



wwPDB X-ray Structure Validation Summary Report

Nov 2, 2024 – 10:26 pm GMT

PDB ID : 2C0U
Title : Crystal Structure of a Covalent Complex of Nitroalkane Oxidase Trapped During Substrate Turnover
Authors : Nagpal, A.; Valley, M.P.; Fitzpatrick, P.F.; Orville, A.M.
Deposited on : 2005-09-07
Resolution : 2.20 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 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

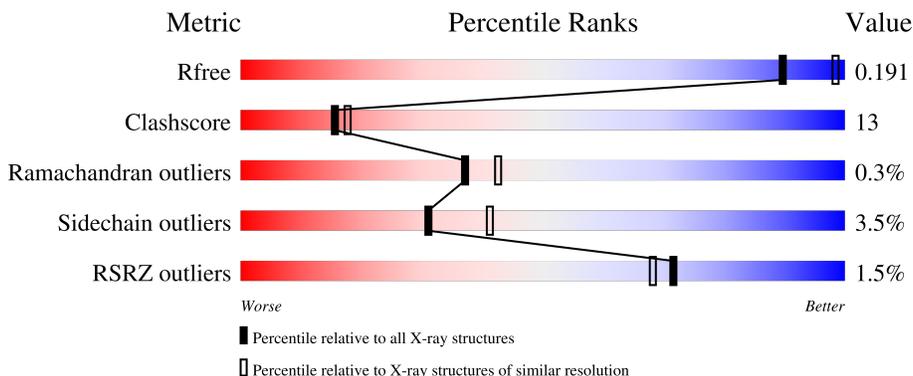
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 $\leq 5\%$. 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	439	 73% 22% ..
1	B	439	 72% 23% ..
1	C	439	 74% 22% ..
1	D	439	 72% 24% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NBT	A	1433	-	-	X	-
3	NBT	B	1433	-	-	X	-
3	NBT	C	1433	-	-	X	-
3	NBT	D	1433	-	-	X	-

2 Entry composition [i](#)

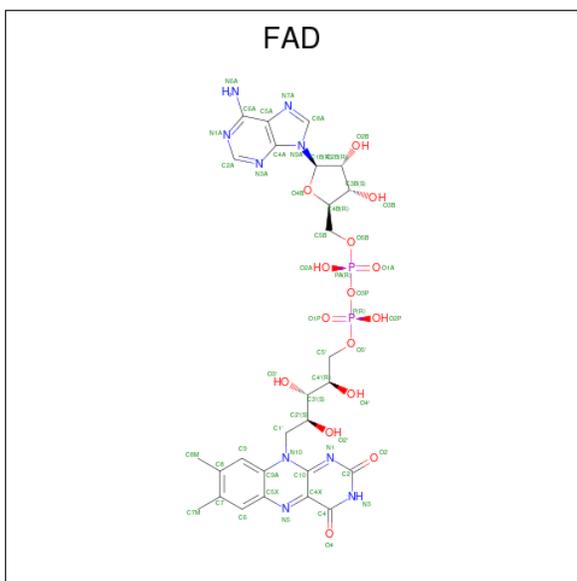
There are 4 unique types of molecules in this entry. The entry contains 14160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITROALKANE OXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	430	Total 3307	C 2095	N 567	O 625	S 7	Se 13	0	0	0
1	B	430	Total 3307	C 2095	N 567	O 625	S 7	Se 13	0	0	0
1	C	430	Total 3307	C 2095	N 567	O 625	S 7	Se 13	0	0	0
1	D	430	Total 3307	C 2095	N 567	O 625	S 7	Se 13	0	0	0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



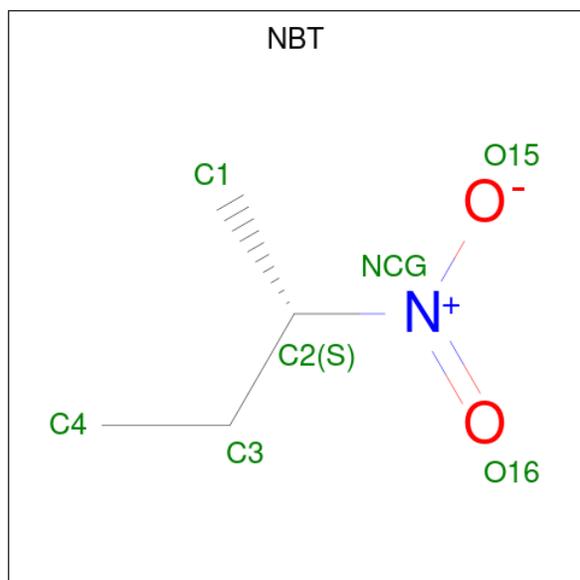
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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 (2S)-2-NITROBUTANE (three-letter code: NBT) (formula: C₄H₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	4	1	2		
3	B	1	Total	C	N	O	0	0
			7	4	1	2		
3	C	1	Total	C	N	O	0	0
			7	4	1	2		
3	D	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total	O	0	0
			171	171		
4	B	175	Total	O	0	0
			175	175		
4	C	204	Total	O	0	0
			204	204		

Continued on next page...

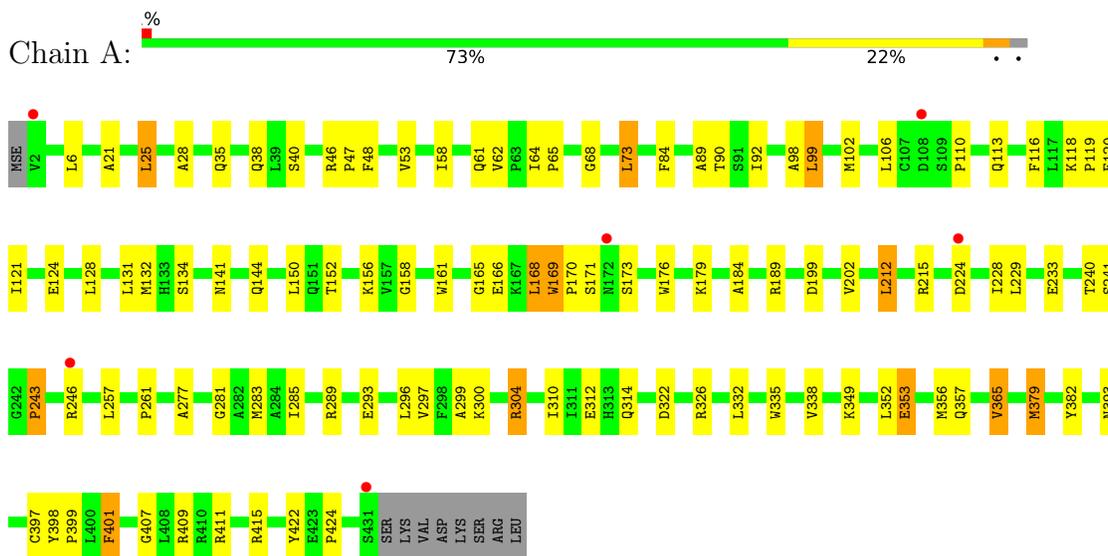
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	142	Total 142	O 142	0	0

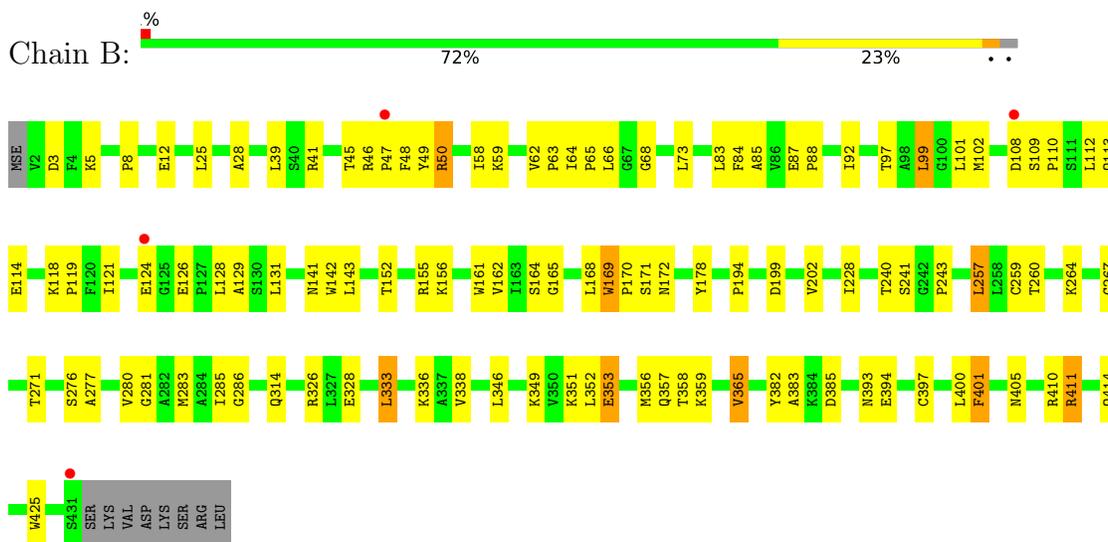
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

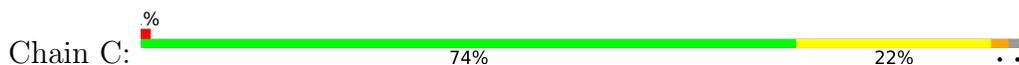
- Molecule 1: NITROALKANE OXIDASE



- Molecule 1: NITROALKANE OXIDASE



- Molecule 1: NITROALKANE OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.39Å 163.74Å 173.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.20) 99.8 (40.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.232 0.189 , 0.191	Depositor DCC
R_{free} test set	6564 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtrriage
Anisotropy	0.287	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14160	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: NBT, 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	0.36	0/3363	0.54	0/4542
1	B	0.36	0/3363	0.55	0/4542
1	C	0.38	0/3363	0.56	0/4542
1	D	0.33	0/3363	0.51	0/4542
All	All	0.36	0/13452	0.54	0/18168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3307	0	3319	94	0
1	B	3307	0	3319	89	0
1	C	3307	0	3319	94	0
1	D	3307	0	3319	86	0
2	A	53	0	31	6	0
2	B	53	0	31	9	0
2	C	53	0	31	7	0
2	D	53	0	31	5	0
3	A	7	0	8	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	8	4	0
3	C	7	0	8	4	0
3	D	7	0	8	4	0
4	A	171	0	0	8	0
4	B	175	0	0	9	0
4	C	204	0	0	7	0
4	D	142	0	0	0	0
All	All	14160	0	13432	356	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 13.

The worst 5 of 356 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:D:5:LYS:HE3	1:D:6:LEU:H	1.33	0.94
1:B:141:ASN:HD21	2:B:1432:FAD:H61A	1.17	0.89
1:B:102:MSE:HG3	4:B:2121:HOH:O	1.72	0.87
1:D:36:LYS:H	1:D:36:LYS:HZ2	1.19	0.86
1:B:92:ILE:HG21	1:B:240:THR:HG22	1.58	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	428/439 (98%)	416 (97%)	10 (2%)	2 (0%)	25 28
1	B	428/439 (98%)	415 (97%)	12 (3%)	1 (0%)	44 52
1	C	428/439 (98%)	416 (97%)	11 (3%)	1 (0%)	44 52
1	D	428/439 (98%)	418 (98%)	9 (2%)	1 (0%)	44 52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1712/1756 (98%)	1665 (97%)	42 (2%)	5 (0%)	37 42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	TRP
1	B	169	TRP
1	C	169	TRP
1	D	169	TRP
1	A	243	PRO

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	355/350 (101%)	343 (97%)	12 (3%)	32 42
1	B	355/350 (101%)	343 (97%)	12 (3%)	32 42
1	C	355/350 (101%)	341 (96%)	14 (4%)	27 37
1	D	355/350 (101%)	344 (97%)	11 (3%)	35 47
All	All	1420/1400 (101%)	1371 (96%)	49 (4%)	31 41

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	128	LEU
1	C	391	LEU
1	C	172	ASN
1	C	346	LEU
1	C	411	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	43	GLN
1	D	10	GLN
1	C	137	ASN
1	C	393	ASN
1	D	55	HIS

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 oligosaccharides 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
2	FAD	D	1432	3	53,58,58	1.03	3 (5%)	68,89,89	1.30	7 (10%)
3	NBT	B	1433	2	4,6,6	4.54	1 (25%)	3,7,7	0.51	0
3	NBT	D	1433	2	4,6,6	4.54	1 (25%)	3,7,7	0.54	0
2	FAD	A	1432	3	53,58,58	1.06	3 (5%)	68,89,89	1.31	8 (11%)
2	FAD	B	1432	3	53,58,58	1.04	3 (5%)	68,89,89	1.28	7 (10%)
3	NBT	A	1433	2	4,6,6	4.53	1 (25%)	3,7,7	0.53	0
3	NBT	C	1433	2	4,6,6	4.56	1 (25%)	3,7,7	0.52	0
2	FAD	C	1432	3	53,58,58	1.04	3 (5%)	68,89,89	1.30	8 (11%)

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	D	1432	3	-	7/30/50/50	0/6/6/6
3	NBT	B	1433	2	-	1/4/6/6	-
3	NBT	D	1433	2	-	0/4/6/6	-
2	FAD	A	1432	3	-	8/30/50/50	0/6/6/6
2	FAD	B	1432	3	-	7/30/50/50	0/6/6/6
3	NBT	A	1433	2	-	0/4/6/6	-
3	NBT	C	1433	2	-	0/4/6/6	-
2	FAD	C	1432	3	-	8/30/50/50	0/6/6/6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1433	NBT	O16-NCG	9.06	1.42	1.22
3	D	1433	NBT	O16-NCG	9.03	1.42	1.22
3	B	1433	NBT	O16-NCG	9.03	1.42	1.22
3	A	1433	NBT	O16-NCG	9.00	1.42	1.22
2	A	1432	FAD	C10-N1	3.57	1.40	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1432	FAD	N3A-C2A-N1A	-4.82	121.14	128.68
2	A	1432	FAD	N3A-C2A-N1A	-4.82	121.15	128.68
2	B	1432	FAD	N3A-C2A-N1A	-4.75	121.26	128.68
2	D	1432	FAD	N3A-C2A-N1A	-4.72	121.30	128.68
2	D	1432	FAD	P-O3P-PA	-3.28	121.58	132.83

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

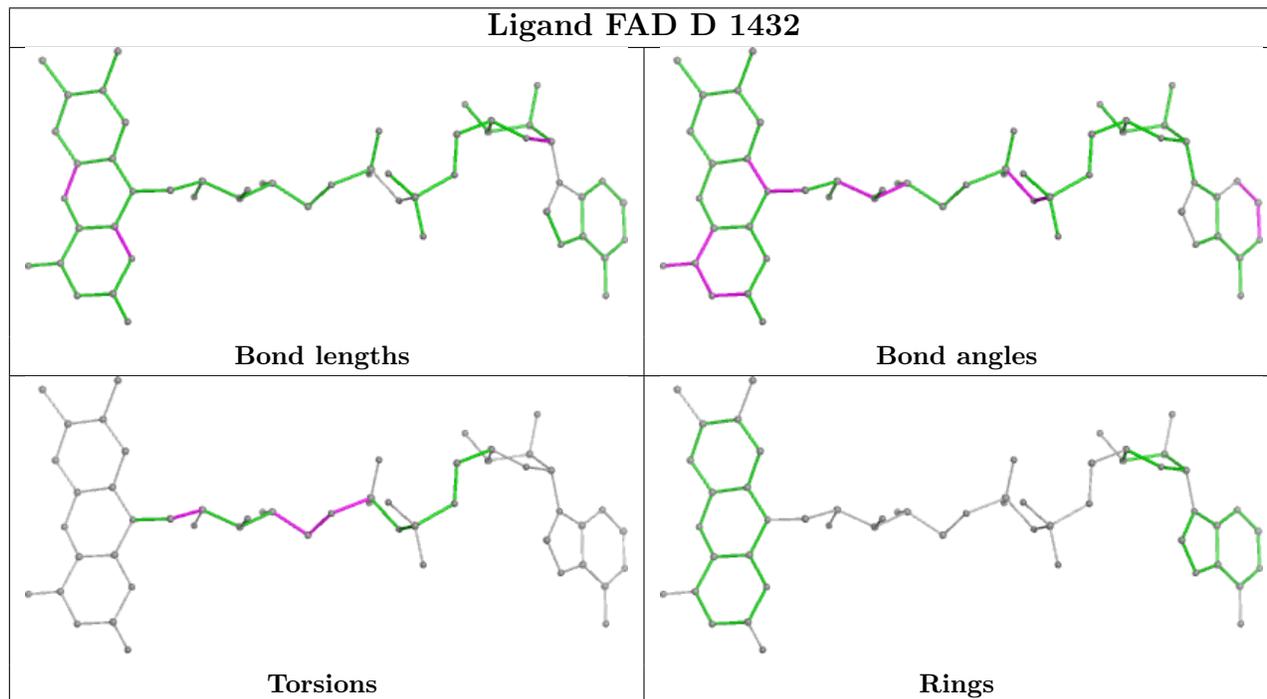
Mol	Chain	Res	Type	Atoms
2	A	1432	FAD	C3'-C4'-C5'-O5'
2	A	1432	FAD	O4'-C4'-C5'-O5'
2	A	1432	FAD	C5'-O5'-P-O2P
2	B	1432	FAD	C3'-C4'-C5'-O5'
2	B	1432	FAD	O4'-C4'-C5'-O5'

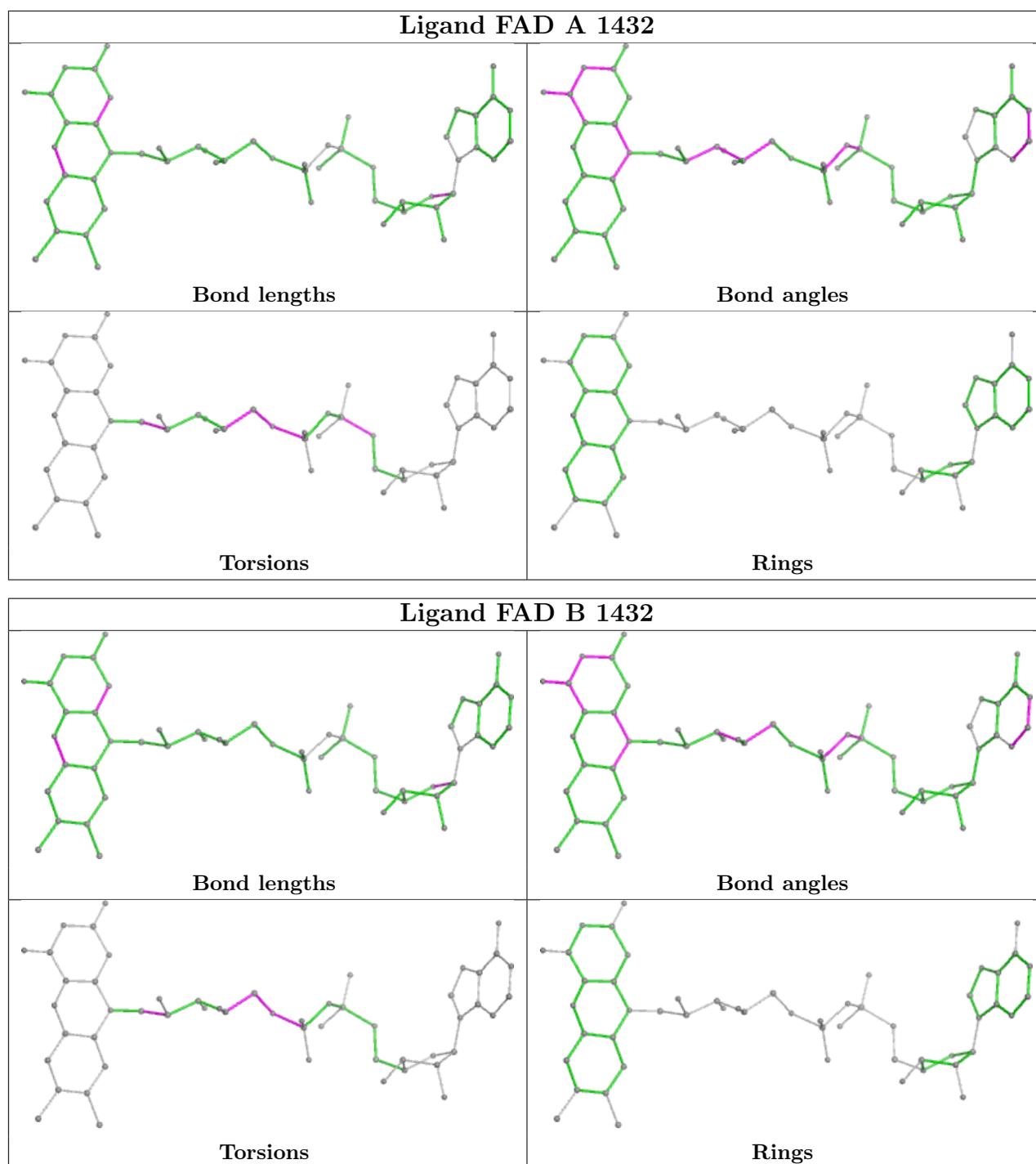
There are no ring outliers.

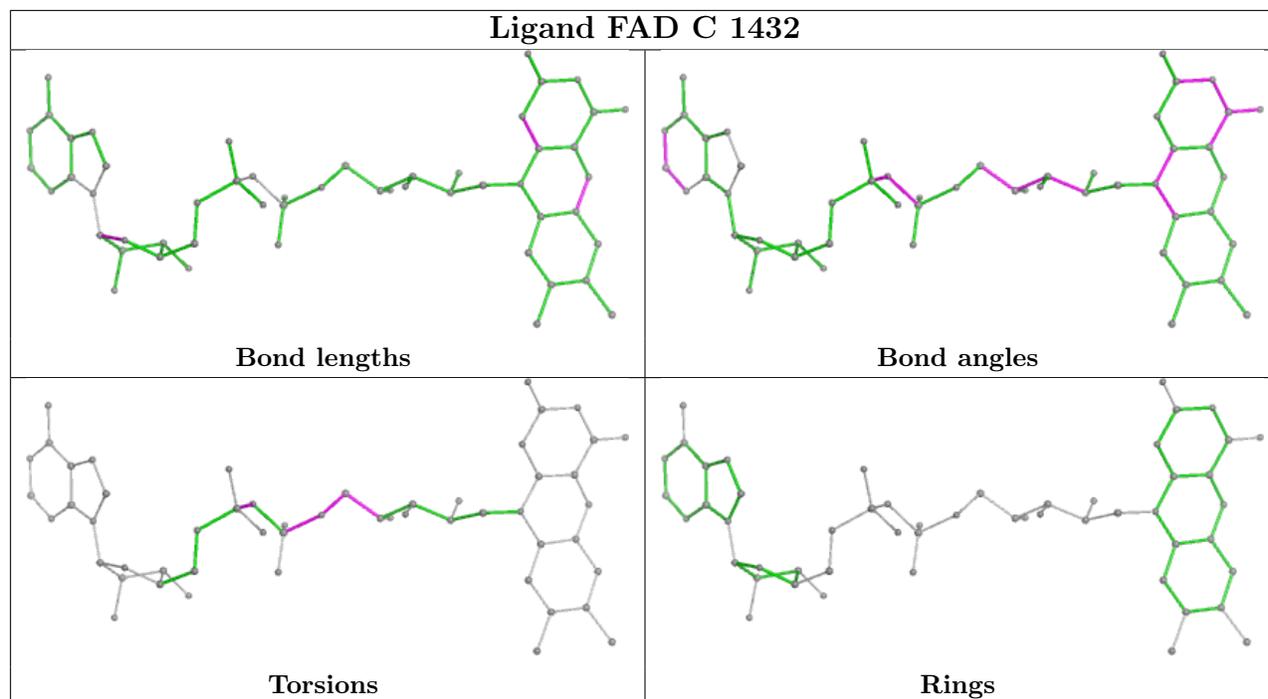
8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1432	FAD	5	0
3	B	1433	NBT	4	0
3	D	1433	NBT	4	0
2	A	1432	FAD	6	0
2	B	1432	FAD	9	0
3	A	1433	NBT	5	0
3	C	1433	NBT	4	0
2	C	1432	FAD	7	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.







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	417/439 (94%)	-0.24	6 (1%) 73 70	18, 30, 50, 66	0
1	B	417/439 (94%)	-0.06	4 (0%) 79 76	20, 32, 51, 70	1 (0%)
1	C	417/439 (94%)	-0.27	5 (1%) 76 73	16, 29, 49, 64	1 (0%)
1	D	417/439 (94%)	0.13	10 (2%) 59 56	22, 36, 56, 68	0
All	All	1668/1756 (94%)	-0.11	25 (1%) 71 68	16, 32, 53, 70	2 (0%)

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	36	LYS	3.5
1	C	21	ALA	3.2
1	D	431	SER	3.1
1	B	431	SER	3.0
1	A	431	SER	2.8

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

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

6.3 Carbohydrates [i](#)

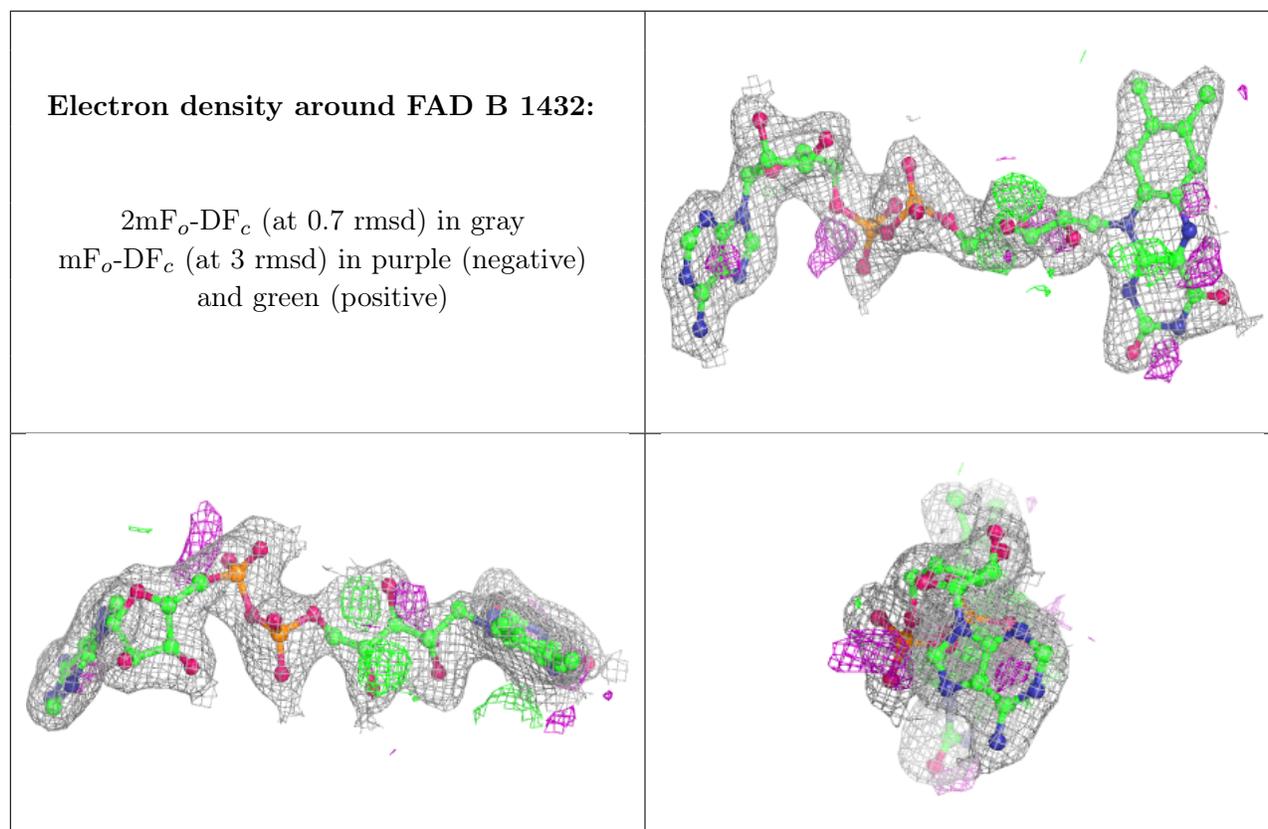
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

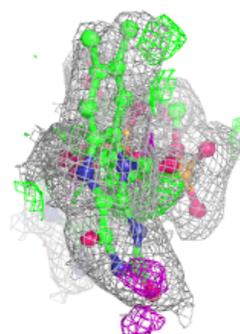
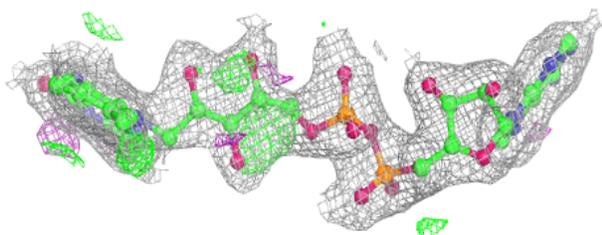
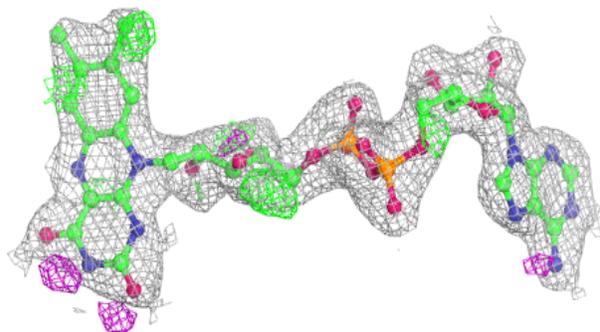
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NBT	B	1433	7/7	0.74	0.36	50,52,76,88	0
3	NBT	D	1433	7/7	0.77	0.29	49,54,75,82	0
3	NBT	C	1433	7/7	0.81	0.27	45,53,71,77	0
3	NBT	A	1433	7/7	0.84	0.26	43,55,76,84	0
2	FAD	B	1432	53/53	0.94	0.10	15,32,44,47	0
2	FAD	D	1432	53/53	0.94	0.09	23,33,44,47	0
2	FAD	C	1432	53/53	0.95	0.08	19,29,40,43	0
2	FAD	A	1432	53/53	0.95	0.08	20,29,40,41	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.

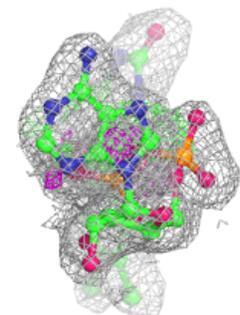
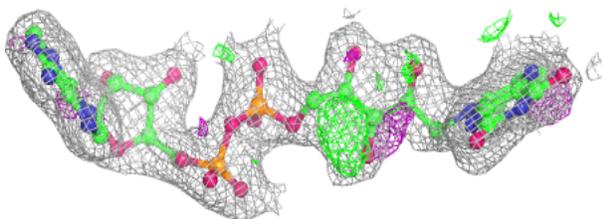
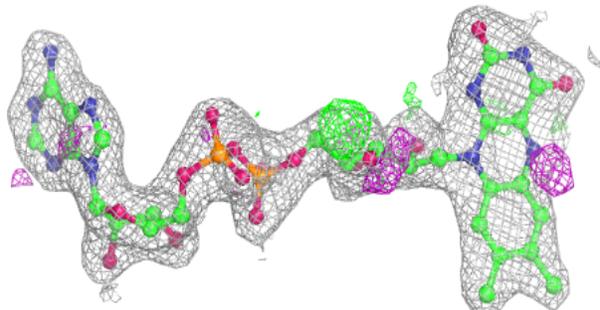


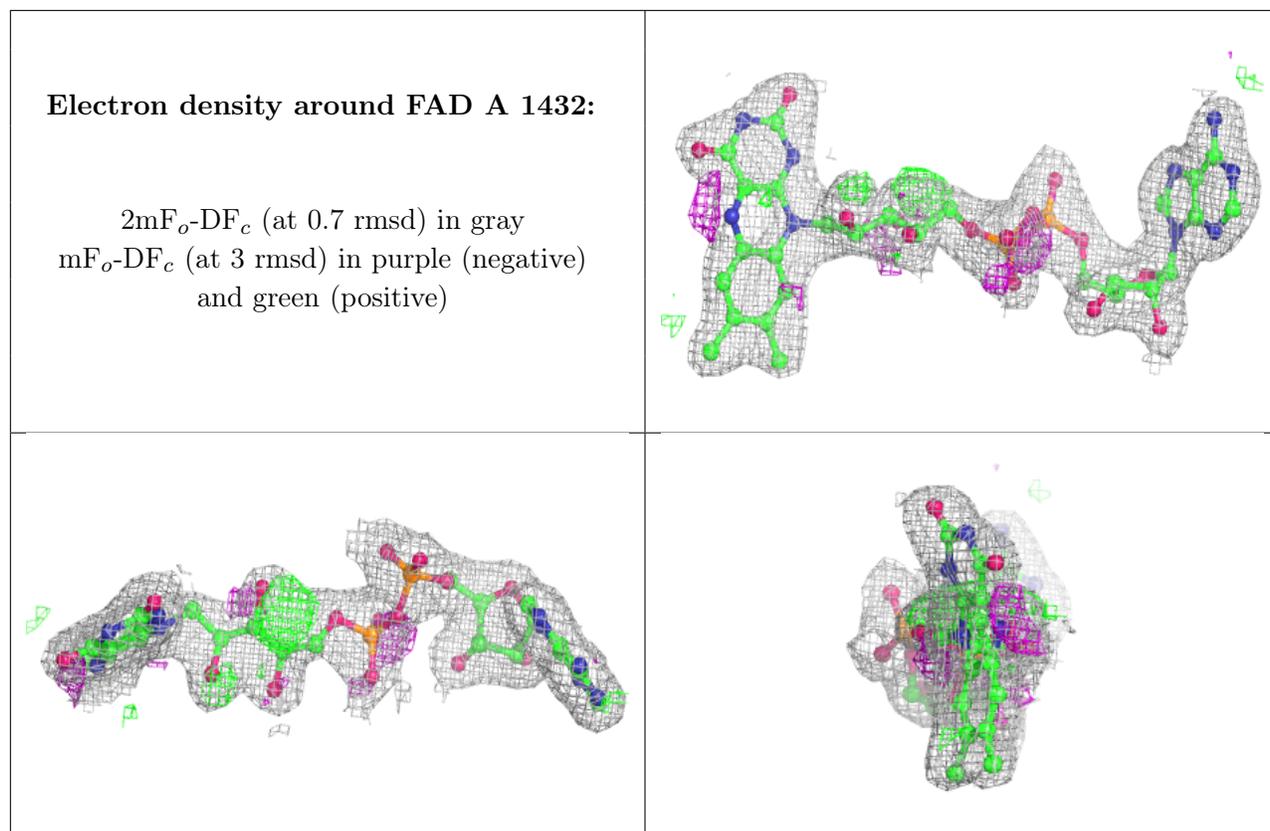
Electron density around FAD D 1432:

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

**Electron density around FAD C 1432:**

$2mF_o-DF_c$ (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.