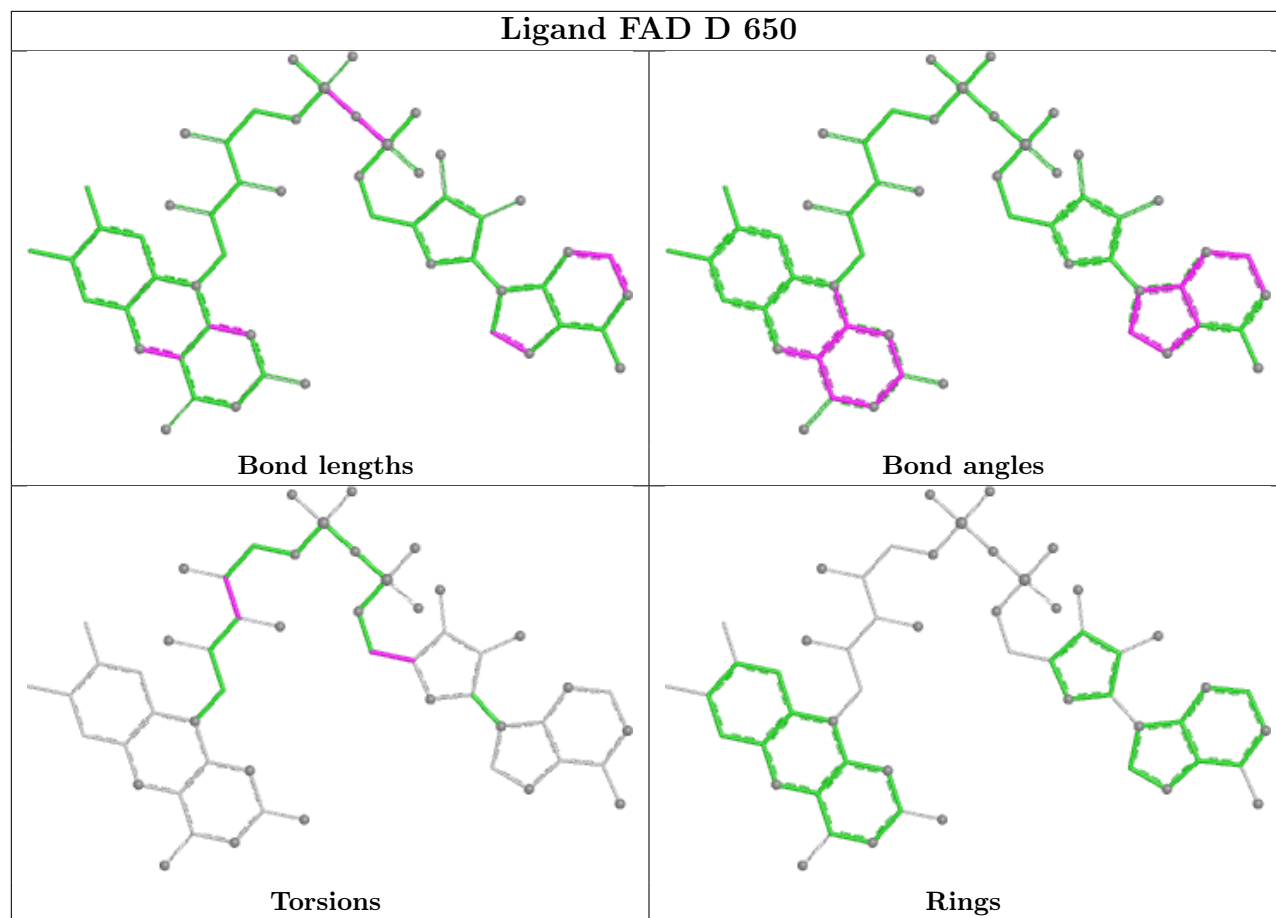
There are no ring outliers.

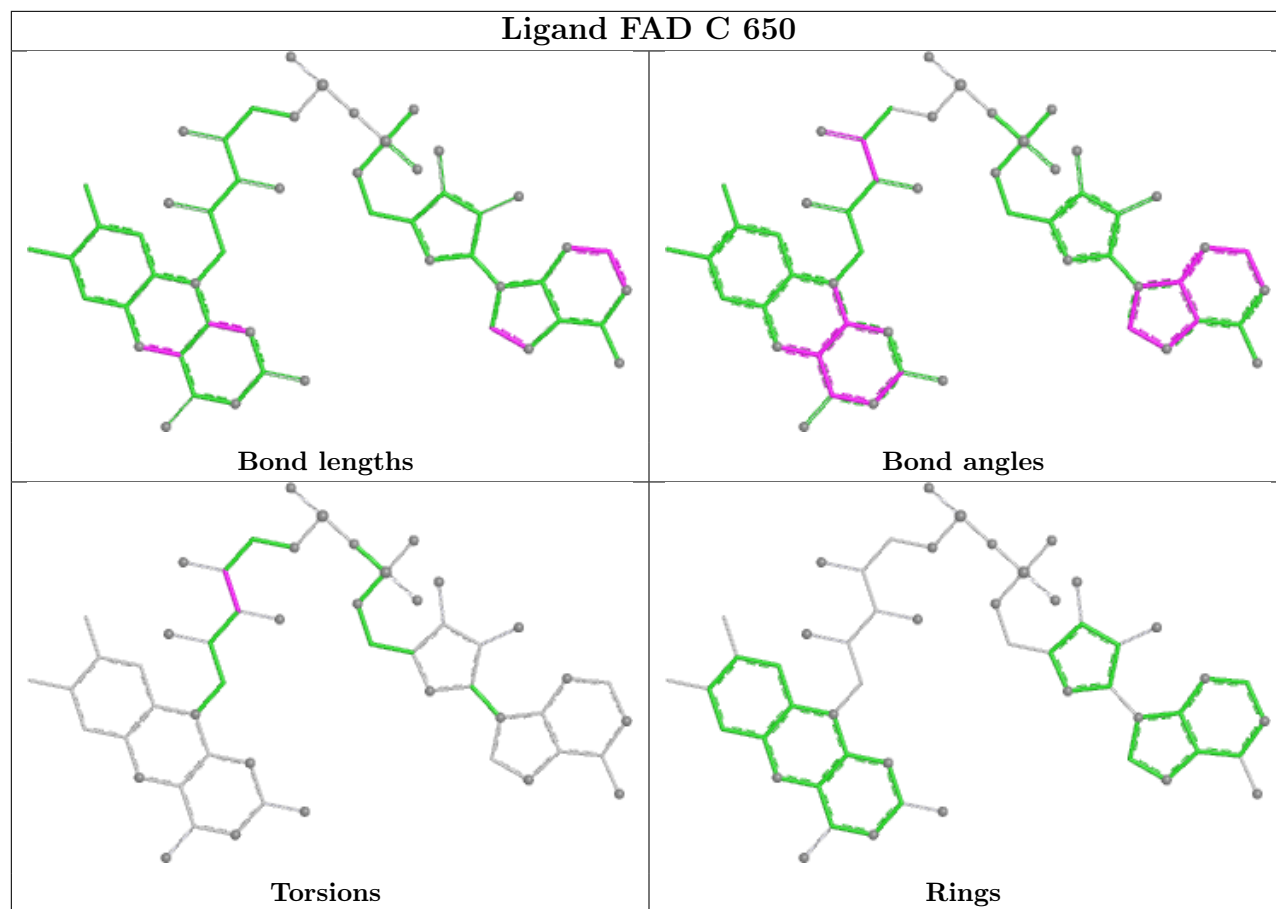
No monomer is involved in short contacts.

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%)	-0.10	7 (1%) 73 70	22, 36, 58, 76	0
1	B	496/511 (97%)	-0.17	4 (0%) 82 80	22, 36, 58, 76	0
1	C	496/511 (97%)	-0.06	10 (2%) 65 61	22, 36, 59, 76	0
1	D	496/511 (97%)	0.11	13 (2%) 57 52	22, 36, 59, 76	0
All	All	1984/2044 (97%)	-0.05	34 (1%) 69 65	22, 36, 58, 76	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	GLY	4.2
1	C	113	GLY	4.1
1	D	164	PHE	4.1
1	A	159	GLU	4.0
1	B	162	ALA	3.3
1	D	42	ILE	3.2
1	B	113	GLY	3.2
1	A	242	GLN	3.1
1	A	240	ARG	3.0
1	A	117	THR	2.9
1	A	146	SER	2.8
1	D	43	GLY	2.7
1	C	164	PHE	2.6
1	D	117	THR	2.6
1	C	163	GLN	2.5
1	C	39	VAL	2.5
1	D	165	PRO	2.5
1	D	146	SER	2.5
1	B	267	ARG	2.4
1	C	44	VAL	2.4
1	D	161	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	44	VAL	2.4
1	C	42	ILE	2.3
1	B	117	THR	2.3
1	D	113	GLY	2.2
1	D	320	LEU	2.2
1	D	162	ALA	2.2
1	A	267	ARG	2.1
1	D	432	GLU	2.1
1	C	165	PRO	2.1
1	C	498	ALA	2.1
1	C	162	ALA	2.1
1	D	316	GLY	2.1
1	C	43	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.

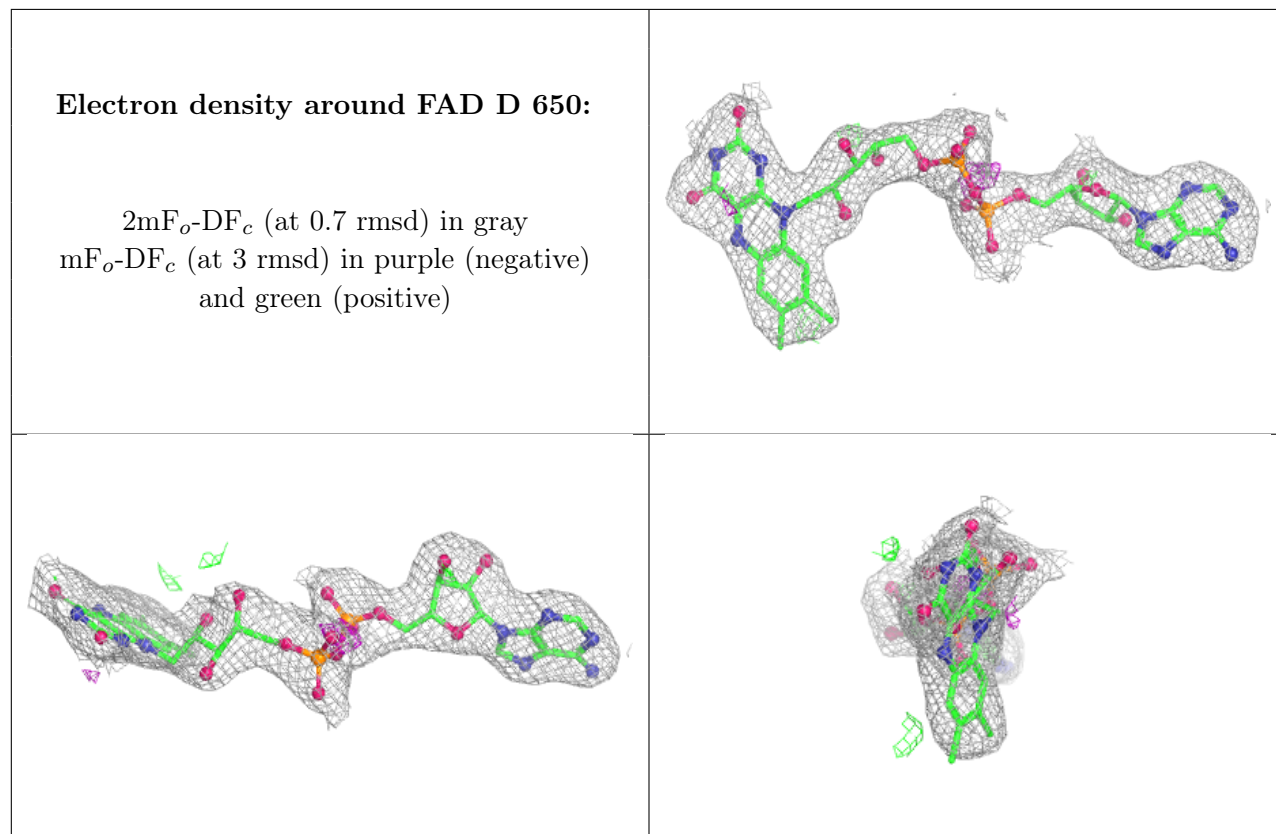
5.4 Ligands [i](#)

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
2	FAD	D	650	53/53	0.92	0.09	22,33,38,43	0
3	CL	C	700	1/1	0.92	0.11	44,44,44,44	0
3	CL	B	700	1/1	0.93	0.11	44,44,44,44	0
2	FAD	C	650	52/53	0.95	0.09	22,33,38,43	0
2	FAD	B	650	53/53	0.95	0.07	22,32,38,43	0
2	FAD	A	650	53/53	0.96	0.07	22,32,38,43	0
3	CL	D	700	1/1	0.96	0.18	45,45,45,45	0
3	CL	A	700	1/1	0.97	0.06	43,43,43,43	0

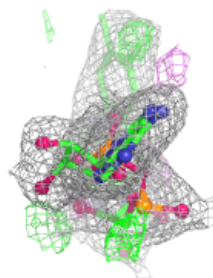
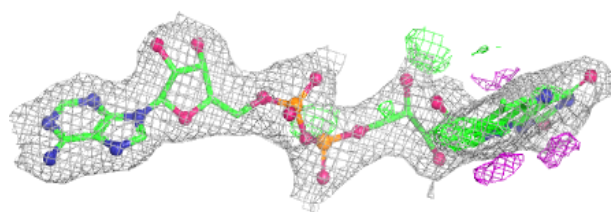
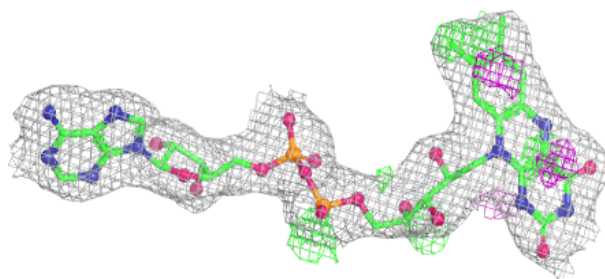
The following is a graphical depiction of the model fit to experimental electron density of all

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.

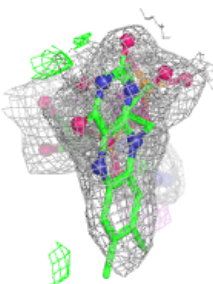
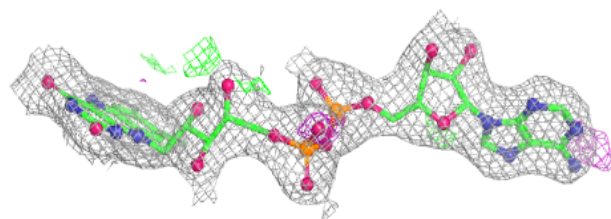
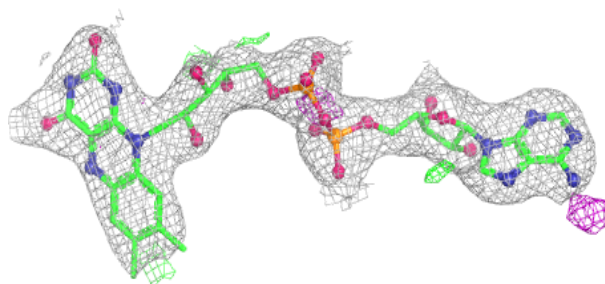


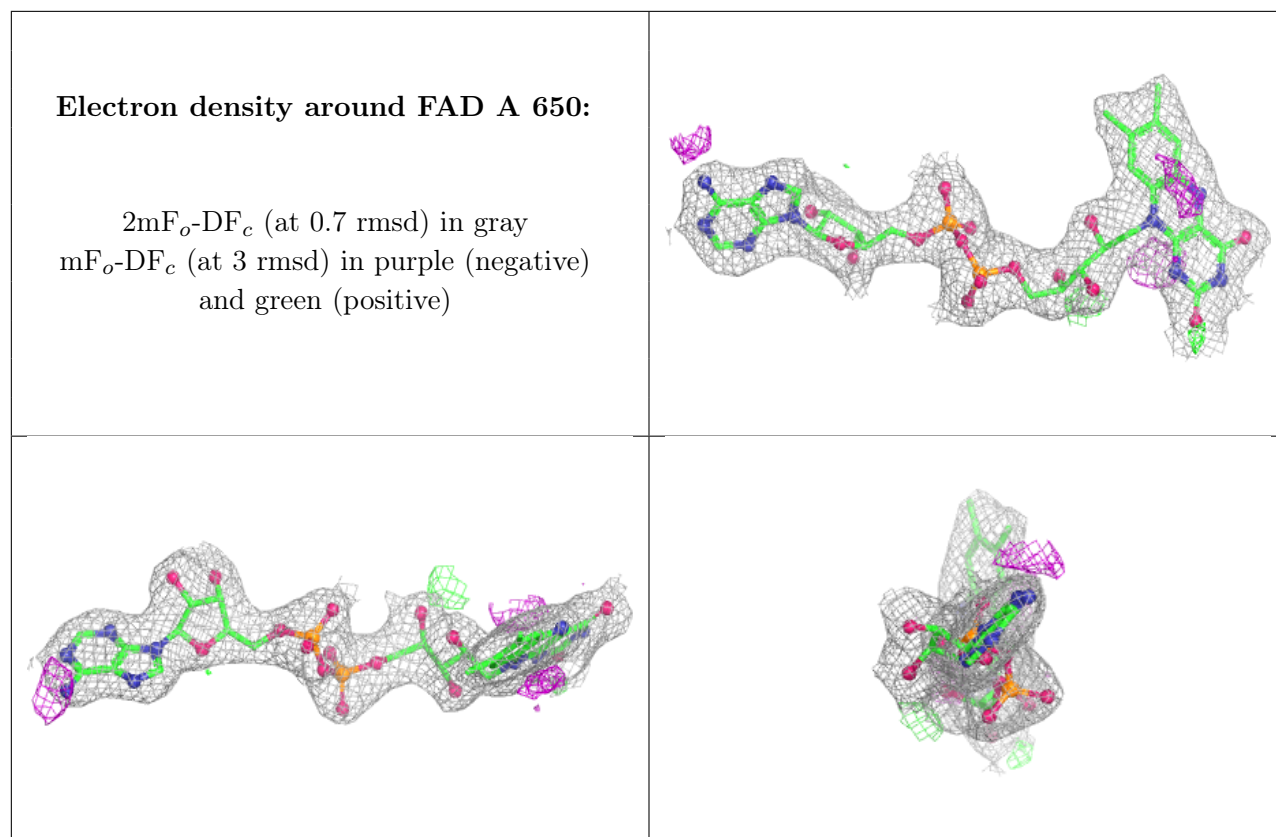
Electron density around FAD C 650:

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

**Electron density around FAD B 650:**

$2mF_o-DF_c$ (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.