wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 01:56 pm GMT

PDB ID	:	1H6V
Title	:	Mammalian thioredoxin reductase
Authors	:	Sandalova, T.; Zhong, L.; Lindqvist, Y.; Holmgren, A.; Schneider, G.
Deposited on	:	2001-06-27
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

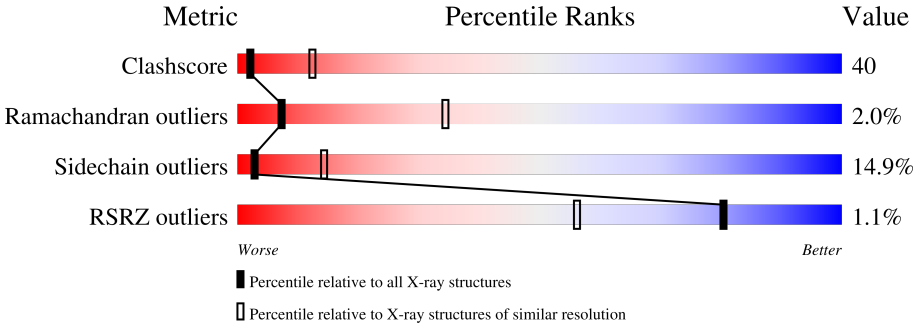
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23075 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 THIOREDOXIN REDUCTASE.

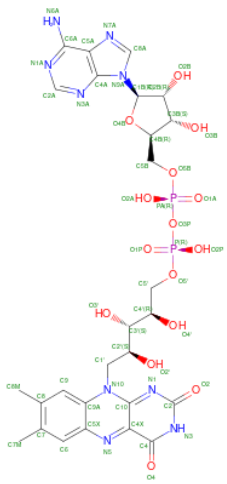
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3764	2391	635	716	22	0	0	0
1	B	487	3753	2387	633	713	20	0	0	0
1	C	482	3707	2356	627	704	20	0	0	0
1	D	487	3753	2387	633	713	20	0	0	0
1	E	491	3773	2397	637	717	22	0	0	0
1	F	490	3764	2391	635	716	22	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ASN	ARG	conflict	UNP O89049
B	52	ASN	ARG	conflict	UNP O89049
C	52	ASN	ARG	conflict	UNP O89049
D	52	ASN	ARG	conflict	UNP O89049
E	52	ASN	ARG	conflict	UNP O89049
F	52	ASN	ARG	conflict	UNP O89049
A	497	CYS	SEL	engineered mutation	UNP O89049
B	497	CYS	SEL	engineered mutation	UNP O89049
C	497	CYS	SEL	engineered mutation	UNP O89049
D	497	CYS	SEL	engineered mutation	UNP O89049
E	497	CYS	SEL	engineered mutation	UNP O89049

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

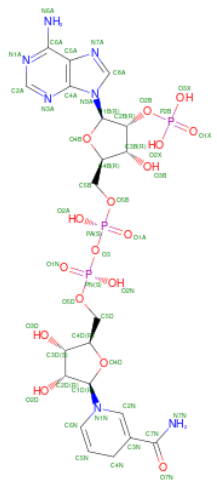
FAD



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

NDP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	39	15	5	16	3	0	0
3	B	1	39	15	5	16	3	0	0
3	C	1	39	15	5	16	3	0	0
3	D	1	39	15	5	16	3	0	0
3	E	1	39	15	5	16	3	0	0
3	F	1	39	15	5	16	3	0	0

- Molecule 4 is water.

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

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.92Å 140.46Å 170.83Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.86 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-3.00) 92.5 (29.86-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.263 0.257 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 4.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23075	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 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	0.92	0/3838	1.07	15/5193 (0.3%)
1	B	0.90	0/3827	1.04	14/5178 (0.3%)
1	C	0.82	1/3779 (0.0%)	1.03	15/5114 (0.3%)
1	D	0.97	3/3827 (0.1%)	1.08	16/5178 (0.3%)
1	E	0.99	2/3847 (0.1%)	1.11	16/5204 (0.3%)
1	F	0.80	0/3838	1.03	14/5193 (0.3%)
All	All	0.90	6/22956 (0.0%)	1.06	90/31060 (0.3%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	489	GLY	C-O	-6.05	1.14	1.23
1	D	410	GLU	CD-OE1	5.80	1.32	1.25
1	D	114	TRP	CB-CG	-5.08	1.41	1.50
1	C	300	ILE	C-O	-5.07	1.13	1.23
1	D	88	TRP	CB-CG	-5.03	1.41	1.50

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	82	ASP	CB-CG-OD2	9.47	126.82	118.30
1	F	229	ASP	CB-CG-OD2	9.21	126.59	118.30
1	F	417	ASP	CB-CG-OD2	8.16	125.65	118.30
1	E	282	ASP	CB-CG-OD2	7.91	125.42	118.30
1	F	466	ASP	CB-CG-OD2	7.83	125.35	118.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	3764	0	3764	309	0
1	B	3753	0	3763	287	0
1	C	3707	0	3721	463	0
1	D	3753	0	3761	294	0
1	E	3773	0	3777	257	0
1	F	3764	0	3764	300	0
2	A	53	0	31	5	0
2	B	53	0	31	10	0
2	C	53	0	31	17	0
2	D	53	0	31	4	0
2	E	53	0	31	3	0
2	F	53	0	31	5	0
3	A	39	0	18	2	0
3	B	39	0	18	8	0
3	C	39	0	18	6	0
3	D	39	0	18	6	0
3	E	39	0	18	1	0
3	F	39	0	18	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	2	0
4	D	1	0	0	0	0
4	E	2	0	0	1	0
4	F	1	0	0	0	0
All	All	23075	0	22844	1832	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 40.

The worst 5 of 1832 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:C:98:TRP:NE1	1:C:190:PRO:HD2	1.54	1.21
1:C:98:TRP:CD1	1:C:189:CYS:HA	1.76	1.20
1:D:477:GLU:O	1:D:480:THR:HG22	1.49	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LEU:HD13	1:C:441:LEU:HD11	1.13	1.12
1:C:98:TRP:CZ3	1:C:102:THR:HG23	1.85	1.12

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	488/499 (98%)	445 (91%)	36 (7%)	7 (1%)	11	43
1	B	485/499 (97%)	436 (90%)	40 (8%)	9 (2%)	8	36
1	C	480/499 (96%)	395 (82%)	70 (15%)	15 (3%)	4	23
1	D	485/499 (97%)	439 (90%)	37 (8%)	9 (2%)	8	36
1	E	489/499 (98%)	441 (90%)	39 (8%)	9 (2%)	8	37
1	F	488/499 (98%)	438 (90%)	40 (8%)	10 (2%)	7	34
All	All	2915/2994 (97%)	2594 (89%)	262 (9%)	59 (2%)	7	34

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	THR
1	A	489	GLY
1	B	92	ASP
1	B	263	THR
1	B	314	GLY

4.3.2 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	406/414 (98%)	352 (87%)	54 (13%)	4 17
1	B	405/414 (98%)	344 (85%)	61 (15%)	3 14
1	C	400/414 (97%)	325 (81%)	75 (19%)	1 8
1	D	405/414 (98%)	342 (84%)	63 (16%)	2 13
1	E	407/414 (98%)	354 (87%)	53 (13%)	4 19
1	F	406/414 (98%)	349 (86%)	57 (14%)	3 16
All	All	2429/2484 (98%)	2066 (85%)	363 (15%)	3 14

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	364	LYS
1	E	308	LYS
1	D	396	GLU
1	E	72	GLN
1	E	450	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	439	HIS
1	F	72	GLN
1	D	494	GLN
1	E	325	ASN
1	F	113	ASN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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 monosaccharides in this entry.

4.6 Ligand geometry (i)

12 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	600	-	53,58,58	1.56	8 (15%)	68,89,89	1.84	16 (23%)
2	FAD	E	600	-	53,58,58	1.43	6 (11%)	68,89,89	1.92	20 (29%)
3	NDP	B	601	-	36,42,52	1.77	9 (25%)	43,65,80	1.52	9 (20%)
3	NDP	C	601	-	36,42,52	1.56	8 (22%)	43,65,80	1.72	10 (23%)
2	FAD	C	600	-	53,58,58	1.31	5 (9%)	68,89,89	1.87	18 (26%)
2	FAD	B	600	-	53,58,58	1.35	7 (13%)	68,89,89	1.94	17 (25%)
3	NDP	A	601	-	36,42,52	1.49	5 (13%)	43,65,80	1.57	7 (16%)
3	NDP	E	601	-	36,42,52	1.48	6 (16%)	43,65,80	1.33	4 (9%)
3	NDP	D	601	-	36,42,52	1.45	5 (13%)	43,65,80	1.67	9 (20%)
2	FAD	F	600	-	53,58,58	1.22	5 (9%)	68,89,89	1.56	10 (14%)
3	NDP	F	601	-	36,42,52	1.55	7 (19%)	43,65,80	1.43	8 (18%)
2	FAD	A	600	-	53,58,58	1.31	5 (9%)	68,89,89	1.78	15 (22%)

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	600	-	-	5/30/50/50	0/6/6/6
2	FAD	E	600	-	-	10/30/50/50	0/6/6/6
3	NDP	B	601	-	-	9/23/56/77	0/4/4/5
3	NDP	C	601	-	-	5/23/56/77	0/4/4/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	600	-	-	10/30/50/50	0/6/6/6
2	FAD	B	600	-	-	3/30/50/50	0/6/6/6
3	NDP	A	601	-	-	13/23/56/77	0/4/4/5
3	NDP	E	601	-	-	5/23/56/77	0/4/4/5
3	NDP	D	601	-	-	12/23/56/77	0/4/4/5
2	FAD	F	600	-	-	10/30/50/50	0/6/6/6
3	NDP	F	601	-	-	6/23/56/77	0/4/4/5
2	FAD	A	600	-	-	9/30/50/50	0/6/6/6

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C2A-N3A	4.49	1.39	1.32
2	E	600	FAD	C2A-N3A	4.48	1.39	1.32
2	B	600	FAD	C2A-N3A	4.41	1.39	1.32
2	D	600	FAD	C2A-N3A	4.29	1.39	1.32
3	C	601	NDP	P2B-O3X	4.17	1.70	1.54

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	P-O3P-PA	-6.71	109.79	132.83
2	D	600	FAD	P-O3P-PA	-6.11	111.86	132.83
2	B	600	FAD	N3A-C2A-N1A	-5.76	119.68	128.68
2	C	600	FAD	N3A-C2A-N1A	-5.64	119.87	128.68
2	F	600	FAD	N3A-C2A-N1A	-5.56	119.99	128.68

There are no chirality outliers.

5 of 97 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	C5'-O5'-P-O2P
2	C	600	FAD	C3B-C4B-C5B-O5B
2	C	600	FAD	N10-C1'-C2'-O2'
2	C	600	FAD	N10-C1'-C2'-C3'

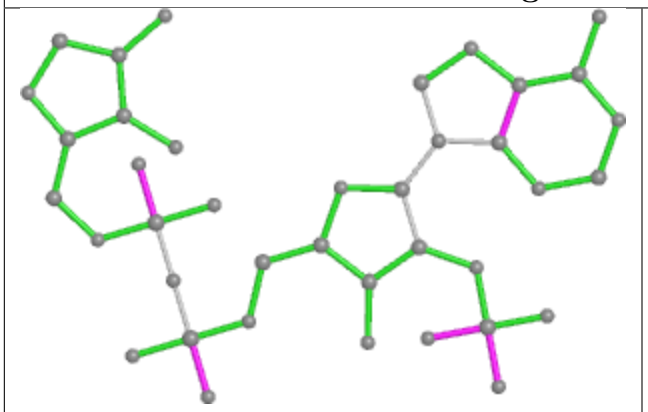
There are no ring outliers.

12 monomers are involved in 71 short contacts:

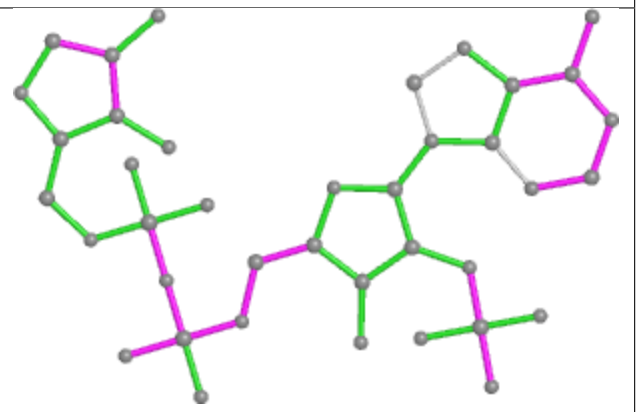
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	FAD	4	0
2	E	600	FAD	3	0
3	B	601	NDP	8	0
3	C	601	NDP	6	0
2	C	600	FAD	17	0
2	B	600	FAD	10	0
3	A	601	NDP	2	0
3	E	601	NDP	1	0
3	D	601	NDP	6	0
2	F	600	FAD	5	0
3	F	601	NDP	4	0
2	A	600	FAD	5	0

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 then 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.

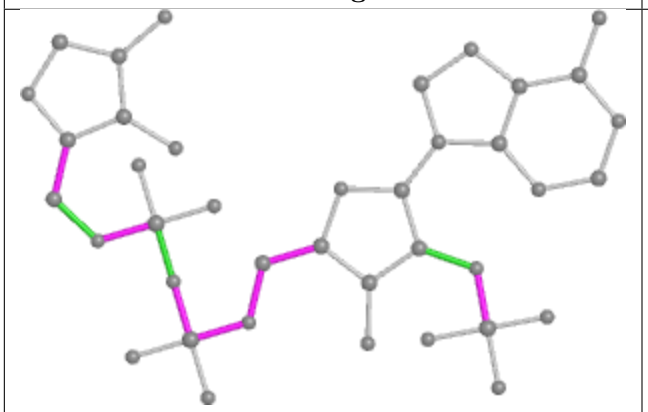
Ligand NDP D 601



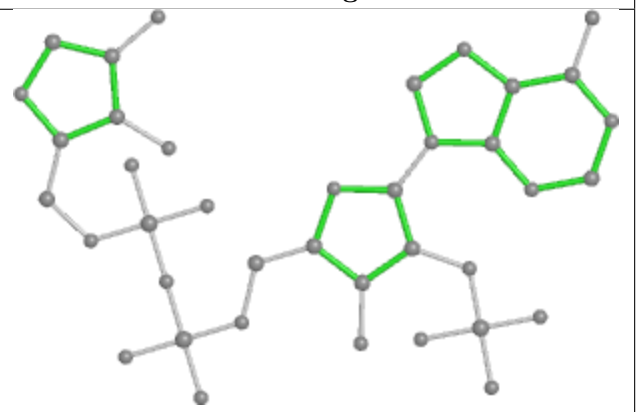
Bond lengths



Bond angles

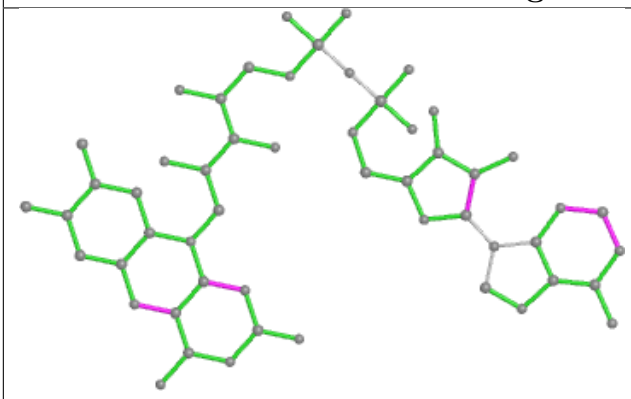


Torsions

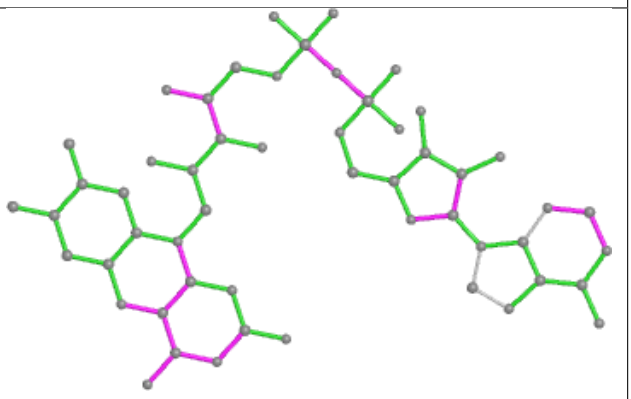


Rings

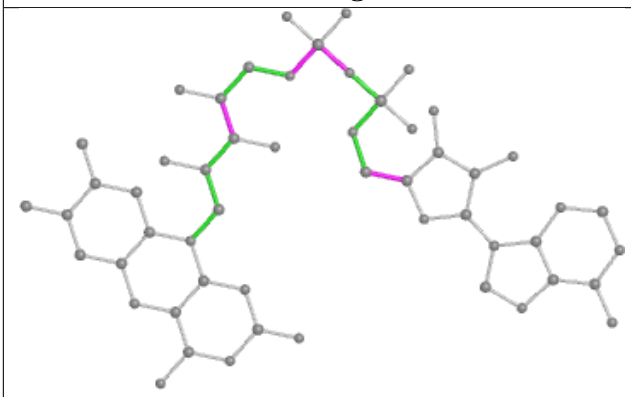
Ligand FAD F 600



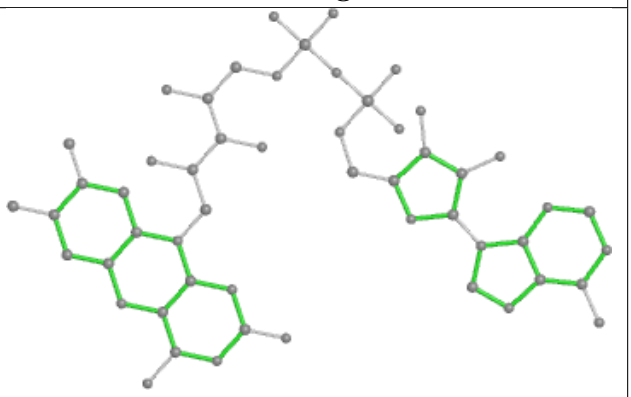
Bond lengths



Bond angles

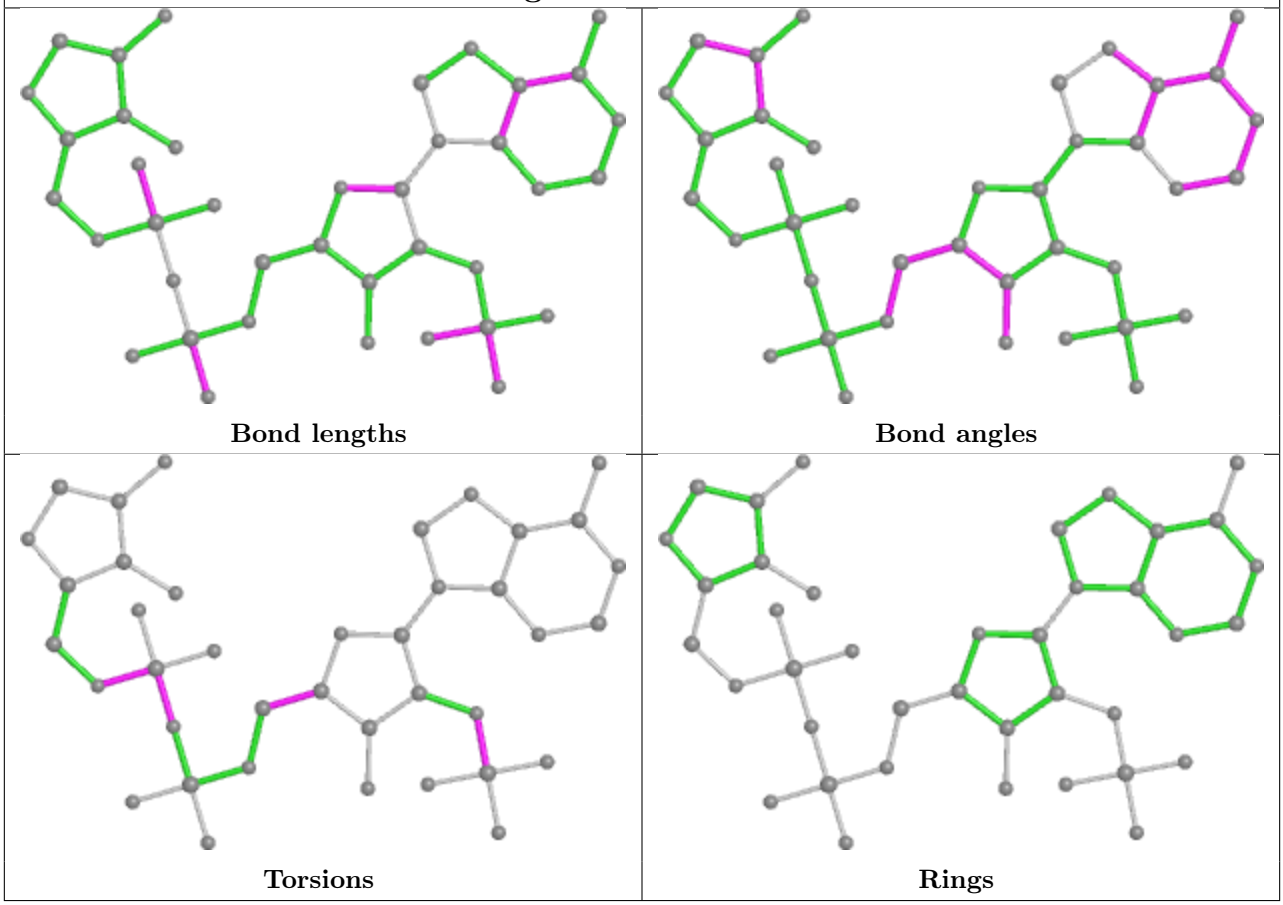


Torsions



Rings

Ligand NDP F 601



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	490/499 (98%)	-0.38	2 (0%)	92	79	7, 13, 20, 48	0
1	B	487/499 (97%)	-0.48	1 (0%)	95	87	6, 13, 20, 39	0
1	C	482/499 (96%)	0.11	16 (3%)	46	20	6, 13, 19, 44	0
1	D	487/499 (97%)	-0.33	4 (0%)	86	65	6, 12, 19, 38	0
1	E	491/499 (98%)	-0.39	4 (0%)	86	65	7, 13, 20, 48	0
1	F	490/499 (98%)	-0.24	6 (1%)	79	54	6, 13, 20, 48	0
All	All	2927/2994 (97%)	-0.29	33 (1%)	80	56	6, 13, 20, 48	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	497	CYS	6.9
1	E	495	SER	5.5
1	C	297	THR	5.1
1	F	495	SER	5.1
1	A	498	CYS	3.6

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 monosaccharides in this entry.

5.4 Ligands (i)

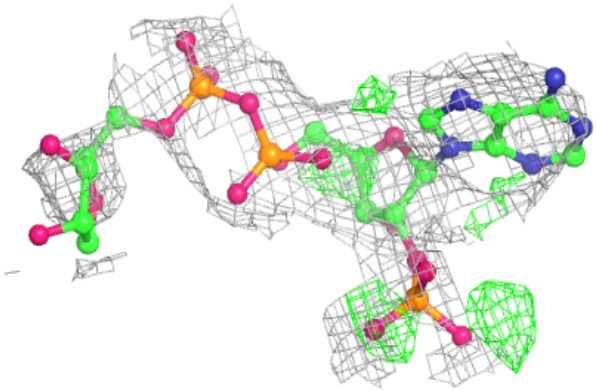
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

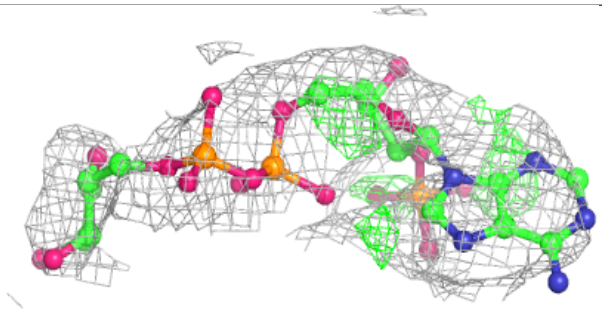
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NDP	C	601	39/48	0.77	0.26	82,92,100,101	0
3	NDP	F	601	39/48	0.78	0.29	72,95,112,112	0
3	NDP	D	601	39/48	0.85	0.20	44,55,77,77	0
3	NDP	A	601	39/48	0.85	0.22	41,49,78,78	0
2	FAD	C	600	53/53	0.86	0.28	34,45,49,51	0
3	NDP	B	601	39/48	0.89	0.22	31,50,69,71	0
3	NDP	E	601	39/48	0.91	0.21	45,52,76,79	0
2	FAD	F	600	53/53	0.92	0.26	27,33,53,55	0
2	FAD	E	600	53/53	0.94	0.28	10,17,54,56	0
2	FAD	A	600	53/53	0.94	0.22	14,24,36,36	0
2	FAD	B	600	53/53	0.95	0.25	18,26,42,46	0
2	FAD	D	600	53/53	0.95	0.29	20,29,40,47	0

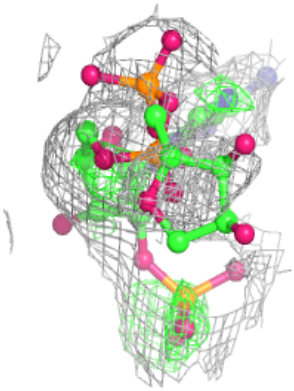
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP C 601:

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

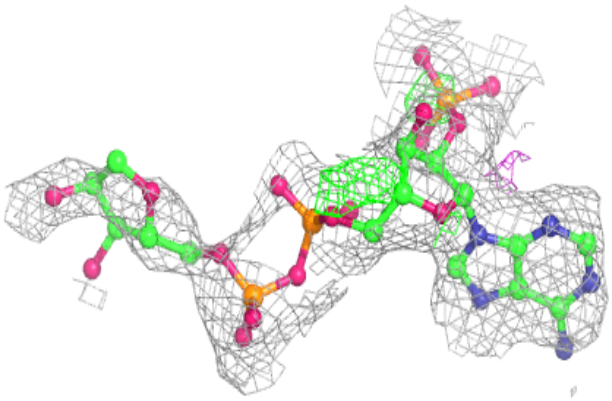


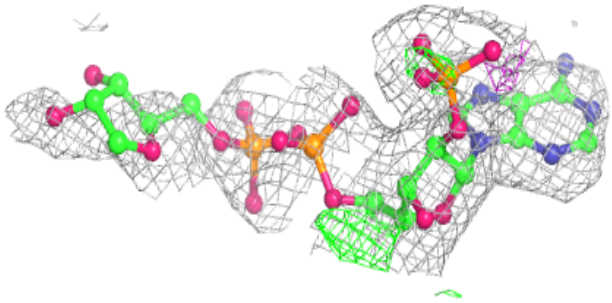


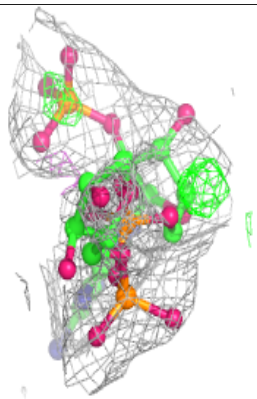


Electron density around NDP F 601:

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

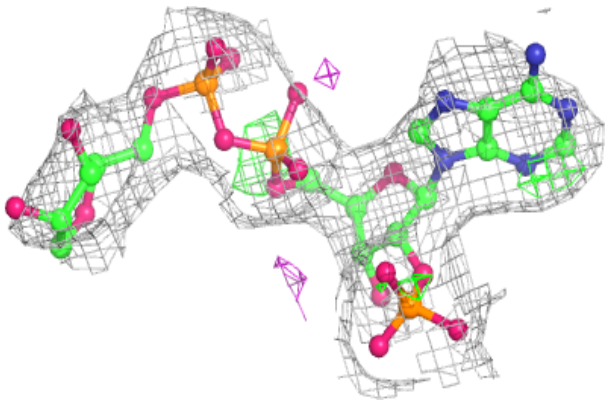


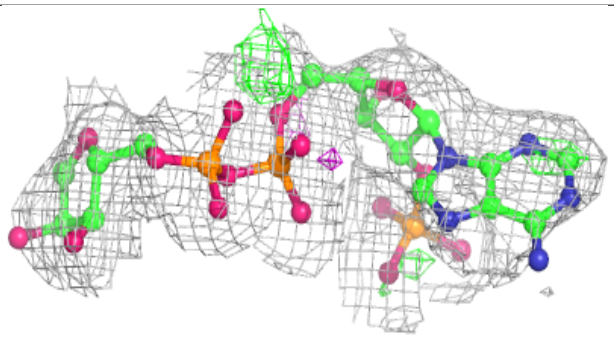


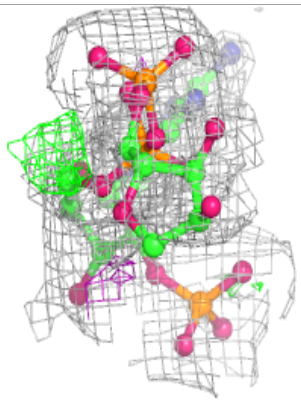


Electron density around NDP D 601:

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

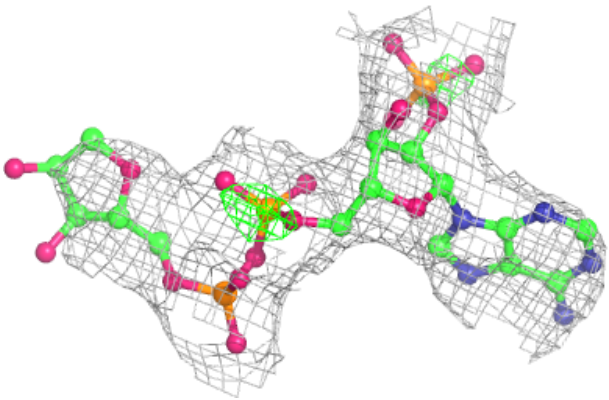


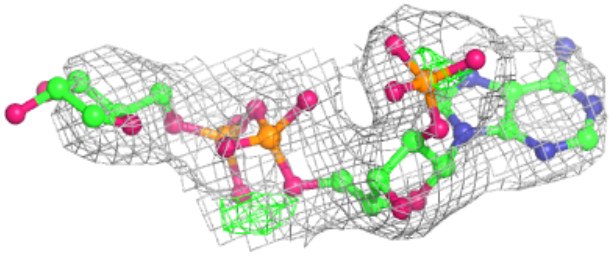


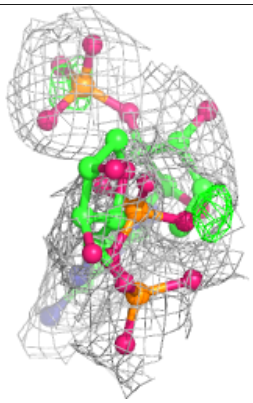


Electron density around NDP A 601:

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

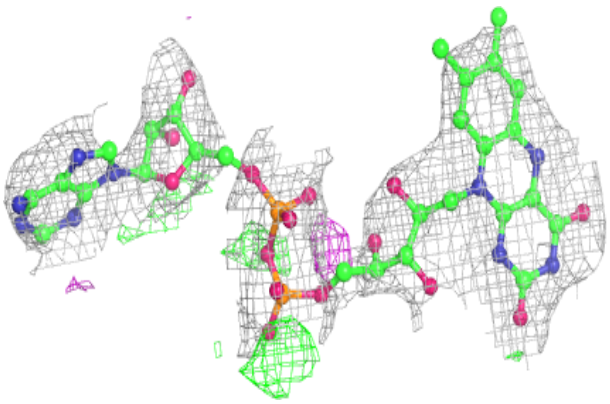


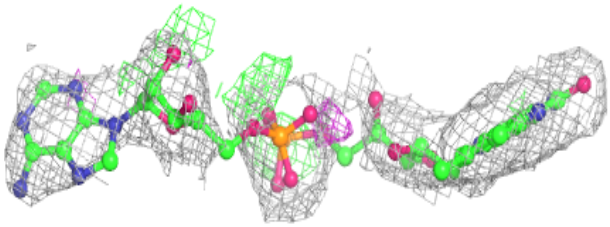


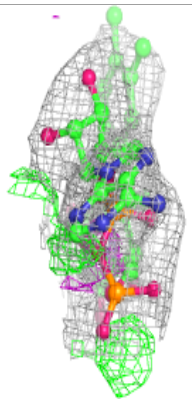


Electron density around FAD C 600:

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

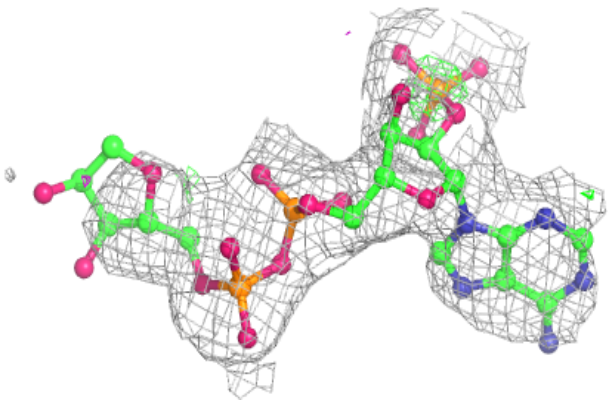


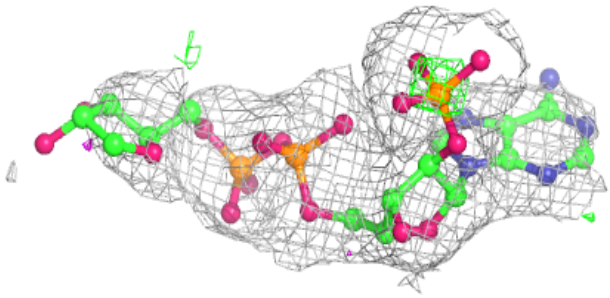


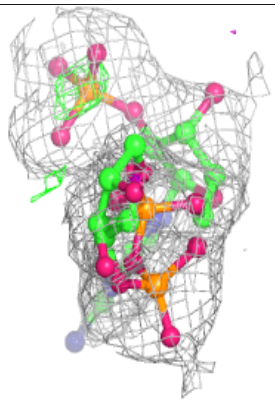


Electron density around NDP B 601:

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

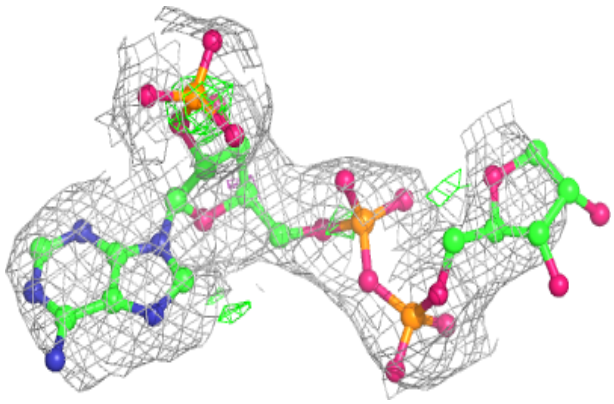


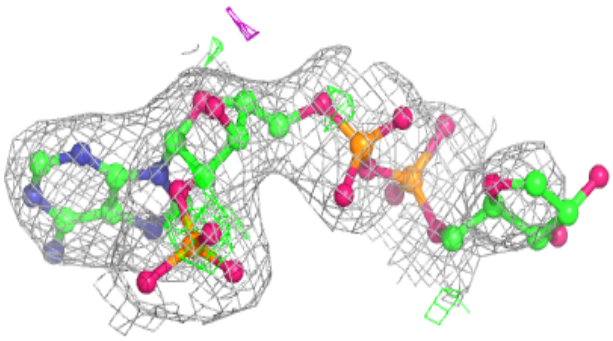


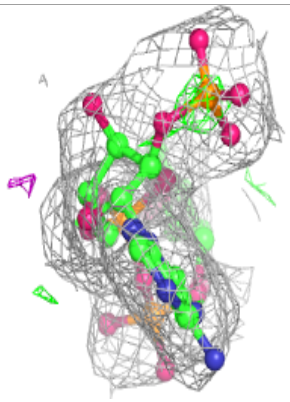


Electron density around NDP E 601:

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

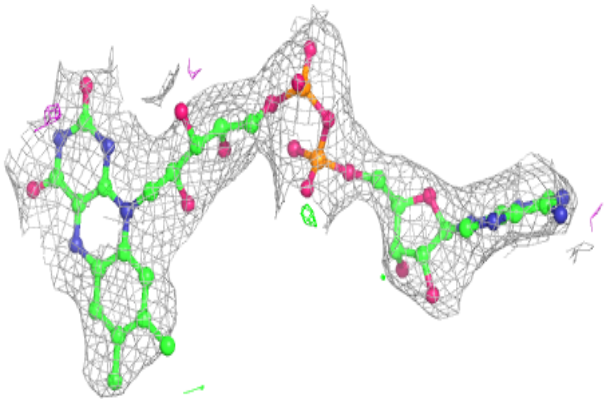


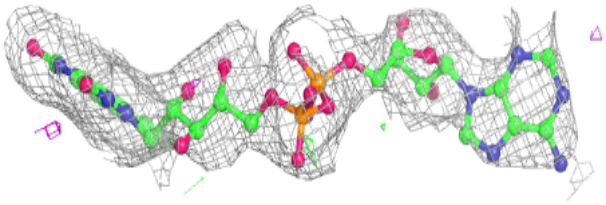


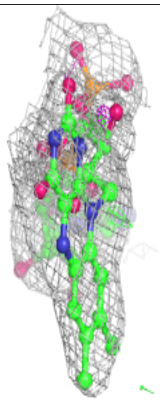


Electron density around FAD F 600:

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

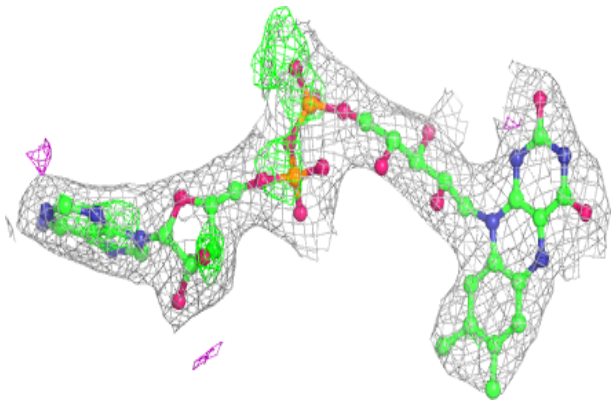


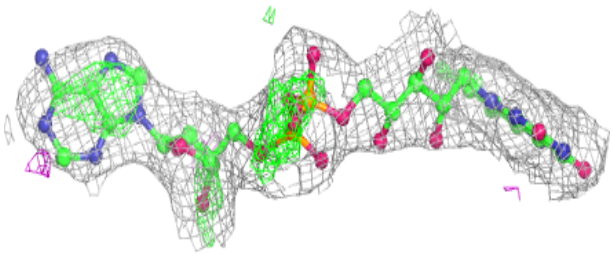


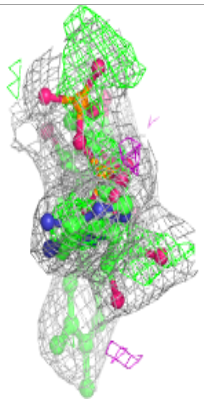


Electron density around FAD E 600:

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

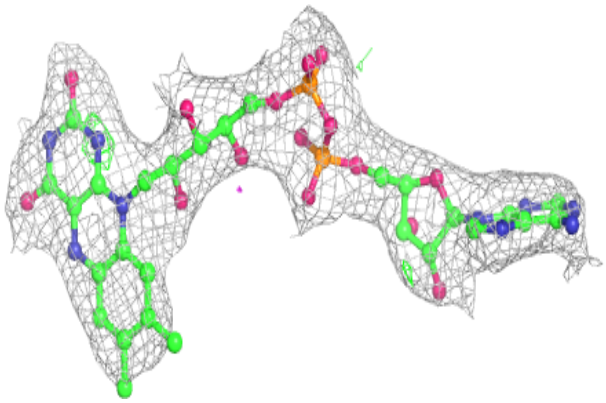


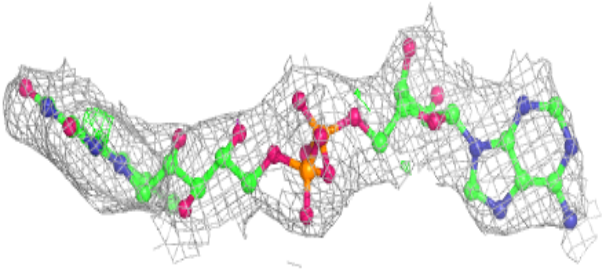


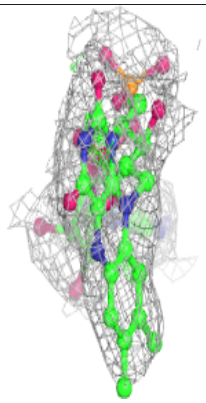


Electron density around FAD A 600:

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

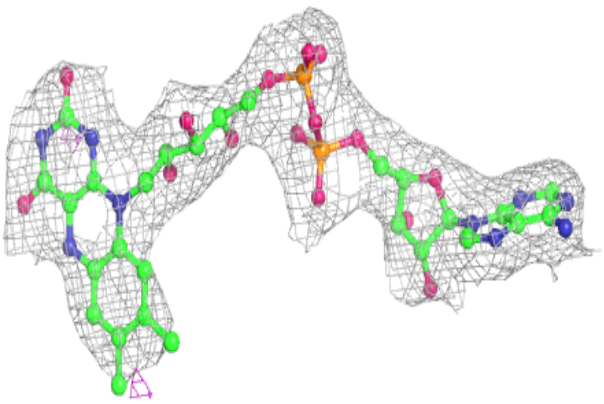


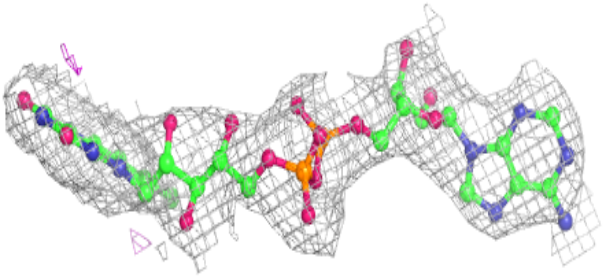


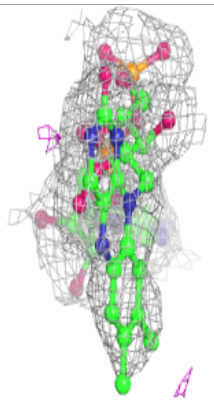


Electron density around FAD B 600:

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

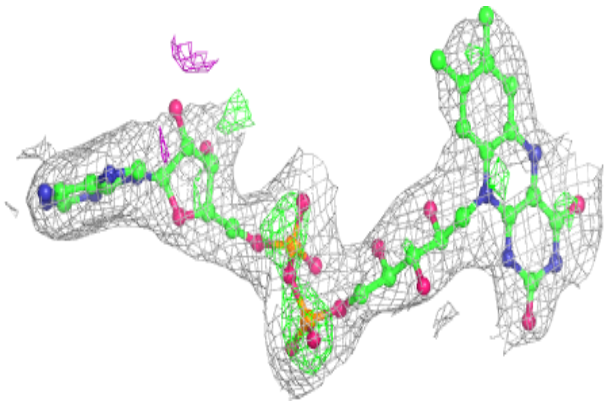


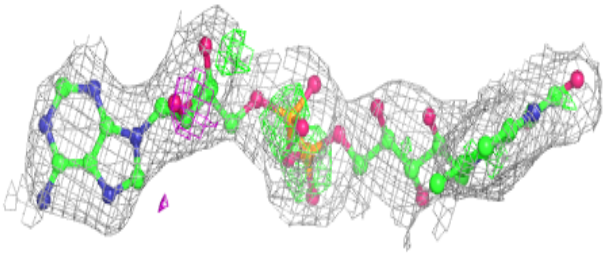


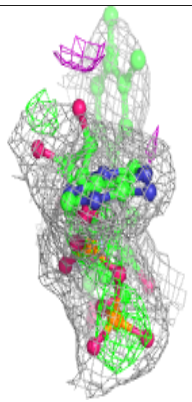


Electron density around FAD D 600:

$2mF_o$-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.