



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 06:16 PM UTC

PDB ID : 2W0H / pdb_00002w0h
Title : X ray structure of Leishmania infantum Trypanothione reductase in complex with antimony and NADPH
Authors : Baiocco, P.; Colotti, G.; Franceschini, S.; Ilari, A.
Deposited on : 2008-08-18
Resolution : 3.00 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

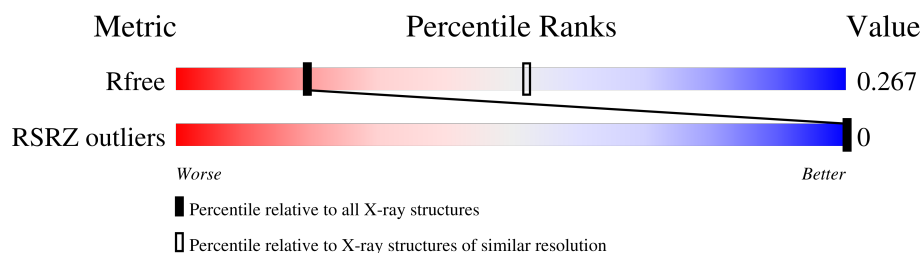
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

2 Entry composition [i](#)

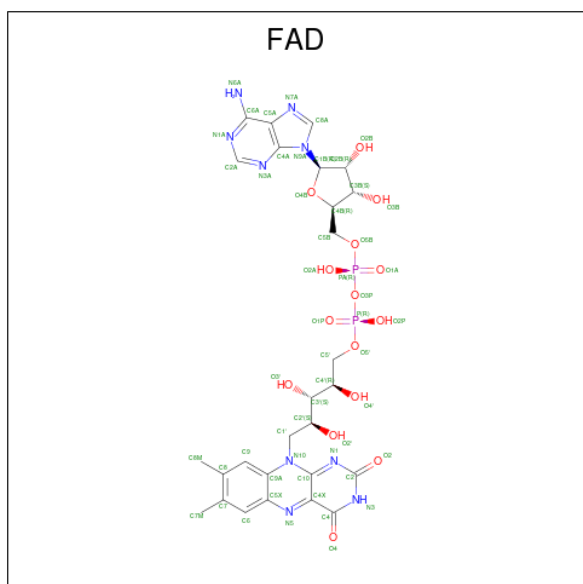
There are 6 unique types of molecules in this entry. The entry contains 7598 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRYPTANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3672	2308	631	707	26			
1	B	487	Total	C	N	O	S	0	0	0
			3686	2317	633	710	26			

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

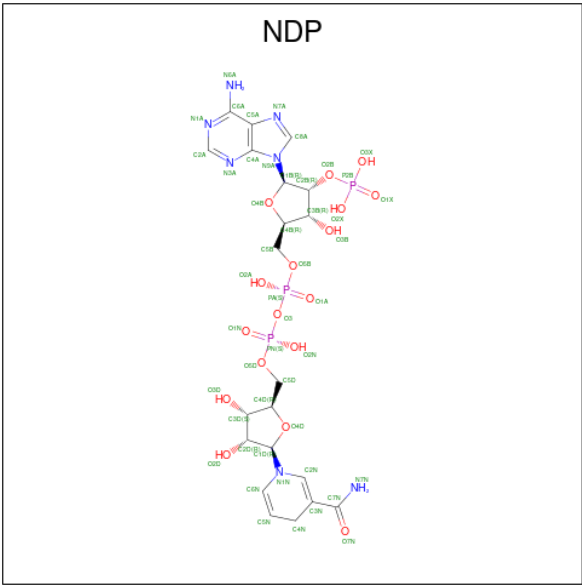


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is ANTIMONY (III) ION (CCD ID: SB) (formula: Sb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Sb	0	0
			1	1		
3	B	1	Total	Sb	0	0
			1	1		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	B	14	Total	O	0	0
			14	14		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	102.94Å 102.94Å 193.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.14 – 3.00 102.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.1 (103.14-3.00) 87.1 (102.94-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.262 0.239 , 0.267	Depositor DCC
R_{free} test set	1788 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7598	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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 8 ligands modelled in this entry, 2 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	$\# Z > 2$
4	NDP	A	1488	-	51,52,52	2.16	15 (29%)	71,80,80	1.51	10 (14%)
2	FAD	A	1486	-	58,58,58	1.16	7 (12%)	85,89,89	1.58	15 (17%)
5	SO4	A	1489	-	4,4,4	0.25	0	6,6,6	0.10	0
4	NDP	B	1488	-	51,52,52	2.15	15 (29%)	71,80,80	1.51	9 (12%)
2	FAD	B	1486	-	58,58,58	1.14	6 (10%)	85,89,89	1.54	16 (18%)
5	SO4	B	1489	-	4,4,4	0.23	0	6,6,6	0.14	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
4	NDP	A	1488	-	4/4/14/17	10/34/77/77	0/5/5/5
4	NDP	B	1488	-	4/4/14/17	10/34/77/77	0/5/5/5
2	FAD	A	1486	-	-	4/34/50/50	0/6/6/6
2	FAD	B	1486	-	-	3/34/50/50	0/6/6/6

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1488	NDP	P2B-O2X	6.49	1.78	1.54
4	A	1488	NDP	P2B-O2X	6.47	1.78	1.54
4	B	1488	NDP	P2B-O3X	6.36	1.78	1.54
4	A	1488	NDP	P2B-O3X	6.30	1.78	1.54
4	A	1488	NDP	PA-O2A	5.10	1.79	1.55
4	B	1488	NDP	PA-O2A	5.09	1.78	1.55
4	A	1488	NDP	PN-O2N	4.99	1.78	1.55
4	B	1488	NDP	PN-O2N	4.93	1.78	1.55
4	A	1488	NDP	C5A-C4A	4.75	1.47	1.39
4	B	1488	NDP	C5A-C4A	4.73	1.47	1.39
2	B	1486	FAD	C4X-N5	3.69	1.38	1.30
2	A	1486	FAD	C4X-N5	3.60	1.38	1.30
2	A	1486	FAD	C10-N1	3.13	1.39	1.33
2	B	1486	FAD	C10-N1	2.97	1.39	1.33
4	B	1488	NDP	P2B-O1X	2.86	1.59	1.50
4	A	1488	NDP	PN-O3	2.83	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1488	NDP	P2B-O1X	2.83	1.59	1.50
4	A	1488	NDP	C5A-C6A	2.82	1.48	1.41
2	B	1486	FAD	C2A-N3A	2.74	1.38	1.33
4	B	1488	NDP	PN-O3	2.74	1.62	1.59
2	B	1486	FAD	C2A-N1A	2.73	1.38	1.33
4	B	1488	NDP	C5A-C6A	2.73	1.48	1.41
2	A	1486	FAD	C2A-N3A	2.69	1.38	1.33
2	A	1486	FAD	C2A-N1A	2.67	1.38	1.33
4	A	1488	NDP	PA-O3	2.60	1.62	1.59
4	A	1488	NDP	PA-O1A	2.47	1.59	1.50
4	B	1488	NDP	PA-O1A	2.46	1.59	1.50
4	B	1488	NDP	PN-O1N	2.44	1.59	1.50
4	A	1488	NDP	PN-O1N	2.43	1.59	1.50
4	A	1488	NDP	C8A-N7A	2.33	1.36	1.31
4	B	1488	NDP	PA-O3	2.31	1.62	1.59
4	A	1488	NDP	C5A-N7A	-2.29	1.34	1.39
2	A	1486	FAD	PA-O3P	2.29	1.62	1.59
4	B	1488	NDP	C5A-N7A	-2.24	1.35	1.39
4	A	1488	NDP	C6N-C5N	2.21	1.39	1.33
4	B	1488	NDP	C8A-N7A	2.21	1.35	1.31
4	B	1488	NDP	C6N-C5N	2.19	1.39	1.33
4	B	1488	NDP	C2N-C3N	2.12	1.41	1.35
2	B	1486	FAD	C8A-N7A	2.12	1.35	1.31
2	A	1486	FAD	P-O3P	2.10	1.61	1.59
2	A	1486	FAD	C8A-N7A	2.09	1.35	1.31
4	A	1488	NDP	C2N-C3N	2.05	1.40	1.35
2	B	1486	FAD	P-O3P	2.00	1.61	1.59

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1488	NDP	C5A-C4A-N3A	-5.92	118.57	126.72
4	A	1488	NDP	C5A-C4A-N3A	-5.84	118.68	126.72
2	B	1486	FAD	N3A-C2A-N1A	-5.63	120.07	128.58
2	A	1486	FAD	N3A-C2A-N1A	-5.57	120.15	128.58
4	B	1488	NDP	N3A-C4A-N9A	4.87	135.46	127.17
2	A	1486	FAD	C5A-C4A-N3A	-4.75	120.18	126.72
2	B	1486	FAD	C5A-C4A-N3A	-4.68	120.27	126.72
4	A	1488	NDP	N3A-C4A-N9A	4.68	135.12	127.17
4	B	1488	NDP	C2A-N3A-C4A	3.97	121.53	111.83
4	A	1488	NDP	C2A-N3A-C4A	3.90	121.36	111.83
2	A	1486	FAD	N9A-C8A-N7A	-3.77	108.59	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1488	NDP	N3A-C2A-N1A	-3.69	123.00	128.58
2	A	1486	FAD	C5A-N7A-C8A	3.62	109.14	103.45
4	A	1488	NDP	N3A-C2A-N1A	-3.58	123.16	128.58
2	B	1486	FAD	N9A-C8A-N7A	-3.51	108.96	113.94
2	B	1486	FAD	C2A-N3A-C4A	3.48	120.33	111.83
2	A	1486	FAD	C2A-N3A-C4A	3.43	120.21	111.83
4	A	1488	NDP	C4A-C5A-N7A	-3.32	106.79	110.58
2	B	1486	FAD	C5A-N7A-C8A	3.31	108.66	103.45
2	A	1486	FAD	C4-N3-C2	-3.16	120.04	125.64
4	B	1488	NDP	C4A-C5A-N7A	-3.11	107.03	110.58
2	A	1486	FAD	N3A-C4A-N9A	3.10	132.44	127.17
2	B	1486	FAD	C4-N3-C2	-3.06	120.20	125.64
2	B	1486	FAD	N3A-C4A-N9A	3.04	132.34	127.17
4	B	1488	NDP	C3D-C2D-C1D	2.79	106.74	101.46
2	A	1486	FAD	C4X-C4-N3	2.76	120.28	113.25
2	A	1486	FAD	C4A-C5A-N7A	-2.74	107.45	110.58
2	B	1486	FAD	C4X-C4-N3	2.70	120.13	113.25
4	A	1488	NDP	C3D-C2D-C1D	2.63	106.45	101.46
4	A	1488	NDP	C4A-N9A-C8A	2.63	108.50	105.74
4	B	1488	NDP	C4A-N9A-C8A	2.62	108.49	105.74
2	B	1486	FAD	C9A-C5X-N5	-2.53	119.77	122.45
4	A	1488	NDP	C5A-N7A-C8A	2.47	107.33	103.45
2	B	1486	FAD	C4A-C5A-N7A	-2.44	107.79	110.58
2	A	1486	FAD	C9A-C5X-N5	-2.44	119.86	122.45
2	A	1486	FAD	C4X-C10-N1	-2.41	118.67	124.59
2	A	1486	FAD	O2A-PA-O3P	2.39	113.74	107.27
4	B	1488	NDP	C5A-N7A-C8A	2.36	107.16	103.45
4	A	1488	NDP	C2B-C1B-N9A	2.36	117.63	113.75
2	B	1486	FAD	C10-C4X-N5	-2.32	120.07	124.81
2	A	1486	FAD	C10-C4X-N5	-2.30	120.10	124.81
2	B	1486	FAD	C4X-C10-N10	2.30	119.78	116.48
2	A	1486	FAD	O4-C4-C4X	-2.25	120.58	126.53
4	A	1488	NDP	C6A-C5A-N7A	2.21	136.35	132.09
2	B	1486	FAD	O4-C4-C4X	-2.20	120.72	126.53
2	B	1486	FAD	C4X-C10-N1	-2.18	119.25	124.59
2	B	1486	FAD	C5X-C9A-N10	2.17	119.93	117.97
2	A	1486	FAD	C6A-C5A-C4A	2.14	120.10	117.18
4	B	1488	NDP	C6A-C5A-N7A	2.09	136.12	132.09
2	B	1486	FAD	O2A-PA-O3P	2.01	112.70	107.27

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1488	NDP	C4B
4	A	1488	NDP	C3B
4	A	1488	NDP	C4D
4	A	1488	NDP	C2B
4	B	1488	NDP	C4B
4	B	1488	NDP	C3B
4	B	1488	NDP	C4D
4	B	1488	NDP	C2B

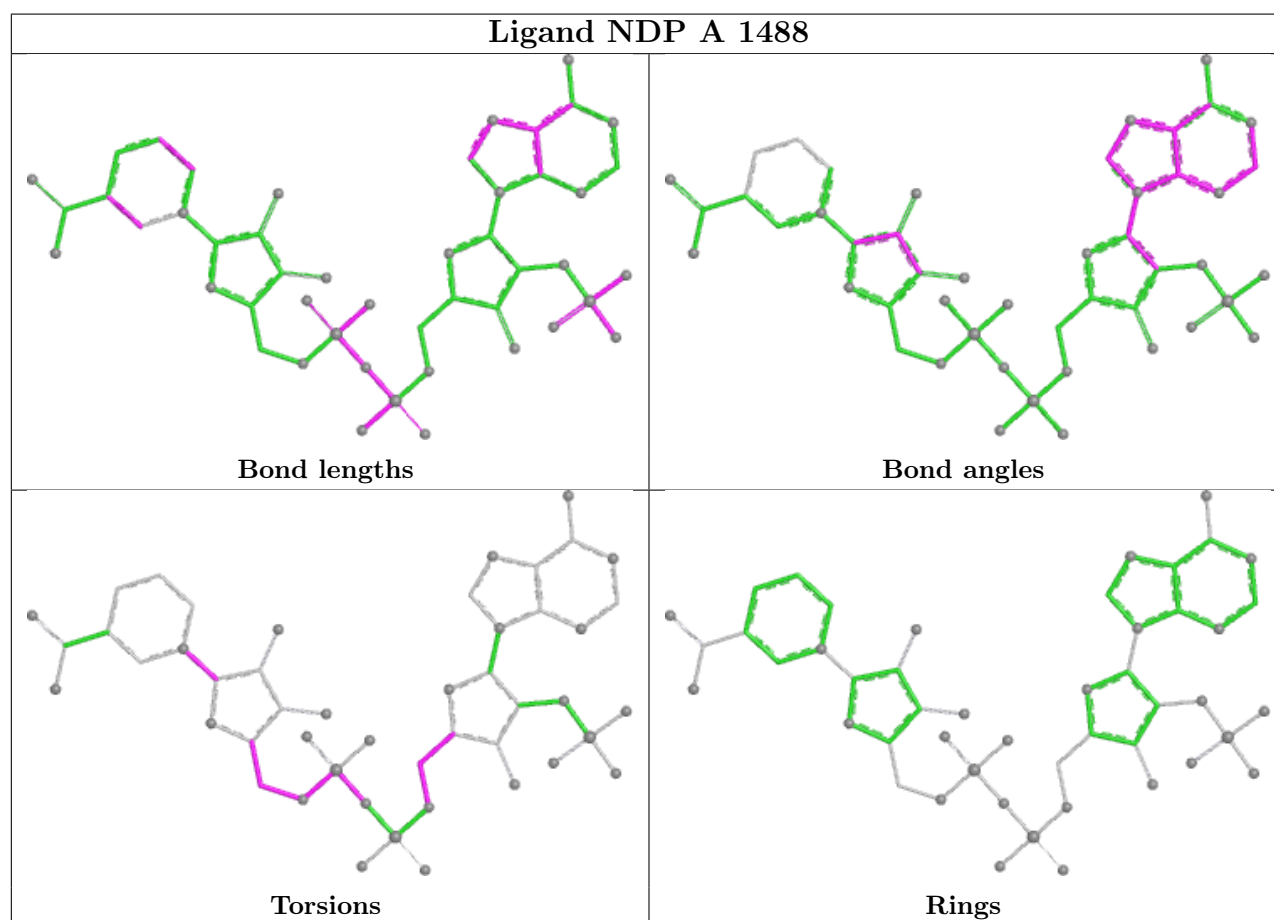
All (27) torsion outliers are listed below:

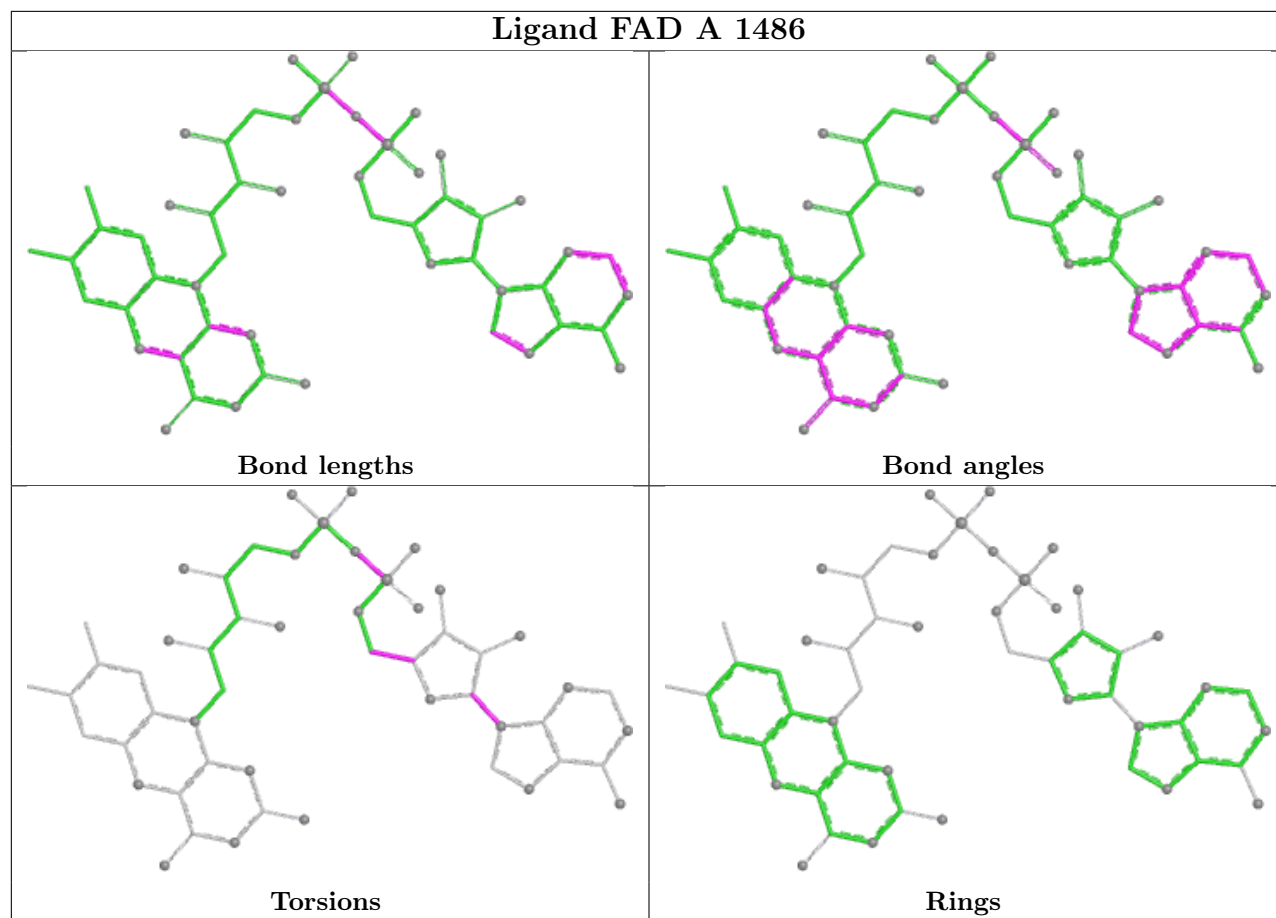
Mol	Chain	Res	Type	Atoms
4	A	1488	NDP	C5D-O5D-PN-O3
4	A	1488	NDP	C5D-O5D-PN-O1N
4	A	1488	NDP	O4D-C1D-N1N-C2N
4	B	1488	NDP	O4D-C1D-N1N-C2N
4	A	1488	NDP	C3D-C4D-C5D-O5D
4	B	1488	NDP	C3D-C4D-C5D-O5D
4	A	1488	NDP	O4D-C4D-C5D-O5D
2	B	1486	FAD	C3B-C4B-C5B-O5B
2	A	1486	FAD	O4B-C4B-C5B-O5B
2	B	1486	FAD	O4B-C4B-C5B-O5B
4	A	1488	NDP	C3B-C4B-C5B-O5B
4	B	1488	NDP	O4D-C4D-C5D-O5D
2	A	1486	FAD	C3B-C4B-C5B-O5B
4	A	1488	NDP	O4B-C4B-C5B-O5B
4	B	1488	NDP	O4B-C4B-C5B-O5B
4	B	1488	NDP	C3B-C4B-C5B-O5B
4	B	1488	NDP	C4D-C5D-O5D-PN
4	B	1488	NDP	C5D-O5D-PN-O3
4	B	1488	NDP	C5D-O5D-PN-O1N
4	B	1488	NDP	C5D-O5D-PN-O2N
4	A	1488	NDP	C4D-C5D-O5D-PN
4	B	1488	NDP	PN-O3-PA-O1A
2	A	1486	FAD	P-O3P-PA-O1A
2	B	1486	FAD	C2B-C1B-N9A-C8A
4	A	1488	NDP	PA-O3-PN-O2N
2	A	1486	FAD	C2B-C1B-N9A-C8A
4	A	1488	NDP	C4B-C5B-O5B-PA

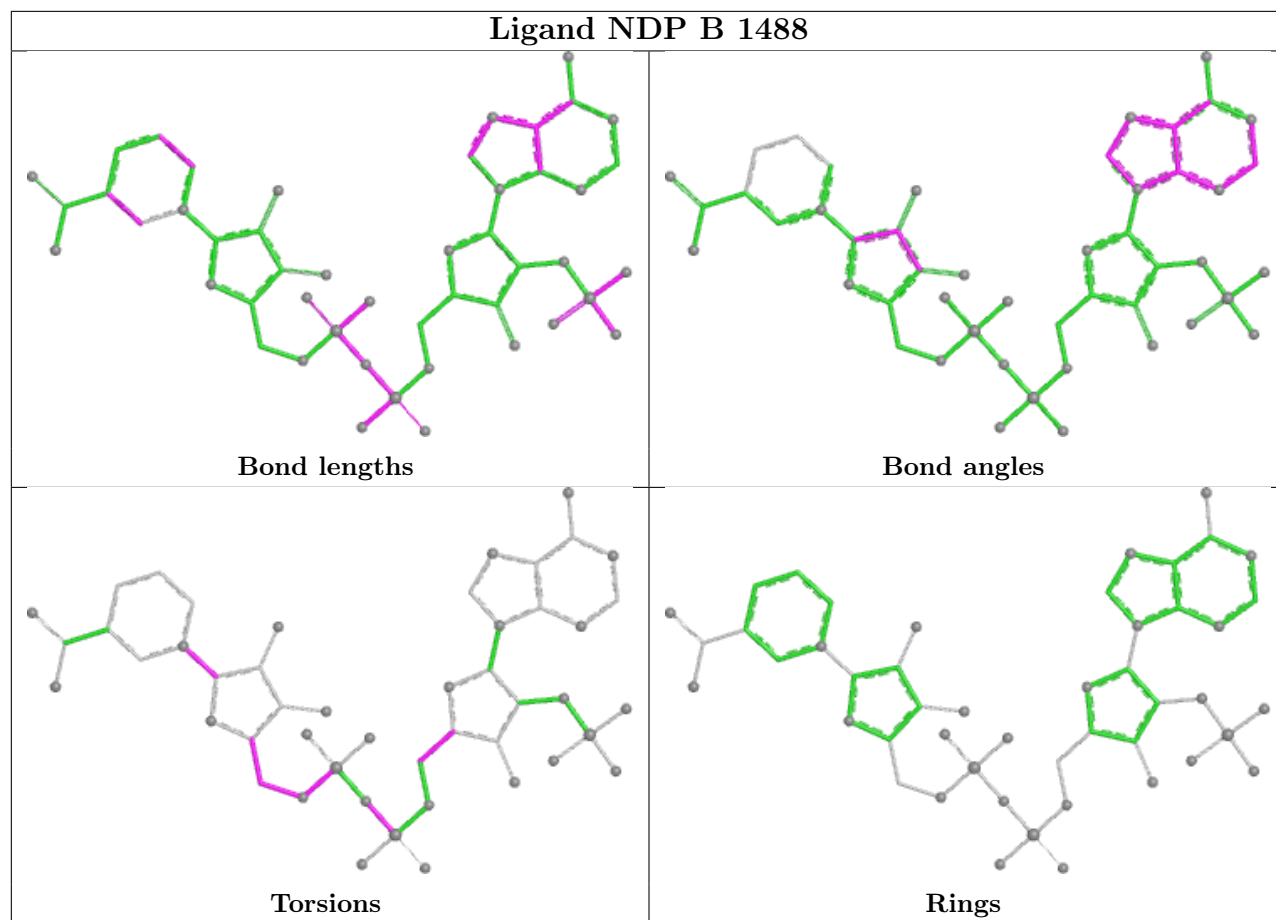
There are no ring outliers.

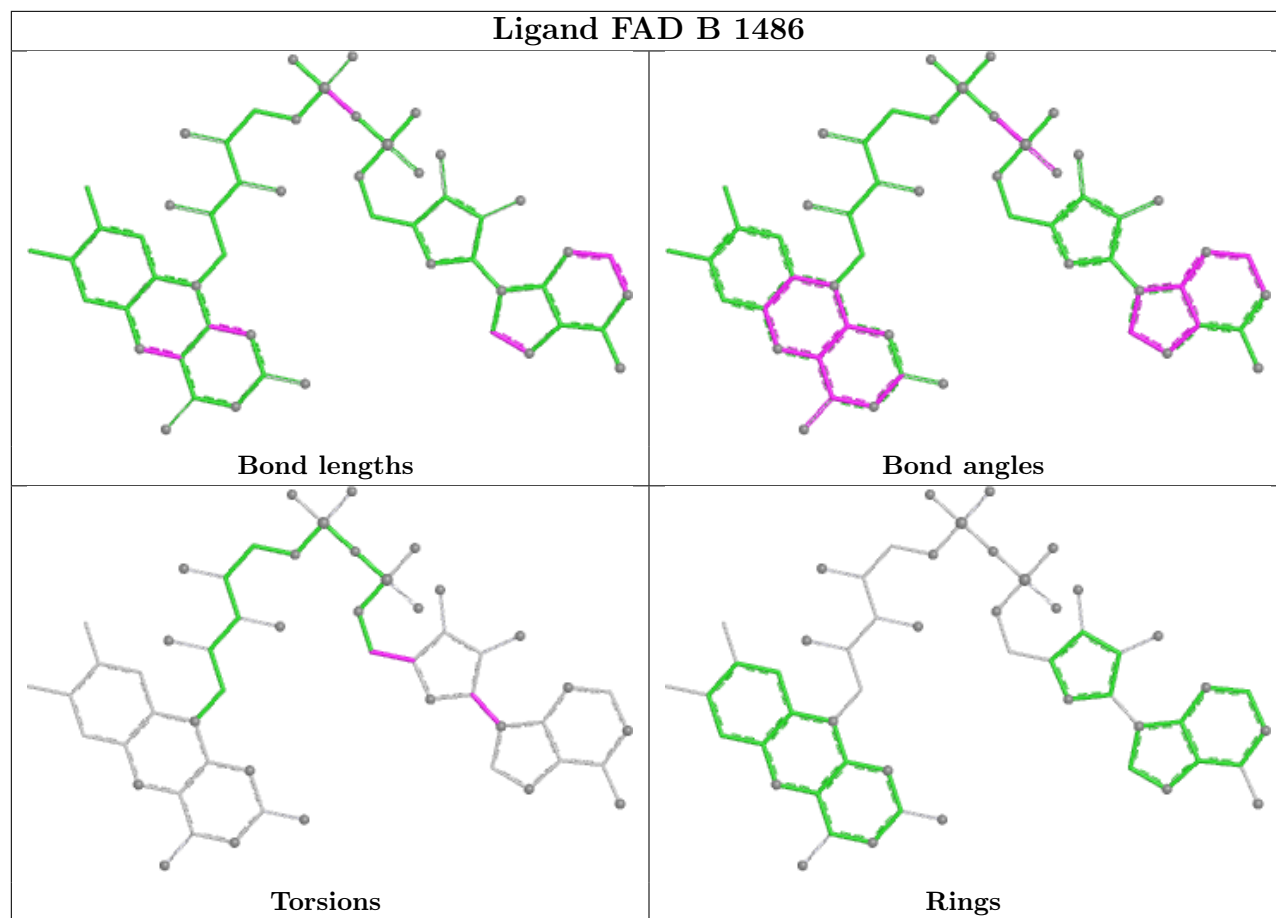
No monomer is involved in short contacts.

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 [i](#)

5.1 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	485/511 (94%)	-1.40	0 100 100	55, 69, 82, 92	0
1	B	487/511 (95%)	-1.39	0 100 100	55, 69, 82, 92	0
All	All	972/1022 (95%)	-1.40	0 100 100	55, 69, 82, 92	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	NDP	A	1488	48/48	0.99	0.03	74,78,82,82	0
4	NDP	B	1488	48/48	0.99	0.04	74,78,82,83	0
5	SO4	A	1489	5/5	0.99	0.06	36,37,37,37	5
5	SO4	B	1489	5/5	0.99	0.06	35,35,36,36	5
2	FAD	A	1486	53/53	1.00	0.03	55,60,65,65	0
2	FAD	B	1486	53/53	1.00	0.03	55,60,65,65	0
3	SB	A	1487	1/1	1.00	0.01	55,55,55,55	1

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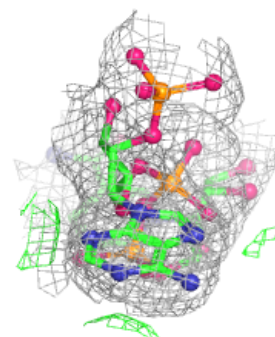
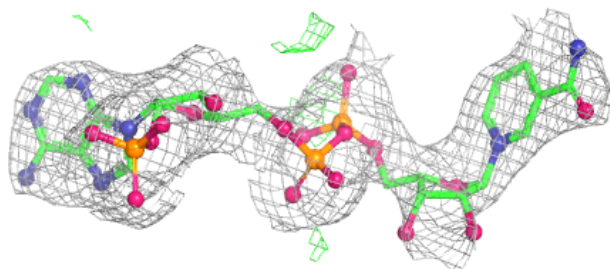
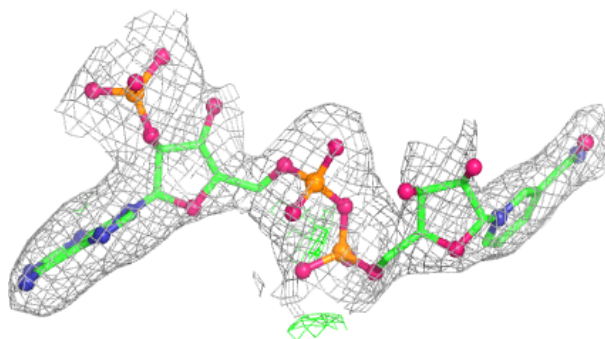
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SB	B	1487	1/1	1.00	0.01	51,51,51,51	1

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.

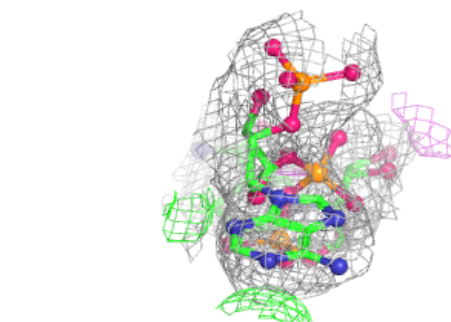
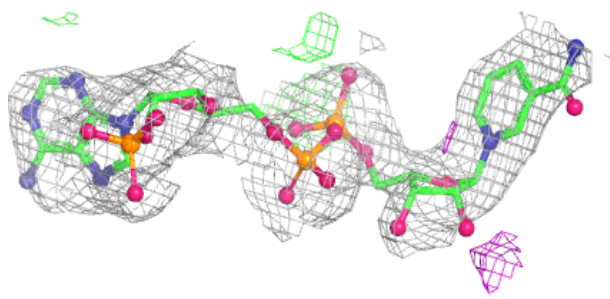
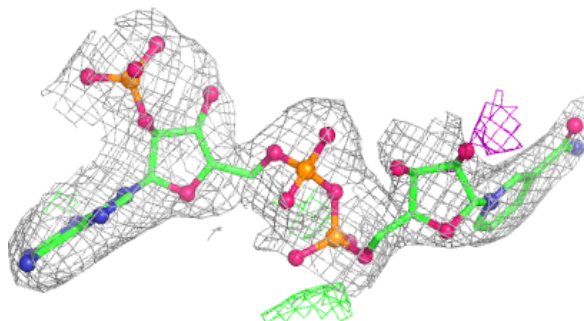
Electron density around NDP A 1488:

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

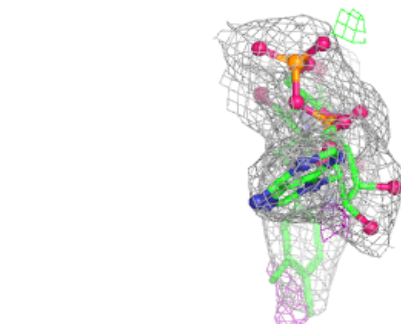
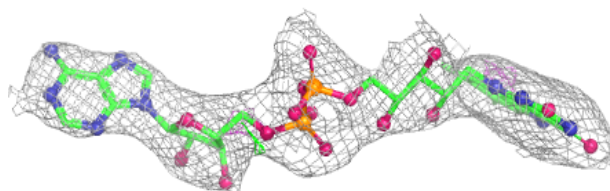
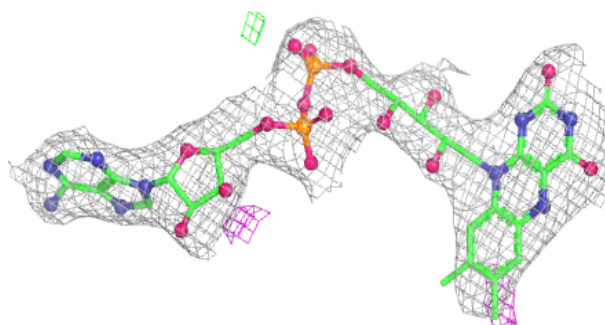


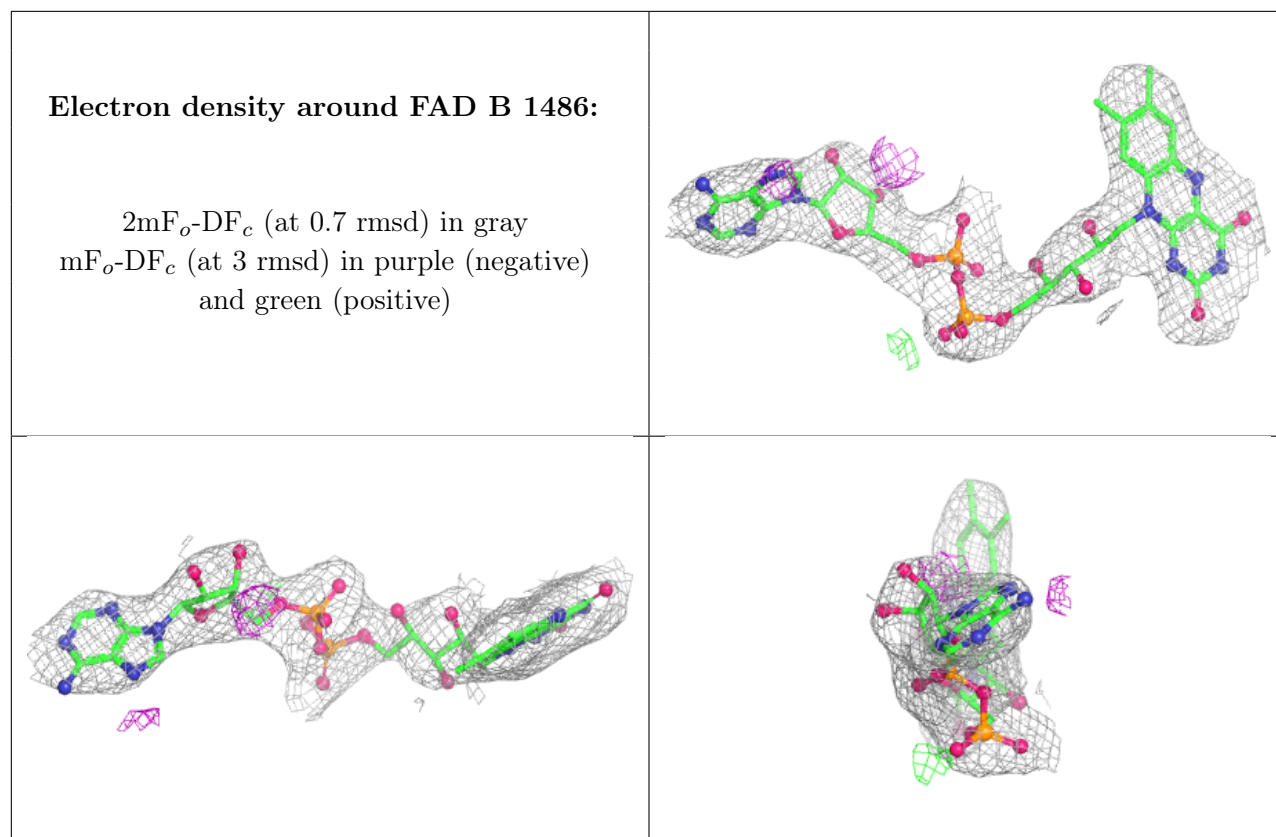
Electron density around NDP B 1488:

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

**Electron density around FAD A 1486:**

$2mF_o-DF_c$ (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.