wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 12:25 PM EDT

PDB ID	:	4LK3
Title	:	Crystal structure of Human UDP-xylose synthase R236A substitution
Authors	:	Walsh Jr., R.M.; Polizzi, S.J.; Wood, Z.A.
Deposited on	:	2013-07-05
Resolution	:	2.64 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:

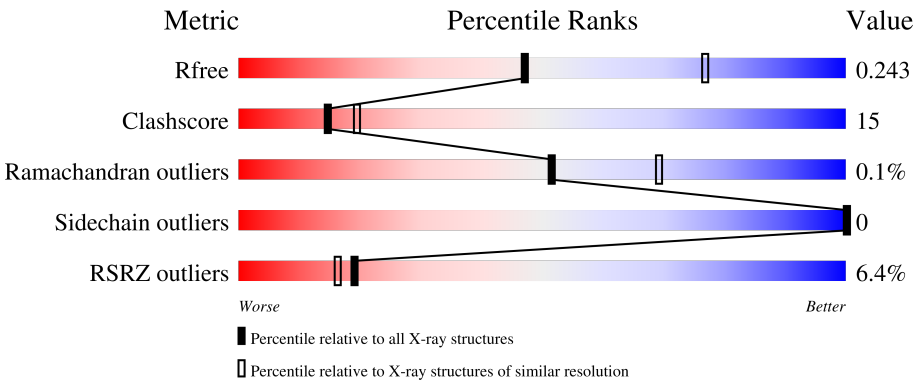
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.64 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	336	11% 53% 26% 21%
1	B	336	3% 65% 16% 18%
1	C	336	.% 67% 14% 19%
1	D	336	.% 61% 20% 19%
1	E	336	7% 61% 19% 20%

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Mol	Chain	Length	Quality of chain
1	F	336	8% 47% 31% 22%

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
5	SO4	A	505	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13434 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 UDP-glucuronic acid decarboxylase 1.

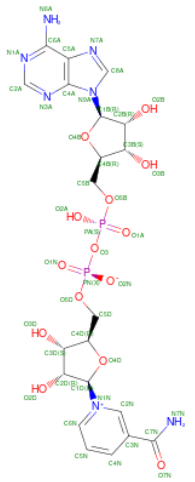
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	2113	1349	367	387	10	0	0	0
1	B	274	2156	1375	374	396	11	0	0	0
1	C	271	2130	1359	368	393	10	0	0	0
1	D	273	2148	1370	373	395	10	0	0	0
1	E	269	2118	1350	369	389	10	0	0	0
1	F	261	2062	1314	360	378	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	ARG	engineered mutation	UNP Q8NBZ7
B	236	ALA	ARG	engineered mutation	UNP Q8NBZ7
C	236	ALA	ARG	engineered mutation	UNP Q8NBZ7
D	236	ALA	ARG	engineered mutation	UNP Q8NBZ7
E	236	ALA	ARG	engineered mutation	UNP Q8NBZ7
F	236	ALA	ARG	engineered mutation	UNP Q8NBZ7

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

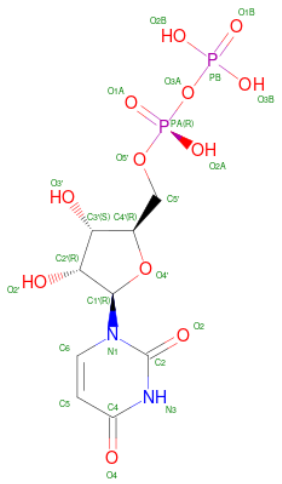
NAD



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0
2	B	1	44	21	7	14	2	0	0
2	C	1	44	21	7	14	2	0	0
2	D	1	44	21	7	14	2	0	0
2	E	1	44	21	7	14	2	0	0
2	F	1	44	21	7	14	2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

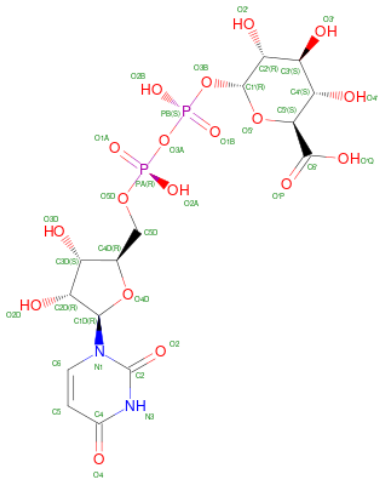
UDP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	B	1	25	9	2	12	2	0	0
			Total	C	N	O	P		
3	D	1	25	9	2	12	2	0	0

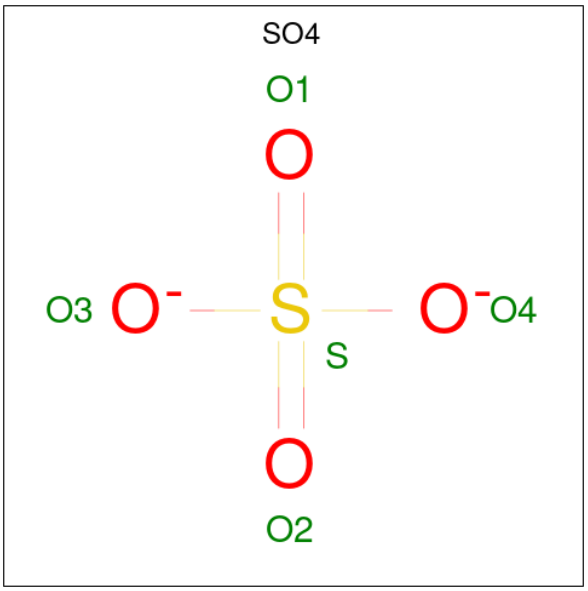
- Molecule 4 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: $C_{15}H_{22}N_2O_{18}P_2$).

UGA



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	37	15	2	18	2	0	0
4	B	1	37	15	2	18	2	0	0
4	C	1	37	15	2	18	2	0	0
4	D	1	37	15	2	18	2	0	0
4	E	1	37	15	2	18	2	0	0
4	F	1	37	15	2	18	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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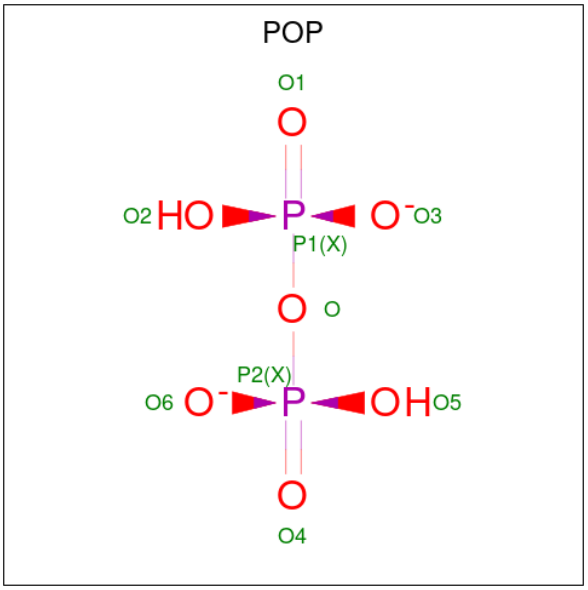
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 9 7 2	0	0
6	E	1	Total O P 9 7 2	0	0
6	F	1	Total O P 9 7 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	32	Total O 32 32	0	0
7	C	31	Total O 31 31	0	0
7	D	9	Total O 9 9	0	0

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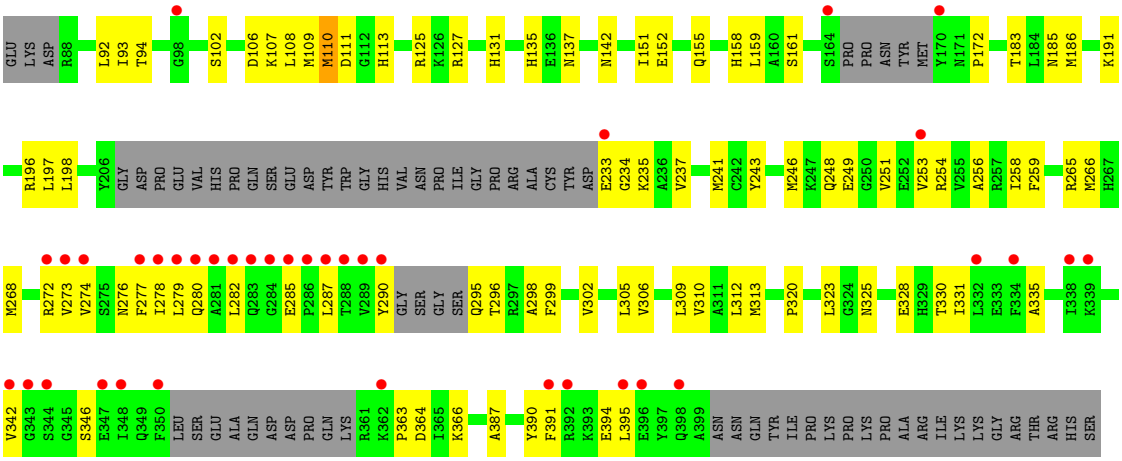
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	E	2	2	2	0	0

3 Residue-property plots (i)

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.

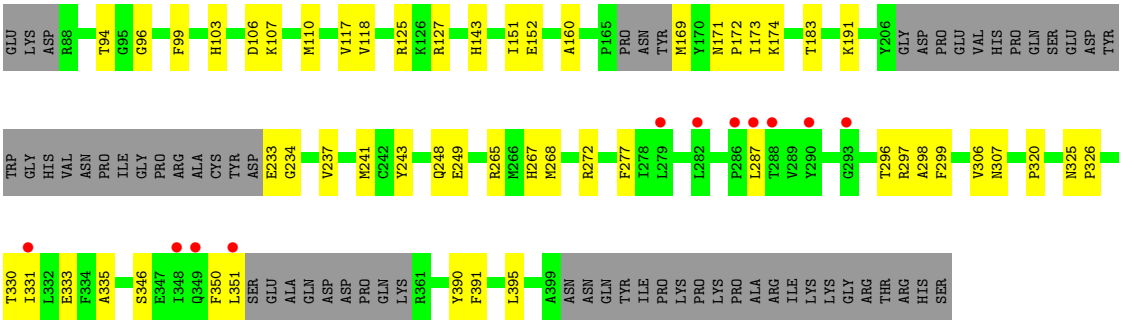
• Molecule 1: UDP-glucuronic acid decarboxylase 1

Chain A:



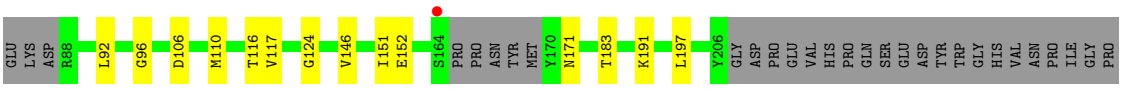
• Molecule 1: UDP-glucuronic acid decarboxylase 1

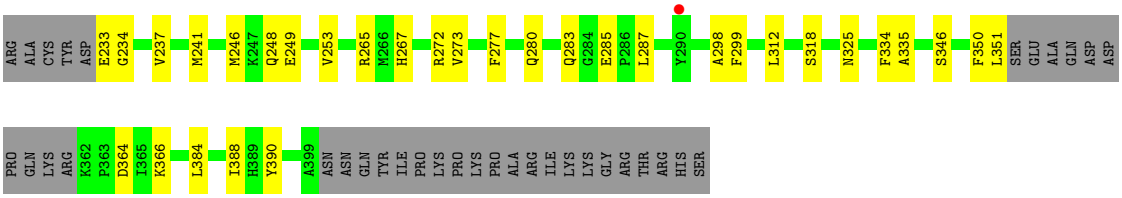
Chain B:



• Molecule 1: UDP-glucuronic acid decarboxylase 1

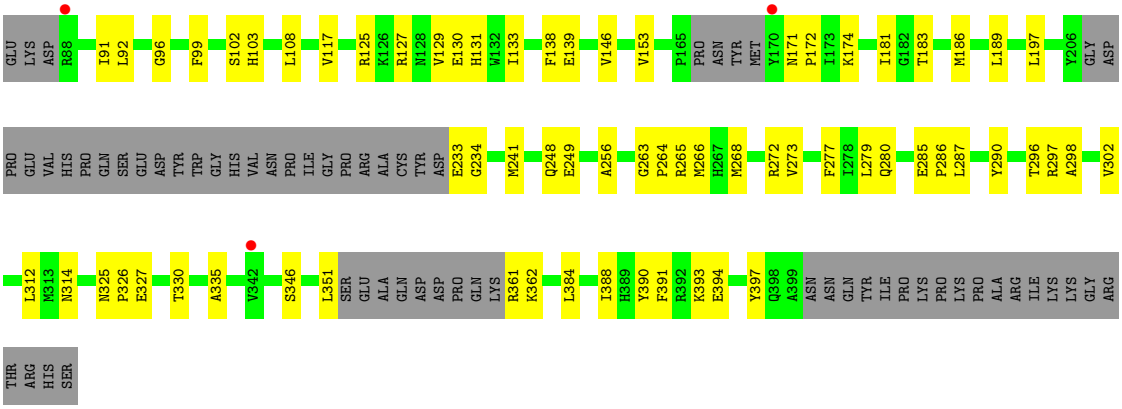
Chain C:





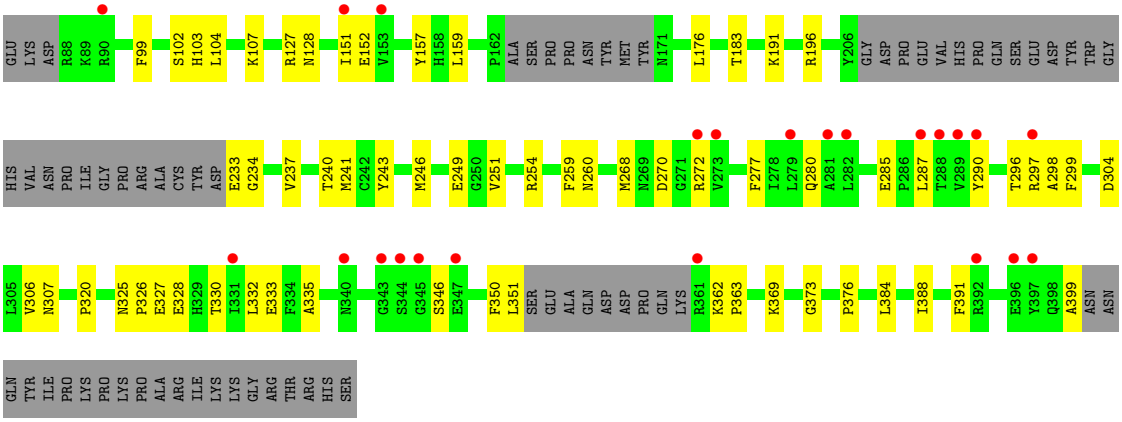
• Molecule 1: UDP-glucuronic acid decarboxylase 1

Chain D:



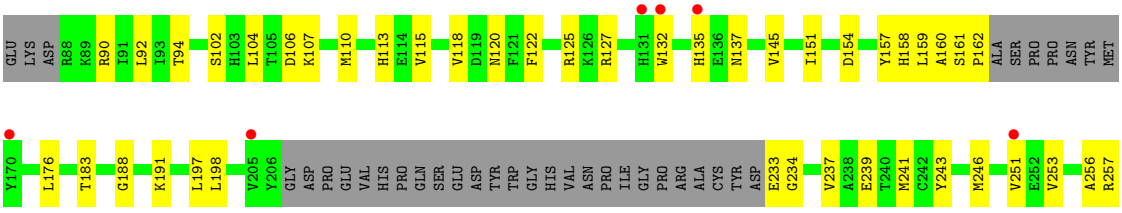
• Molecule 1: UDP-glucuronic acid decarboxylase 1

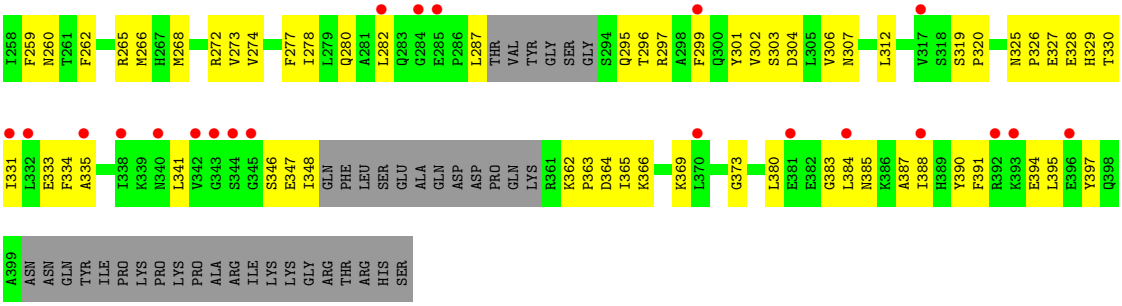
Chain E:



• Molecule 1: UDP-glucuronic acid decarboxylase 1

Chain F:




I258 F259 N260 T261 F262
R265 M266 H267 M268
R272 V273 V274
F277 I278 L279 Q280 A281 L282 Q283 G284 E285 P286 L287 THR VAL TYR GLY SER GLY S294 Q295 T296 R297 A298 F299 Q300 Y301 V302 S303 D304 L305 V306 N307
L312
V317 S318 S319 P320
N325 P326 E327 E328 H329 T330
I331 L332 E333 F334 A335
I338 K339 N340 L341 V342 G343 S344 G345 S346 E347 I348 GLN PHE LEU SER GLU ALA GLN ASP ASP PRO GLN LYS R361 K362 P363 D364 I365 K366
K369 L370
G373
L380 E381 E382 G383 L384 N385 K386 A387 I388 H389 Y390 F391 R392 K393 E394 L395 E396 Y397 Q398
A399 ASN ASN GLN TYR ILE PRO LYS PRO LYS PRO ALA ARG ILE LYS LYS GLY ARG THR ARG HIS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.57Å 92.07Å 290.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.37 – 2.64 38.90 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.37-2.64) 95.6 (38.90-2.64)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.198 , 0.245 0.197 , 0.243	Depositor DCC
R_{free} test set	3330 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13434	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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.

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: UGA, SO4, NAD, UDP, POP

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	0.48	0/2152	0.67	0/2905
1	B	0.57	0/2197	0.73	0/2967
1	C	0.56	0/2170	0.72	0/2931
1	D	0.50	0/2189	0.67	1/2957 (0.0%)
1	E	0.48	0/2157	0.66	0/2912
1	F	0.47	0/2099	0.70	0/2832
All	All	0.51	0/12964	0.69	1/17504 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	314	ASN	O-C-N	-5.18	114.41	122.70

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	2113	0	2123	88	0
1	B	2156	0	2167	47	0
1	C	2130	0	2138	46	0
1	D	2148	0	2158	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2118	0	2132	57	0
1	F	2062	0	2076	108	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	3	0
3	A	25	0	11	1	0
3	B	25	0	11	0	0
3	D	25	0	11	2	0
4	A	37	0	19	2	0
4	B	37	0	19	2	0
4	C	37	0	19	0	0
4	D	37	0	19	1	0
4	E	37	0	19	0	0
4	F	37	0	19	2	0
5	A	10	0	0	3	0
5	B	10	0	0	1	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	C	9	0	0	2	0
6	E	9	0	0	0	0
6	F	9	0	0	3	0
7	B	32	0	0	2	0
7	C	31	0	0	3	0
7	D	9	0	0	0	0
7	E	2	0	0	0	0
All	All	13434	0	13097	404	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 15.

The worst 5 of 404 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:F:262:PHE:HE2	1:F:299:PHE:CD1	1.43	1.37
1:F:262:PHE:CE2	1:F:299:PHE:CD1	2.34	1.15
1:B:233:GLU:HG2	1:B:234:GLY:H	1.05	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:GLU:HG2	1:F:234:GLY:H	0.94	1.06
1:F:262:PHE:CZ	1:F:272:ARG:HD3	1.90	1.06

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	257/336 (76%)	249 (97%)	7 (3%)	1 (0%)	34	48
1	B	266/336 (79%)	260 (98%)	6 (2%)	0	100	100
1	C	263/336 (78%)	254 (97%)	9 (3%)	0	100	100
1	D	265/336 (79%)	252 (95%)	13 (5%)	0	100	100
1	E	261/336 (78%)	255 (98%)	6 (2%)	0	100	100
1	F	251/336 (75%)	242 (96%)	9 (4%)	0	100	100
All	All	1563/2016 (78%)	1512 (97%)	50 (3%)	1 (0%)	51	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	MET

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	229/289 (79%)	229 (100%)	0	100	100
1	B	234/289 (81%)	234 (100%)	0	100	100
1	C	231/289 (80%)	231 (100%)	0	100	100
1	D	233/289 (81%)	233 (100%)	0	100	100
1	E	230/289 (80%)	230 (100%)	0	100	100
1	F	224/289 (78%)	224 (100%)	0	100	100
All	All	1381/1734 (80%)	1381 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	295	GLN
1	F	135	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

27 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	NAD	B	501	-	42,48,48	0.88	3 (7%)	50,73,73	1.20	2 (4%)
5	SO4	A	504	-	4,4,4	0.17	0	6,6,6	0.28	0
2	NAD	F	501	-	42,48,48	0.82	1 (2%)	50,73,73	1.15	2 (4%)
5	SO4	E	504	-	4,4,4	0.15	0	6,6,6	0.31	0
6	POP	F	503	-	6,8,8	0.72	0	13,13,13	1.36	1 (7%)
4	UGA	A	503	-	32,39,39	0.82	1 (3%)	42,60,60	1.03	4 (9%)
4	UGA	B	503	-	32,39,39	0.83	1 (3%)	42,60,60	1.17	3 (7%)
3	UDP	B	502	-	24,26,26	1.15	3 (12%)	37,40,40	1.62	6 (16%)
2	NAD	A	501	-	42,48,48	0.80	1 (2%)	50,73,73	1.27	3 (6%)
4	UGA	E	503	-	32,39,39	0.82	1 (3%)	42,60,60	1.17	3 (7%)
5	SO4	B	504	-	4,4,4	0.12	0	6,6,6	0.62	0
2	NAD	E	501	-	42,48,48	0.80	0	50,73,73	1.22	5 (10%)
4	UGA	C	502	-	32,39,39	0.77	1 (3%)	42,60,60	1.16	3 (7%)
5	SO4	A	505	-	4,4,4	0.15	0	6,6,6	0.18	0
2	NAD	C	501	-	42,48,48	0.91	2 (4%)	50,73,73	1.27	6 (12%)
4	UGA	F	502	-	32,39,39	0.82	1 (3%)	42,60,60	1.28	3 (7%)
6	POP	C	503	-	6,8,8	0.69	0	13,13,13	1.30	1 (7%)
4	UGA	D	503	-	32,39,39	0.87	1 (3%)	42,60,60	0.98	2 (4%)
3	UDP	A	502	-	24,26,26	1.08	3 (12%)	37,40,40	1.61	7 (18%)
5	SO4	C	504	-	4,4,4	0.12	0	6,6,6	0.39	0
5	SO4	D	505	-	4,4,4	0.36	0	6,6,6	0.49	0
3	UDP	D	502	-	24,26,26	1.07	2 (8%)	37,40,40	1.73	6 (16%)
5	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.49	0
5	SO4	F	504	-	4,4,4	0.18	0	6,6,6	0.17	0
5	SO4	B	505	-	4,4,4	0.20	0	6,6,6	0.41	0
2	NAD	D	501	-	42,48,48	0.78	0	50,73,73	1.24	3 (6%)
6	POP	E	502	-	6,8,8	1.15	0	13,13,13	1.91	3 (23%)

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	UGA	F	502	-	-	5/23/61/61	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POP	C	503	-	-	2/6/6/6	-
6	POP	F	503	-	-	4/6/6/6	-
4	UGA	D	503	-	-	6/23/61/61	0/3/3/3
2	NAD	E	501	-	-	1/26/62/62	0/5/5/5
2	NAD	F	501	-	-	1/26/62/62	0/5/5/5
3	UDP	A	502	-	-	4/16/32/32	0/2/2/2
2	NAD	B	501	-	-	3/26/62/62	0/5/5/5
4	UGA	C	502	-	-	6/23/61/61	0/3/3/3
2	NAD	A	501	-	-	3/26/62/62	0/5/5/5
4	UGA	A	503	-	-	2/23/61/61	0/3/3/3
3	UDP	D	502	-	-	4/16/32/32	0/2/2/2
4	UGA	B	503	-	-	7/23/61/61	0/3/3/3
4	UGA	E	503	-	-	8/23/61/61	0/3/3/3
3	UDP	B	502	-	-	4/16/32/32	0/2/2/2
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
6	POP	E	502	-	-	0/6/6/6	-
2	NAD	C	501	-	-	4/26/62/62	0/5/5/5

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O4B-C1B	2.75	1.44	1.41
3	B	502	UDP	C4-N3	-2.57	1.34	1.38
4	B	503	UGA	C2-N3	-2.51	1.33	1.38
3	B	502	UDP	C2-N1	2.50	1.42	1.38
2	A	501	NAD	C5A-C4A	2.38	1.47	1.40

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	502	POP	P2-O-P1	-4.95	115.83	132.83
3	D	502	UDP	C4-N3-C2	-4.94	120.06	126.58
3	D	502	UDP	N3-C2-N1	4.91	121.40	114.89
4	F	502	UGA	O3A-PB-O3B	-4.90	92.60	102.48
3	B	502	UDP	N3-C2-N1	4.33	120.63	114.89

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	NAD	C5D-O5D-PN-O1N
2	D	501	NAD	C5B-O5B-PA-O2A
2	D	501	NAD	C5D-O5D-PN-O1N
3	B	502	UDP	C5'-O5'-PA-O1A
3	B	502	UDP	C5'-O5'-PA-O2A

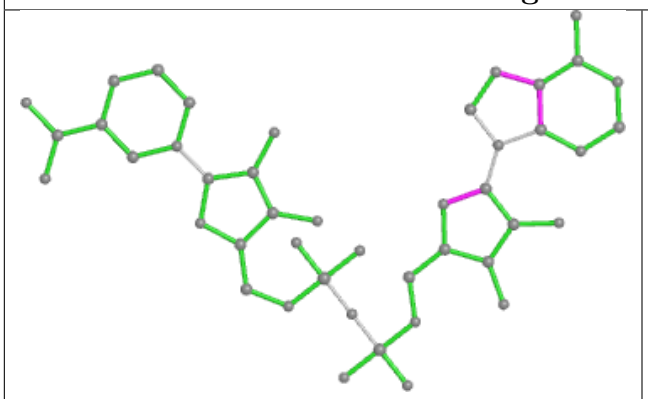
There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	NAD	3	0
6	F	503	POP	3	0
4	A	503	UGA	2	0
4	B	503	UGA	2	0
5	B	504	SO4	1	0
5	A	505	SO4	3	0
2	C	501	NAD	1	0
4	F	502	UGA	2	0
6	C	503	POP	2	0
4	D	503	UGA	1	0
3	A	502	UDP	1	0
3	D	502	UDP	2	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 NAD B 501



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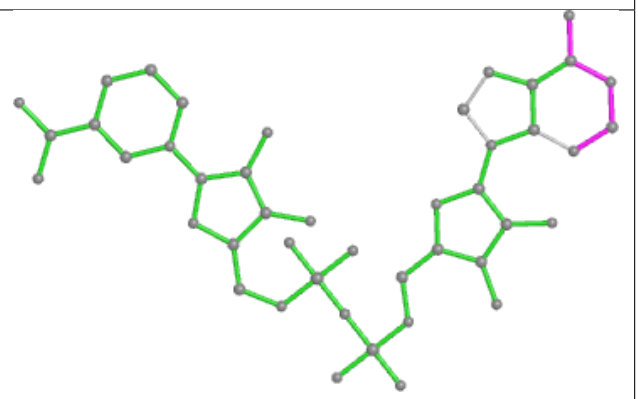
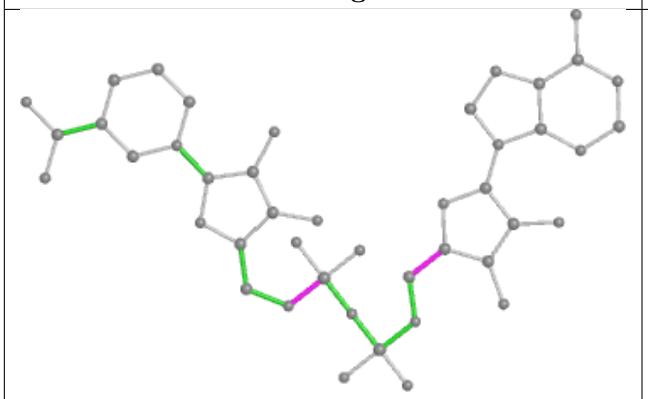
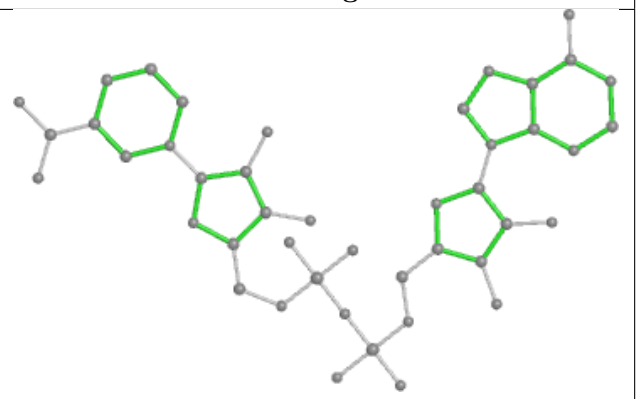


Bond angles

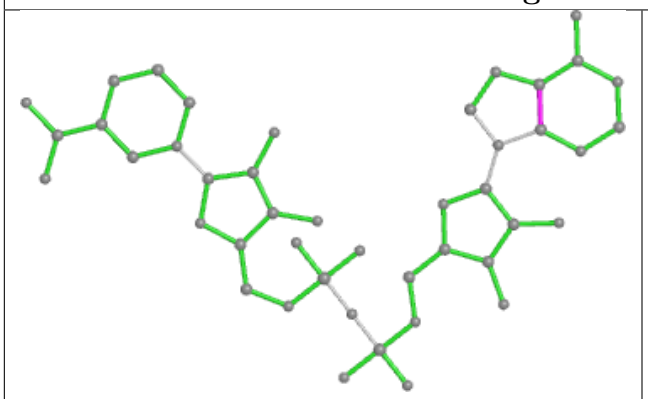


Torsions



Rings

Ligand NAD F 501



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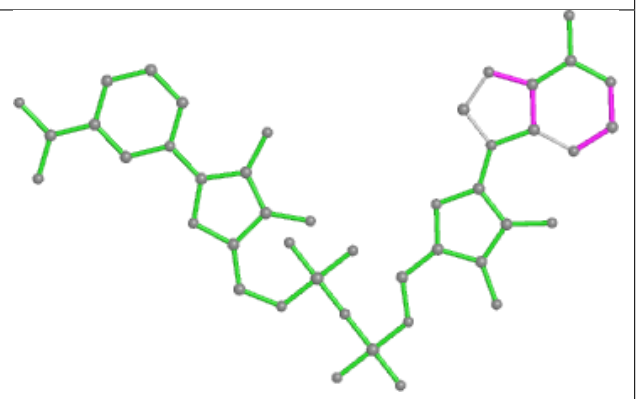

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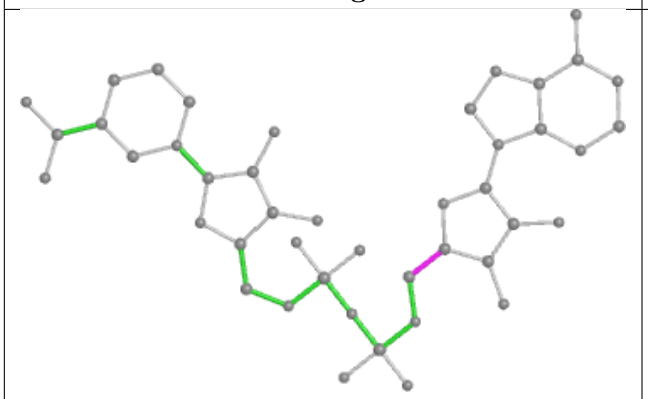

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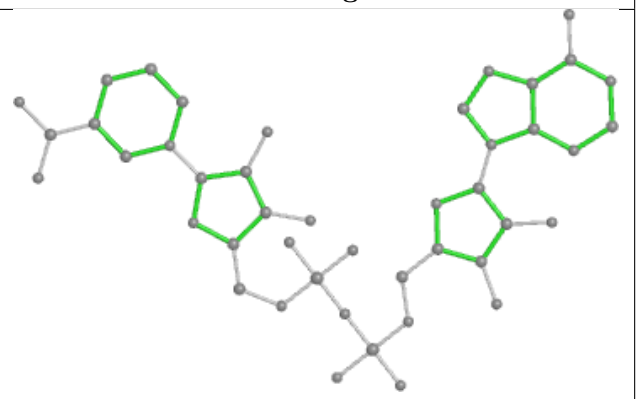
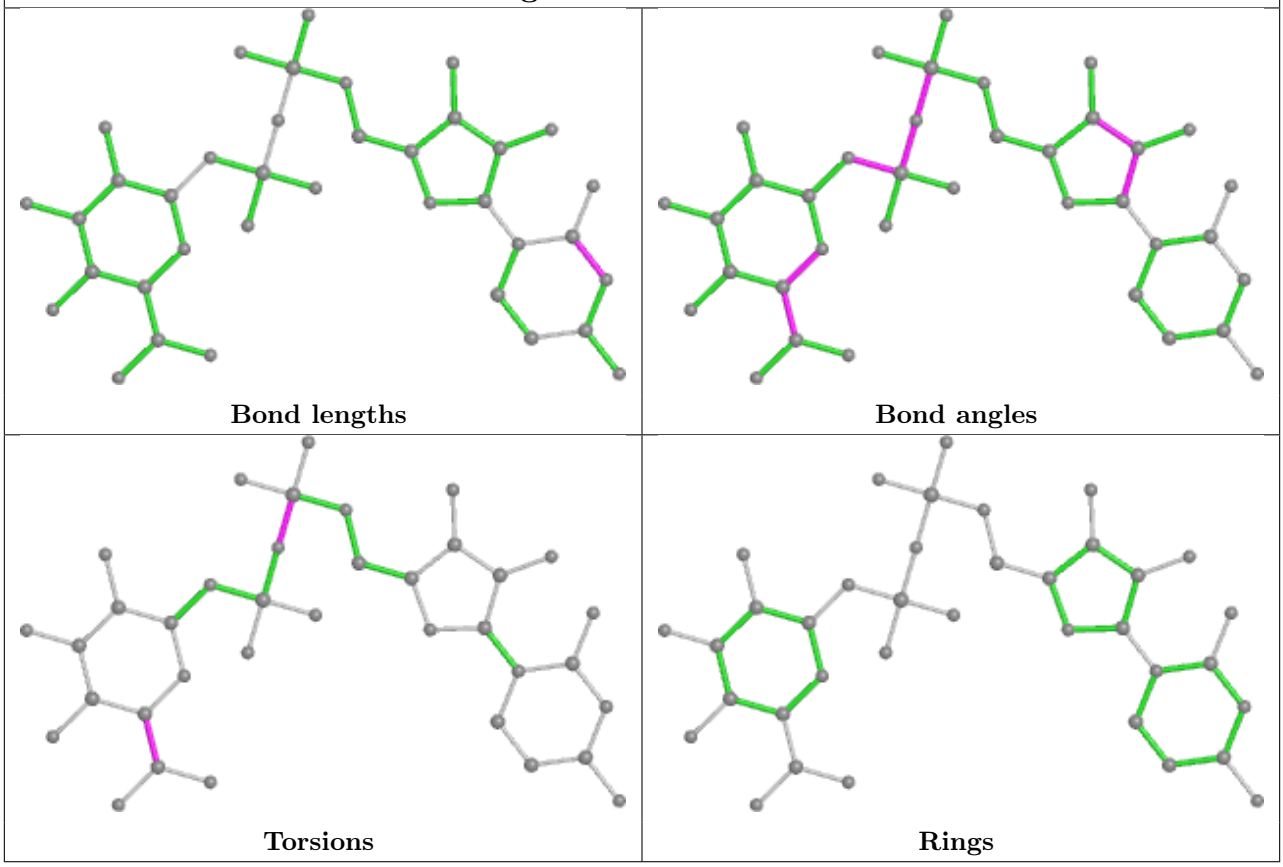


Rings

Ligand UGA A 503



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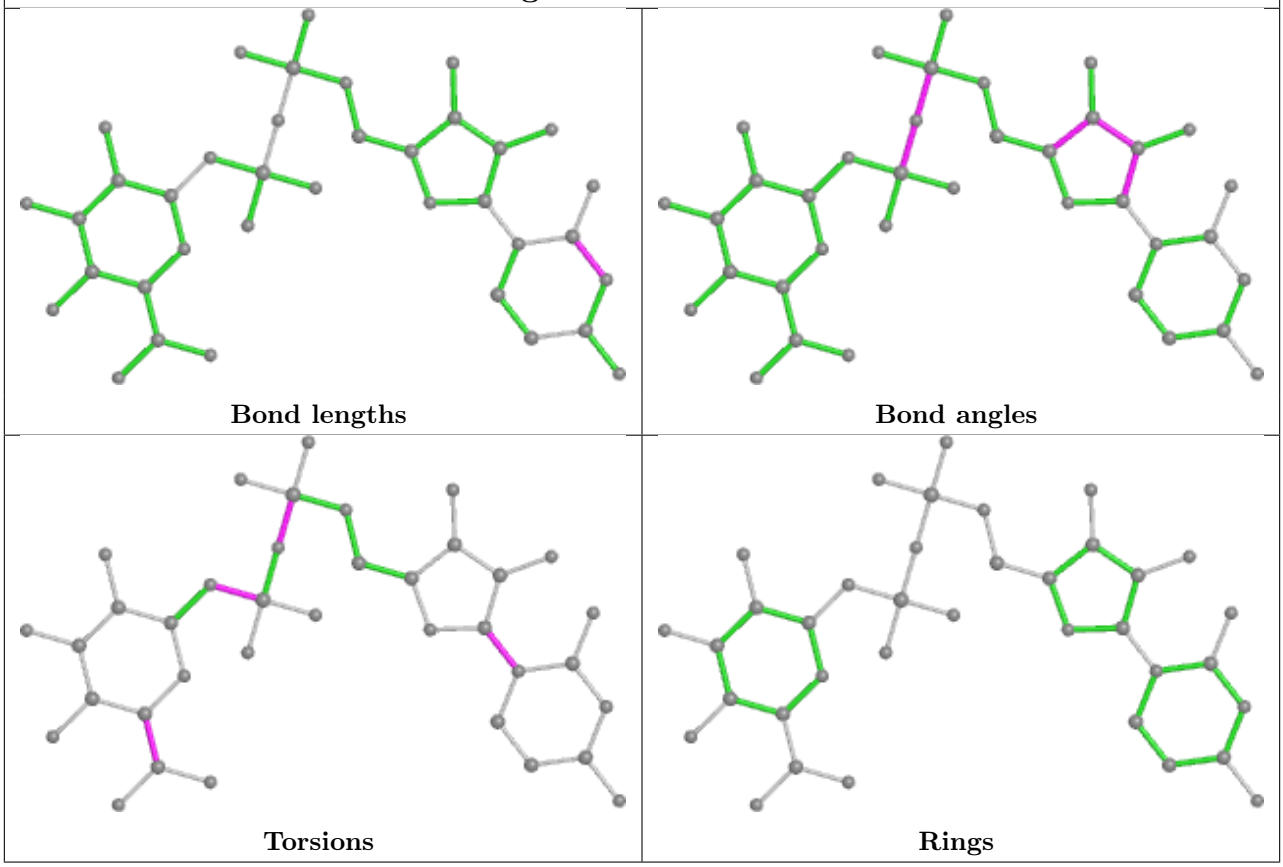

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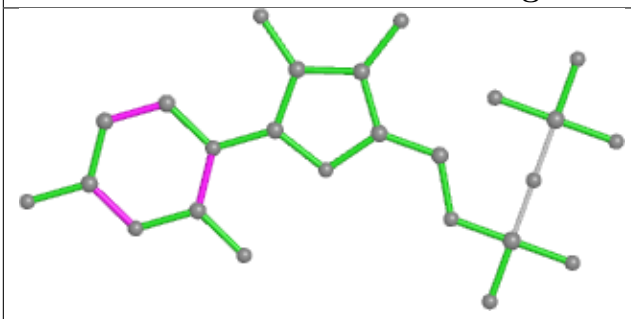

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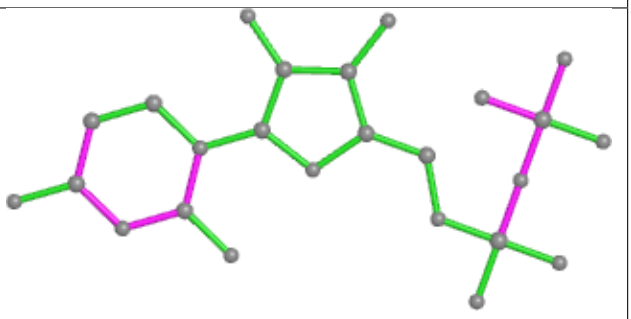
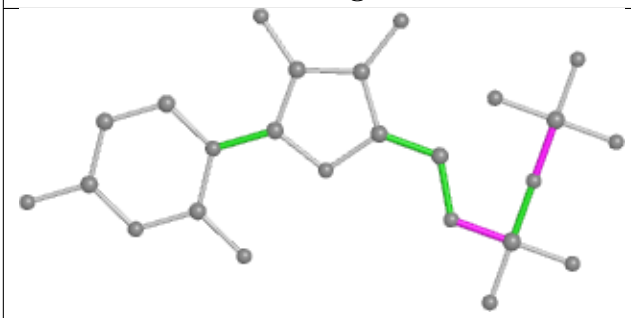
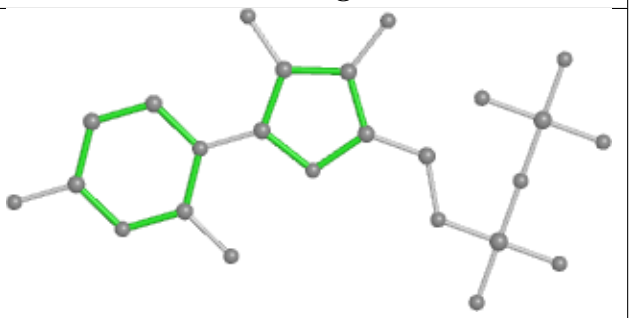


Bond angles

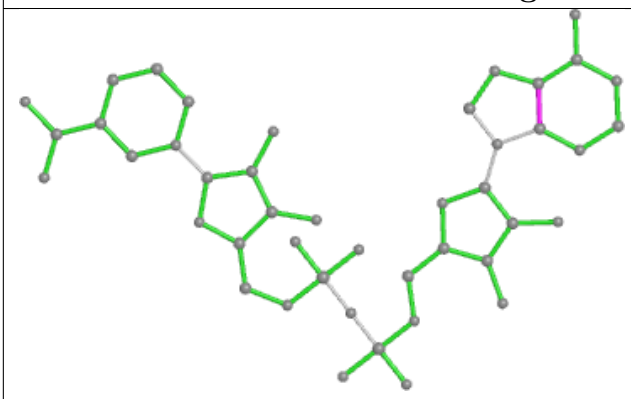


Torsions



Rings

Ligand NAD A 501



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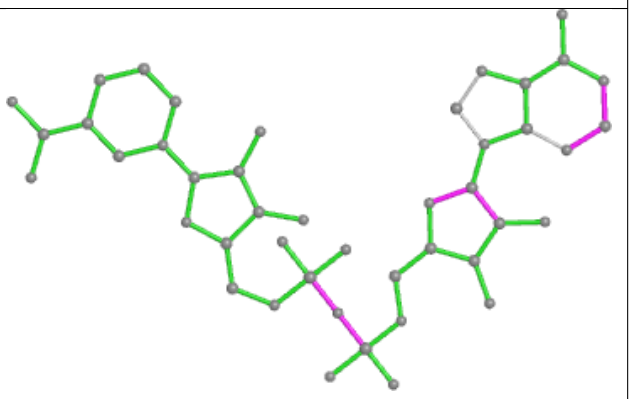

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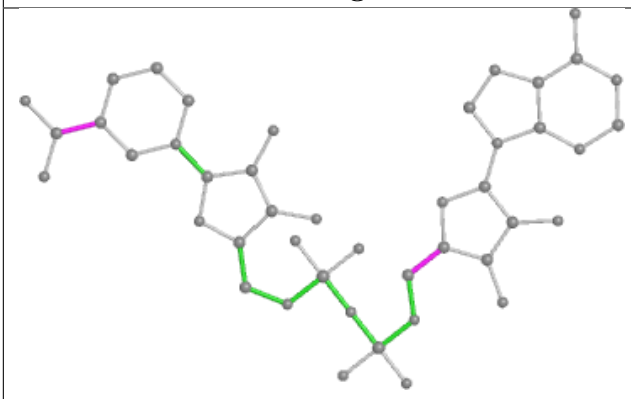

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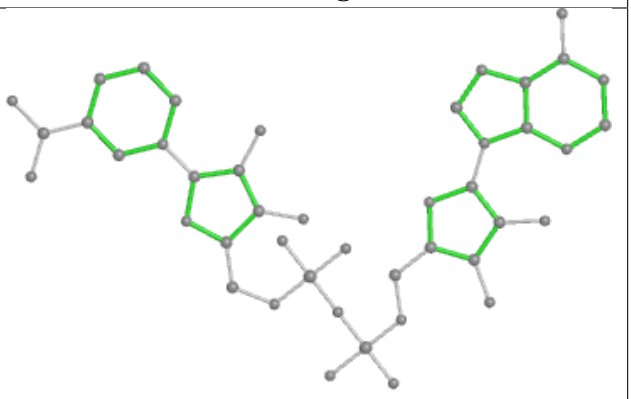
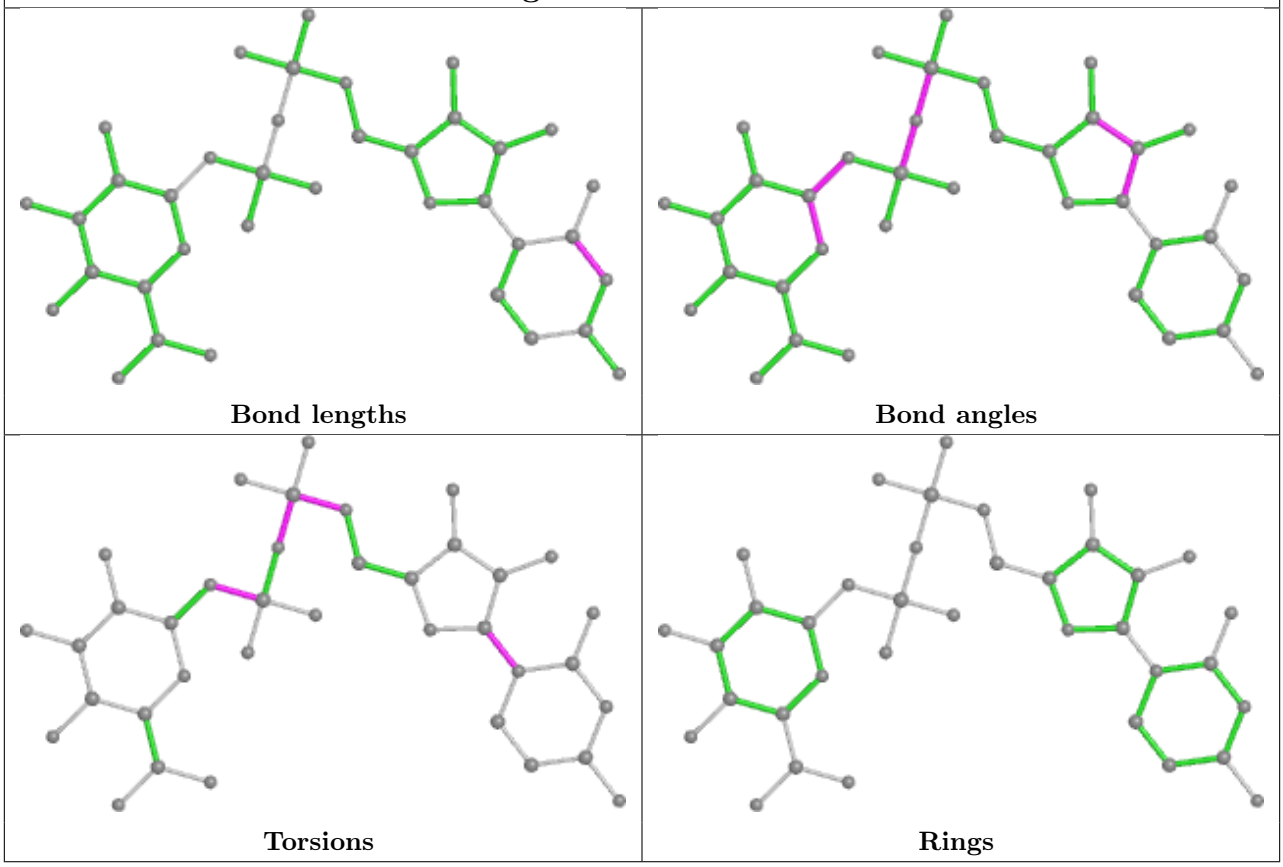


Rings

Ligand UGA E 503



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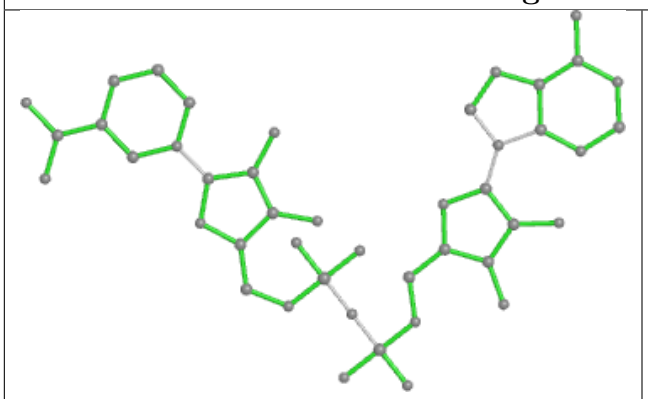
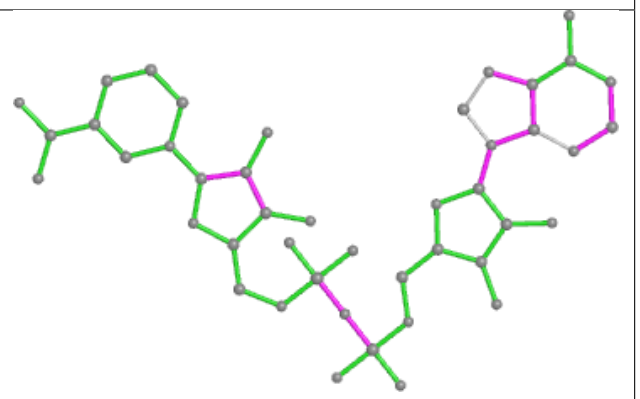


Bond lengths



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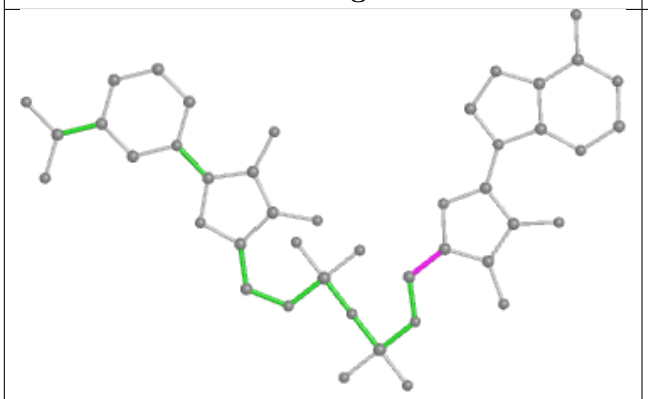

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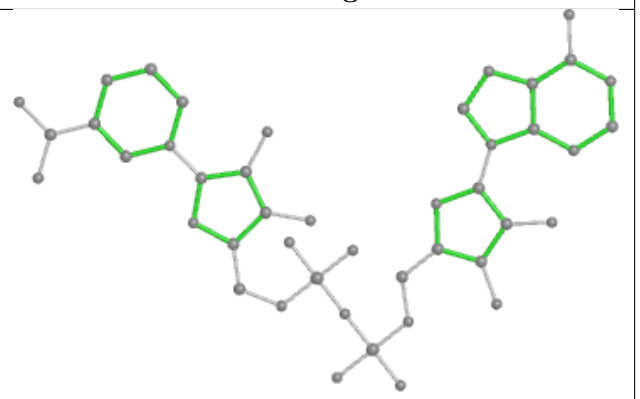
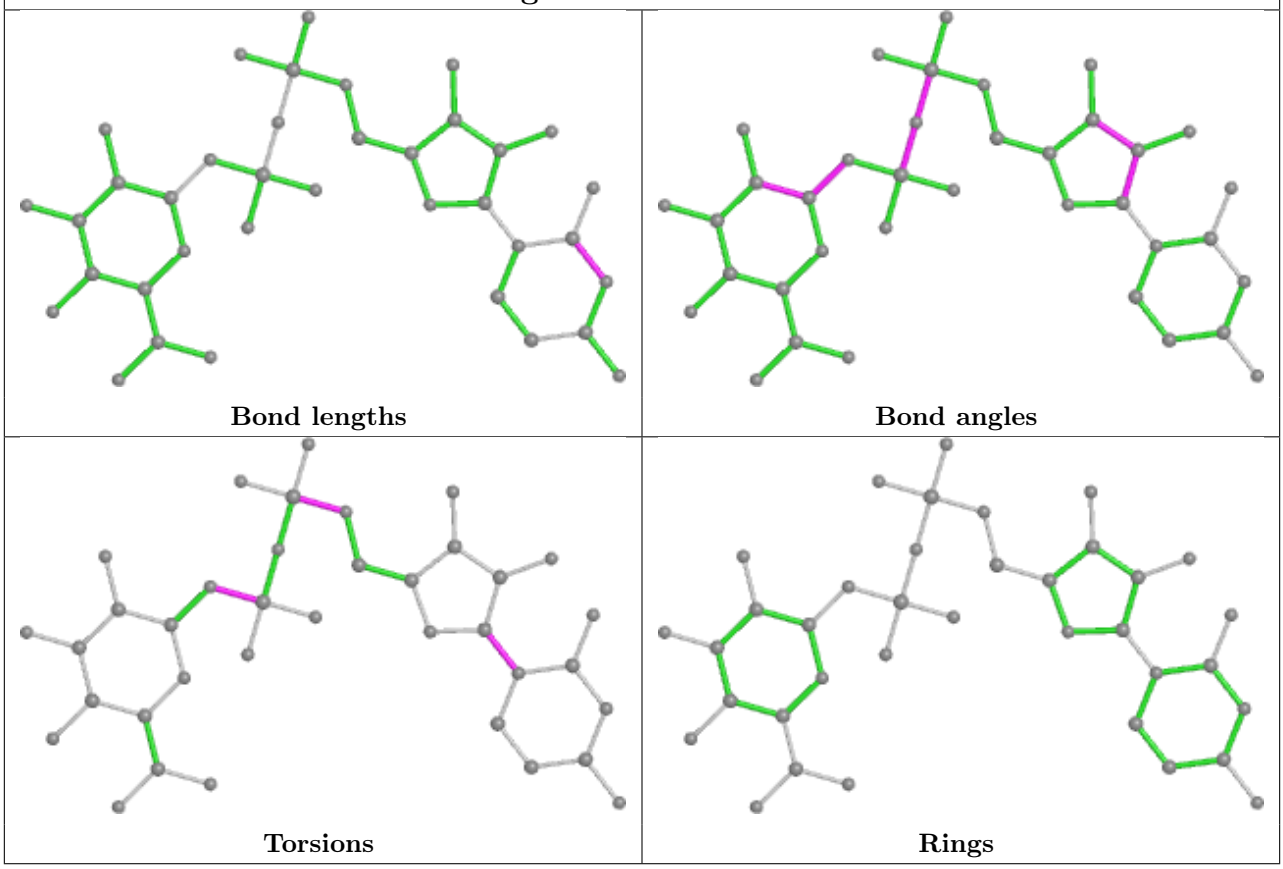


Rings

Ligand UGA C 502



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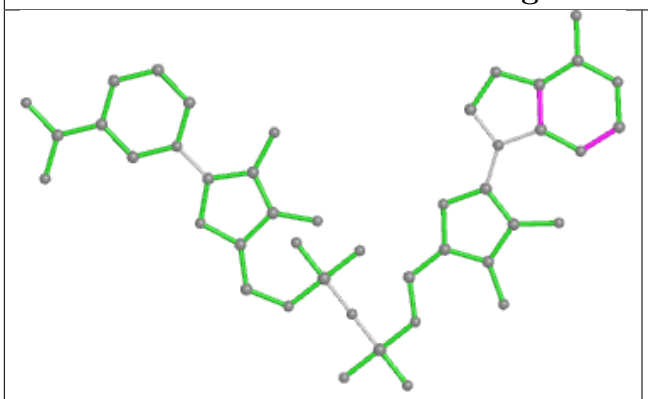

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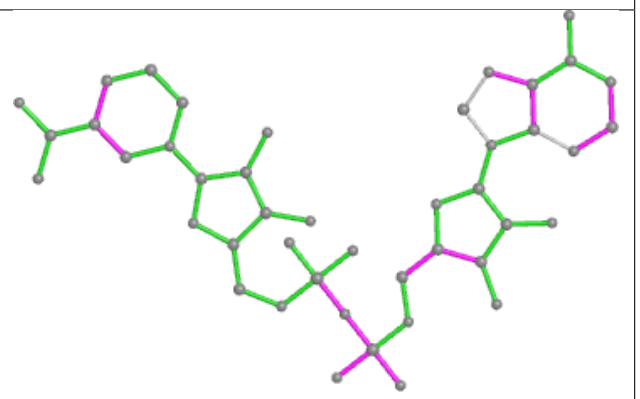

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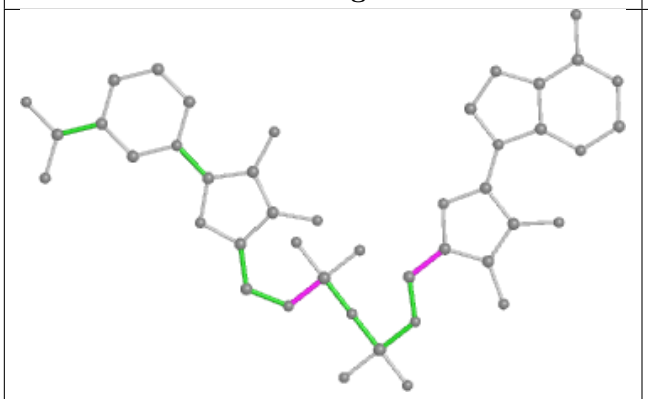

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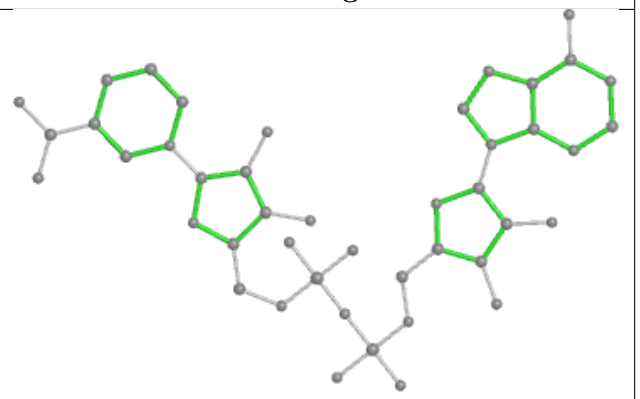

Rings

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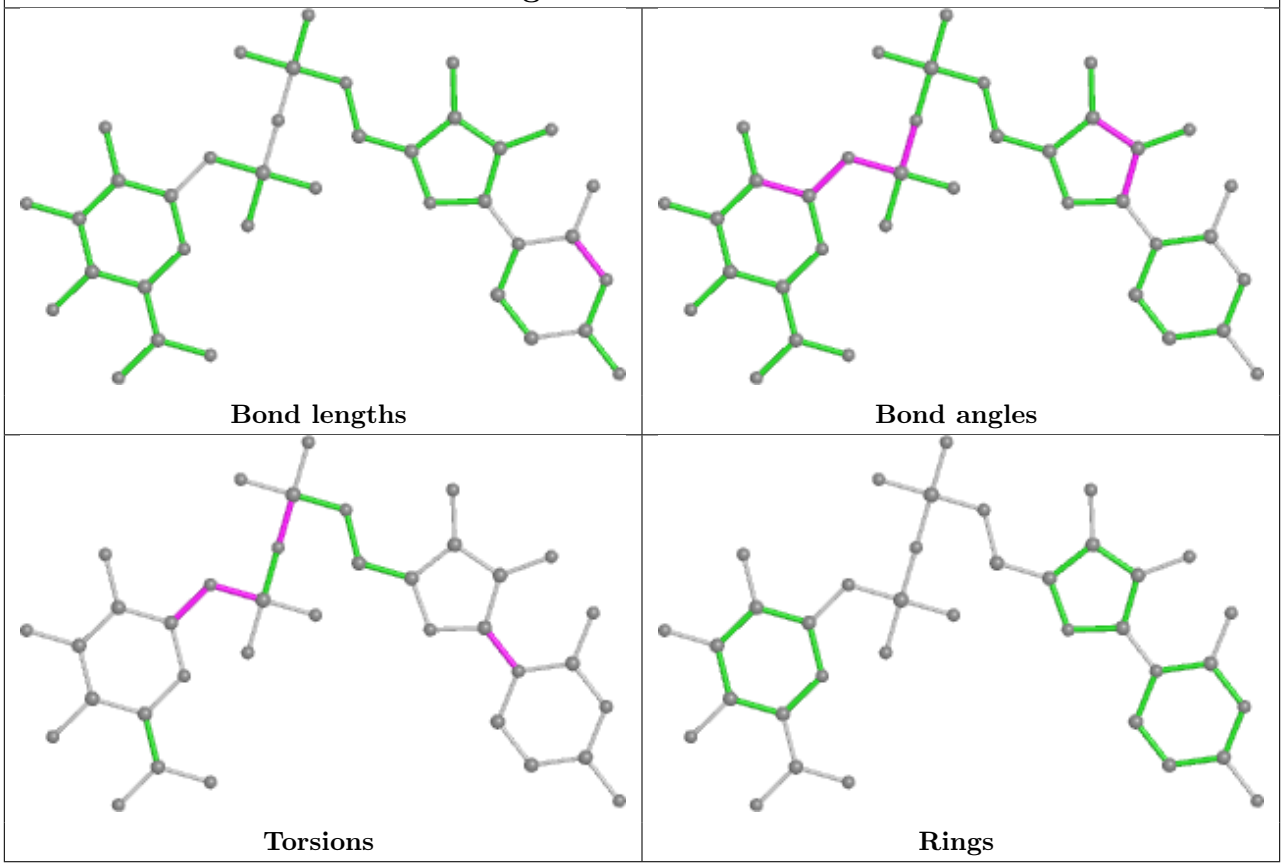

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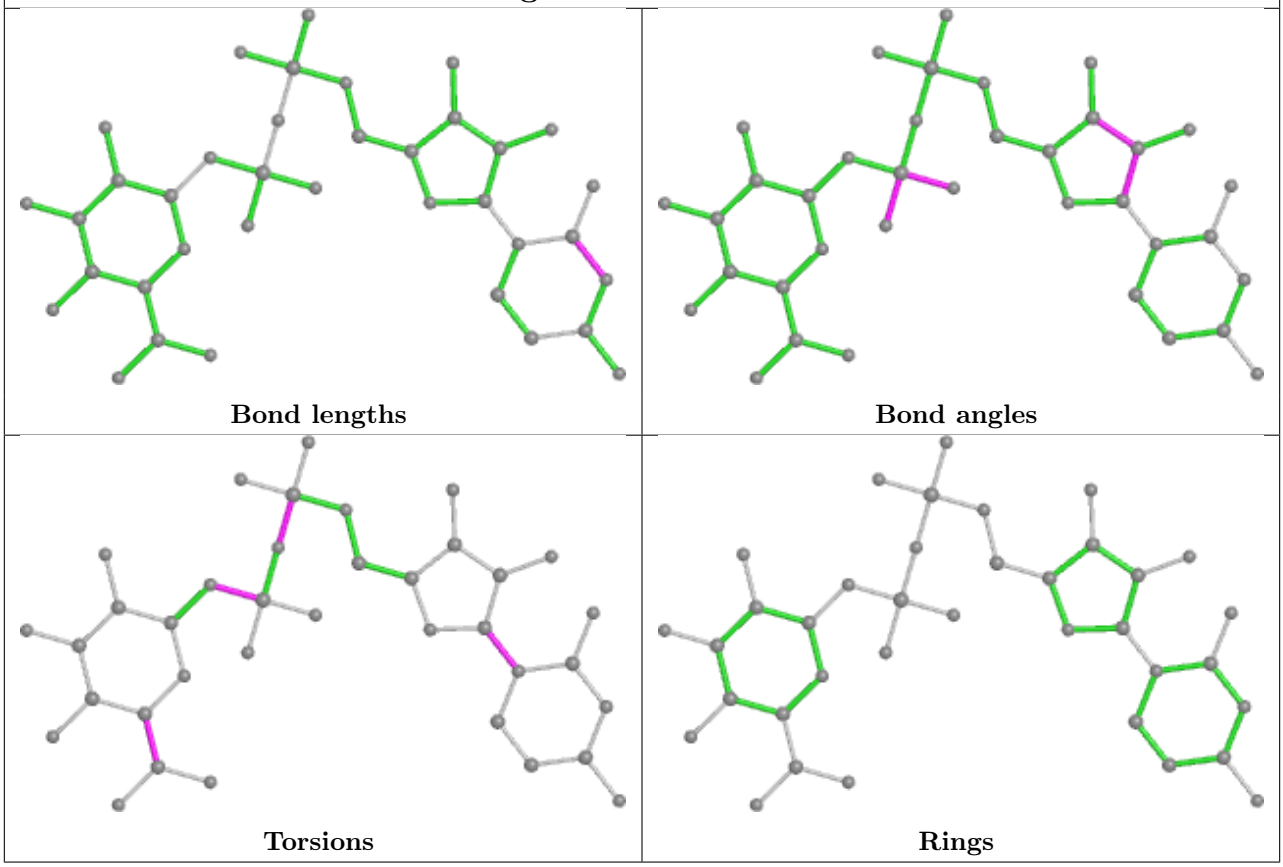
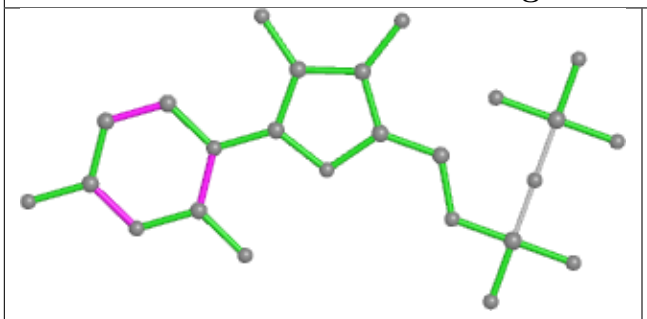
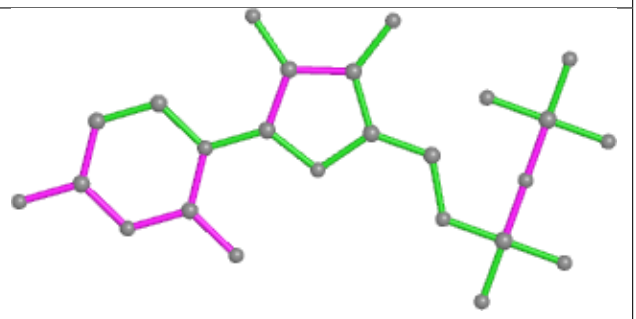


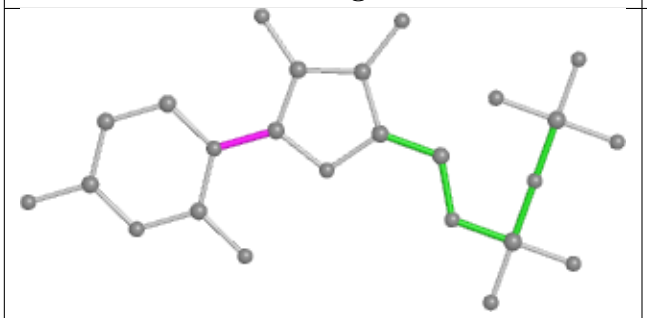
Ligand UDP A 502



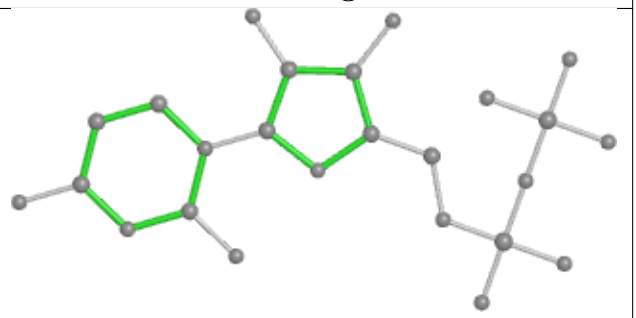
Bond lengths



Bond angles

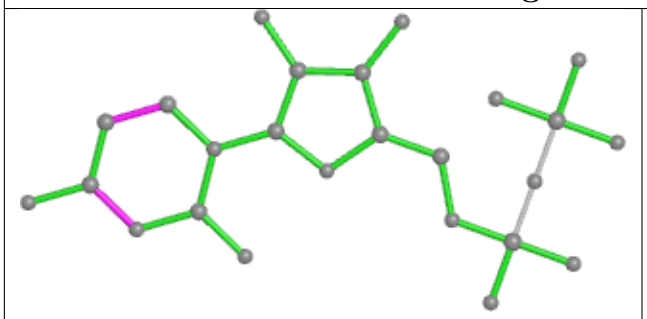


Torsions

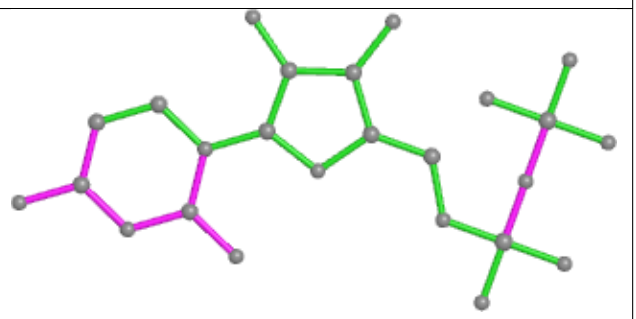


Rings

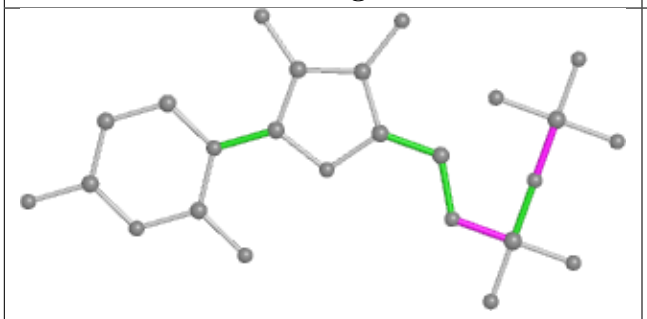
Ligand UDP D 502



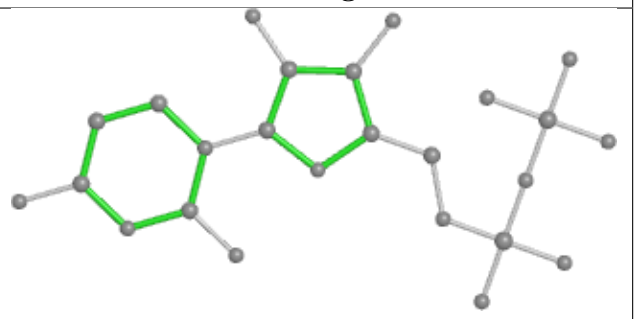
Bond lengths



Bond angles

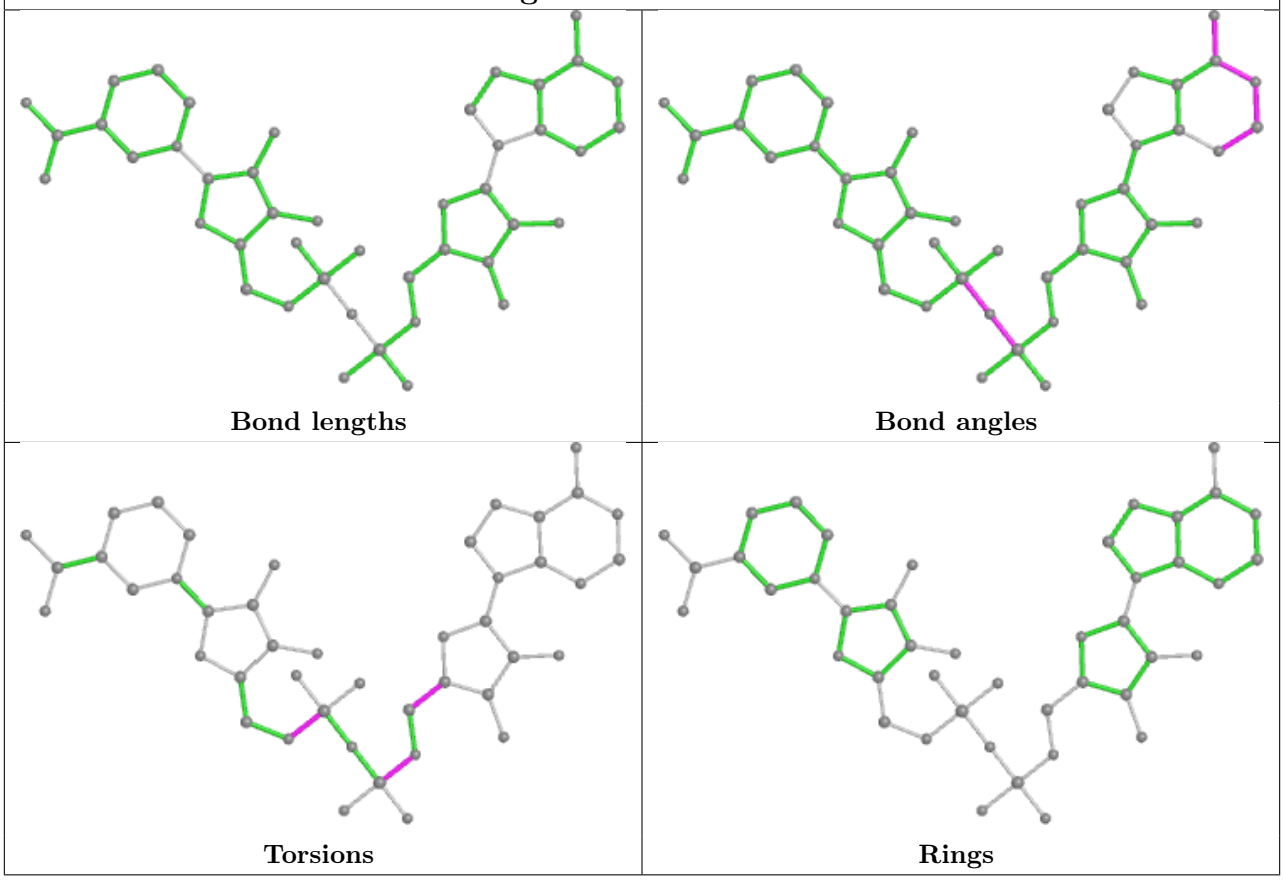


Torsions



Rings

Ligand NAD D 501



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	267/336 (79%)	0.54	38 (14%)	2	1	45, 83, 138, 167	0
1	B	274/336 (81%)	0.16	11 (4%)	38	35	33, 54, 104, 131	0
1	C	271/336 (80%)	-0.21	2 (0%)	87	86	38, 59, 95, 130	0
1	D	273/336 (81%)	-0.00	3 (1%)	80	78	40, 65, 111, 126	0
1	E	269/336 (80%)	0.45	23 (8%)	10	8	57, 89, 127, 152	0
1	F	261/336 (77%)	0.55	27 (10%)	6	4	63, 105, 136, 168	0
All	All	1615/2016 (80%)	0.24	104 (6%)	19	16	33, 75, 126, 168	0

The worst 5 of 104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	282	LEU	6.2
1	B	290	TYR	5.7
1	F	131	HIS	5.6
1	A	338	ILE	5.3
1	A	395	LEU	5.3

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)

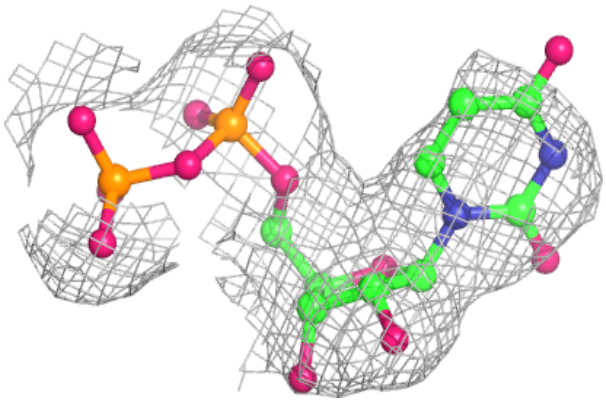
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

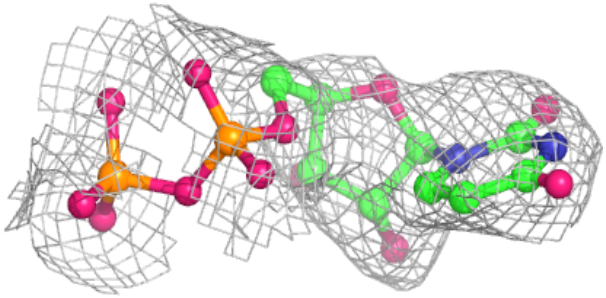
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UDP	A	502	25/25	0.82	0.24	100,124,141,142	0
3	UDP	B	502	25/25	0.82	0.35	81,108,119,173	0
3	UDP	D	502	25/25	0.82	0.23	84,100,120,147	0
5	SO4	F	504	5/5	0.84	0.18	121,123,127,128	0
6	POP	E	502	9/9	0.85	0.14	71,81,135,148	3
6	POP	F	503	9/9	0.85	0.26	86,91,184,186	3
5	SO4	E	504	5/5	0.86	0.24	109,118,119,123	0
5	SO4	A	504	5/5	0.86	0.14	132,135,137,140	0
6	POP	C	503	9/9	0.87	0.17	64,95,130,200	1
5	SO4	D	505	5/5	0.92	0.23	88,96,98,107	0
5	SO4	C	504	5/5	0.92	0.23	79,90,95,100	0
4	UGA	F	502	37/37	0.93	0.17	90,98,139,142	0
5	SO4	B	504	5/5	0.94	0.16	77,78,85,97	0
4	UGA	A	503	37/37	0.94	0.18	70,87,112,114	0
4	UGA	E	503	37/37	0.95	0.19	60,81,112,120	0
5	SO4	A	505	5/5	0.95	0.17	95,96,100,102	0
4	UGA	D	503	37/37	0.96	0.13	40,59,90,93	0
2	NAD	E	501	44/44	0.96	0.19	51,67,89,94	0
2	NAD	F	501	44/44	0.96	0.19	54,76,103,105	0
5	SO4	D	504	5/5	0.96	0.33	75,83,84,87	0
4	UGA	B	503	37/37	0.96	0.16	36,69,115,120	0
4	UGA	C	502	37/37	0.97	0.15	45,63,114,118	0
2	NAD	D	501	44/44	0.97	0.19	36,51,71,88	0
2	NAD	A	501	44/44	0.97	0.22	47,67,76,84	0
5	SO4	B	505	5/5	0.98	0.16	56,62,73,75	0
2	NAD	C	501	44/44	0.98	0.18	25,42,58,77	0
2	NAD	B	501	44/44	0.98	0.18	23,40,51,63	0

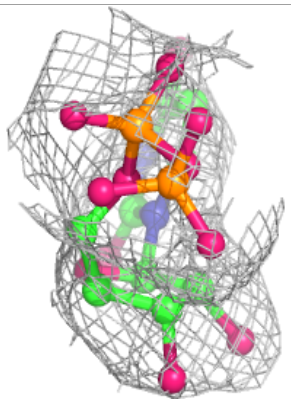
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP A 502:

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







Electron density around UDP B 502:

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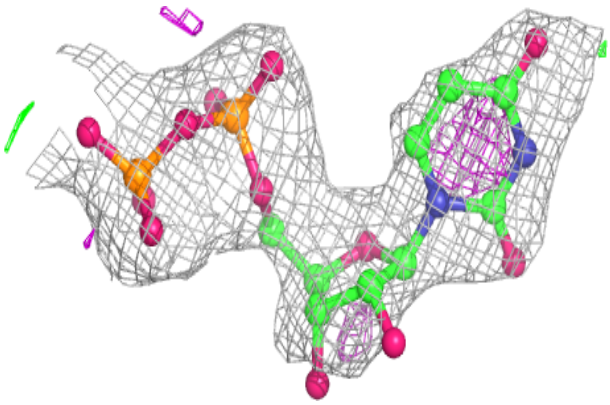
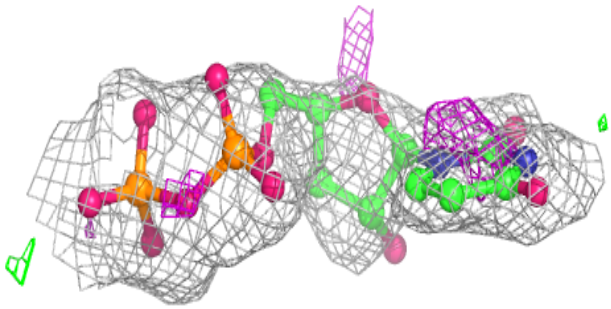
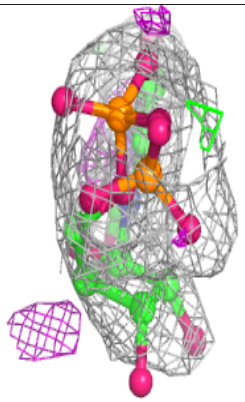
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UDP D 502:

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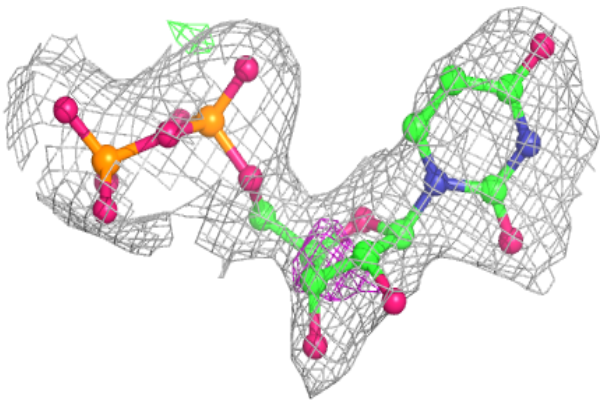
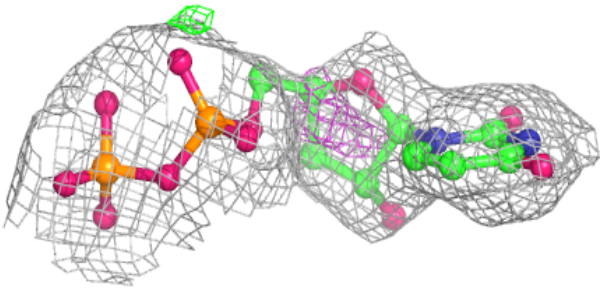
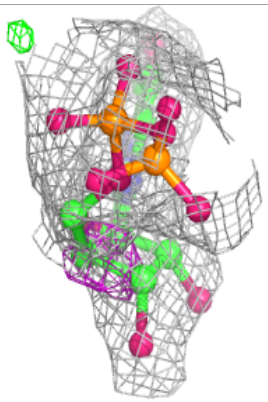
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UGA F 502:

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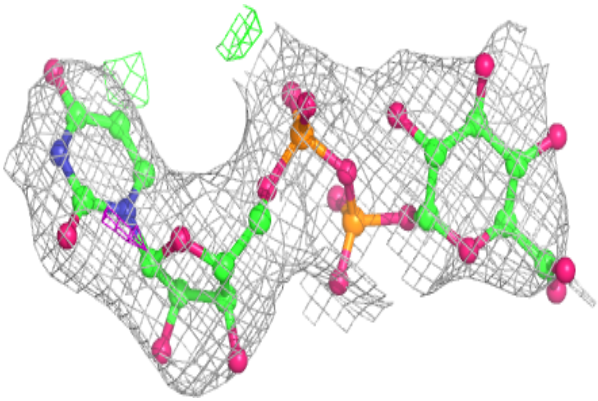
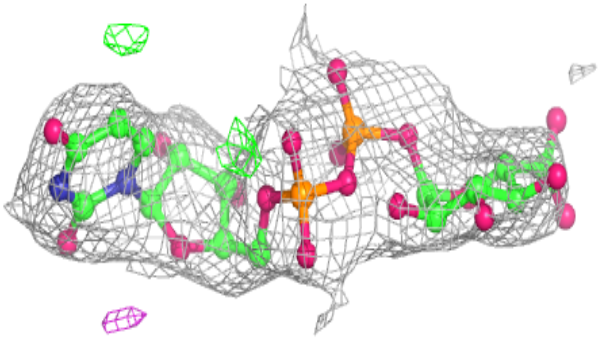
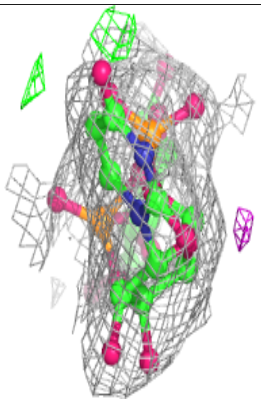
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

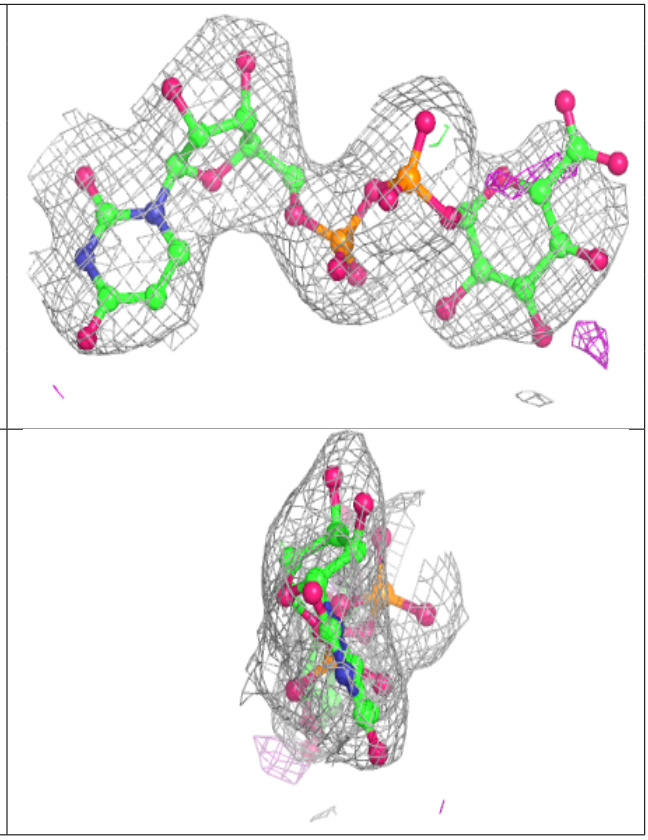


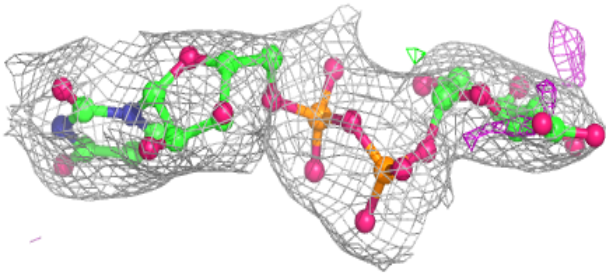




Electron density around UGA A 503:

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





Electron density around UGA E 503:

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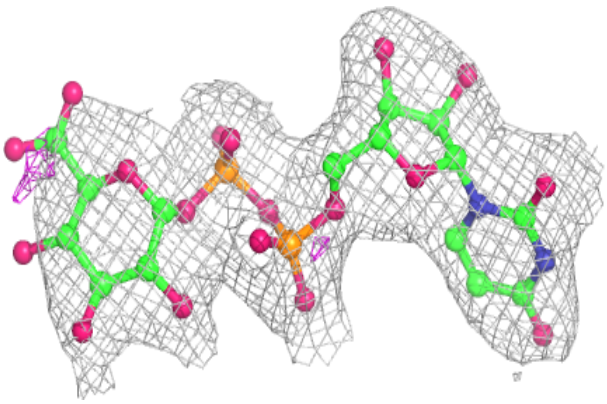
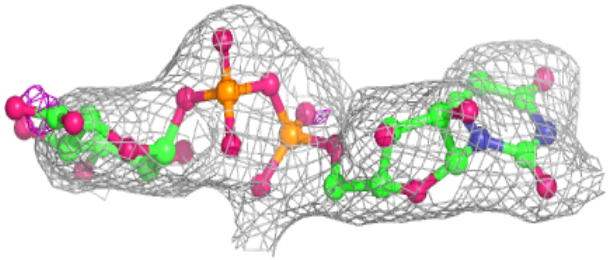
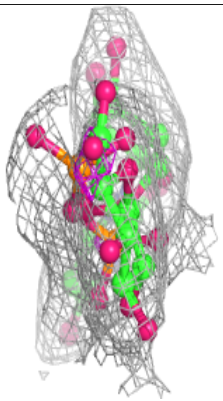
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UGA D 503:

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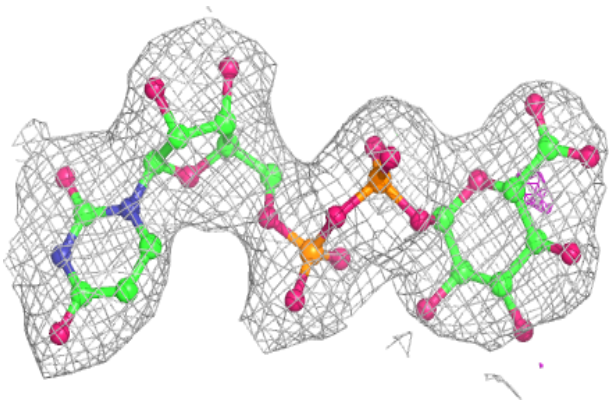
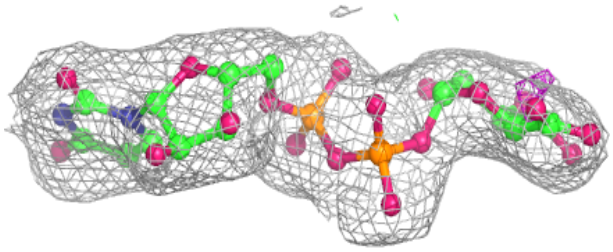
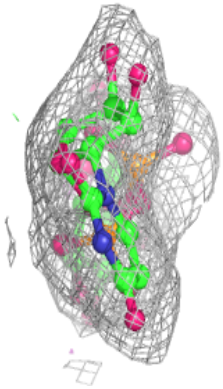
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAD E 501:

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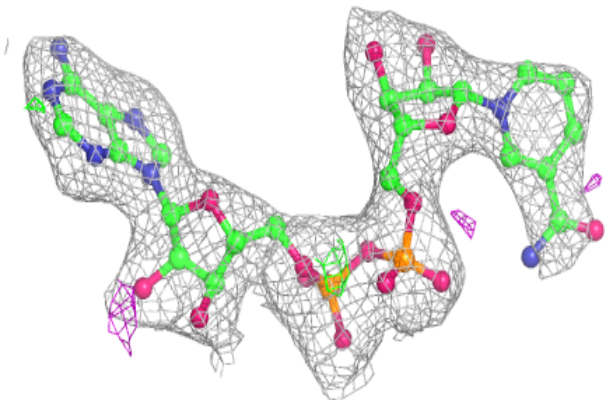
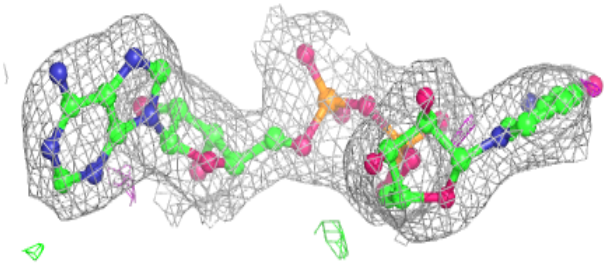
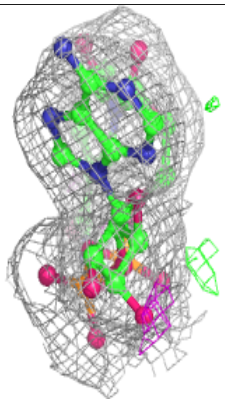
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

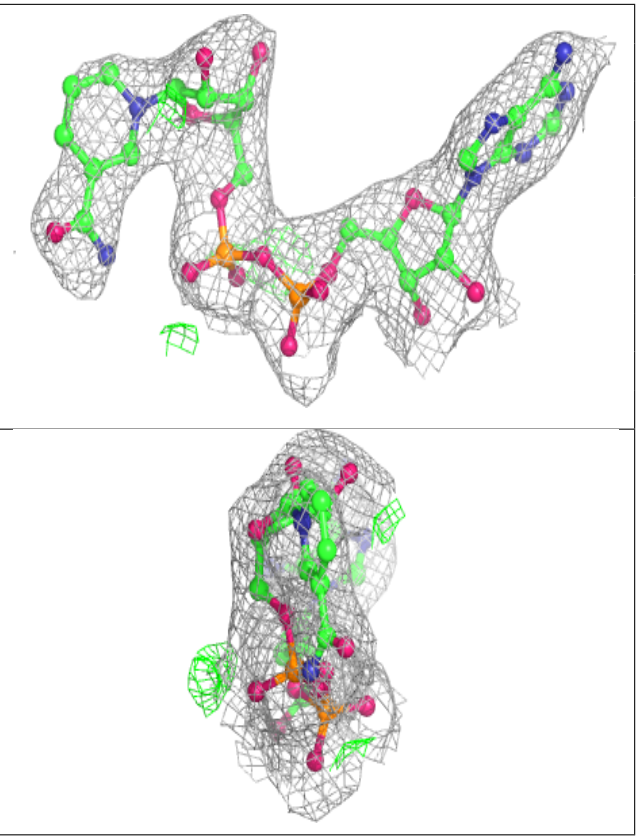






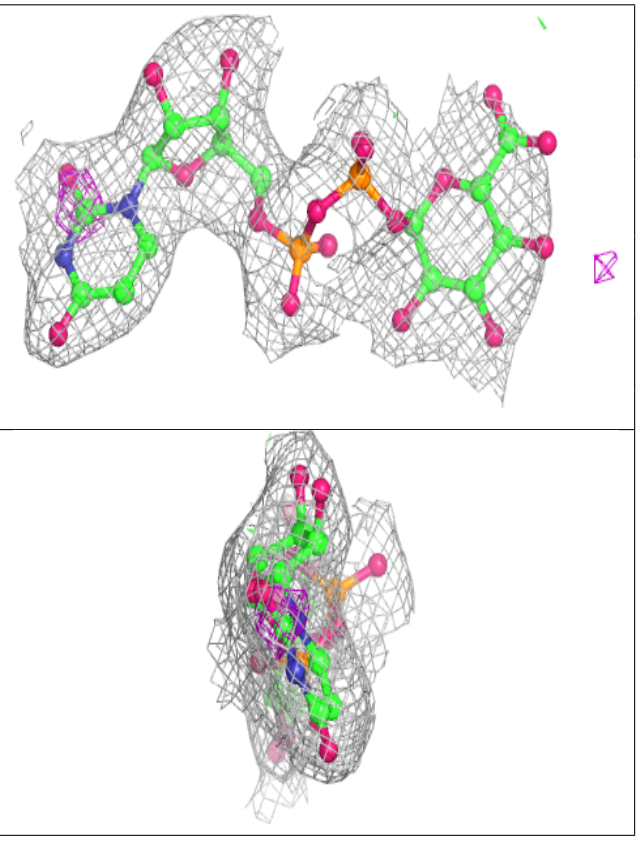
Electron density around NAD F 501:

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



Electron density around UGA B 503:

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



Electron density around UGA C 502:

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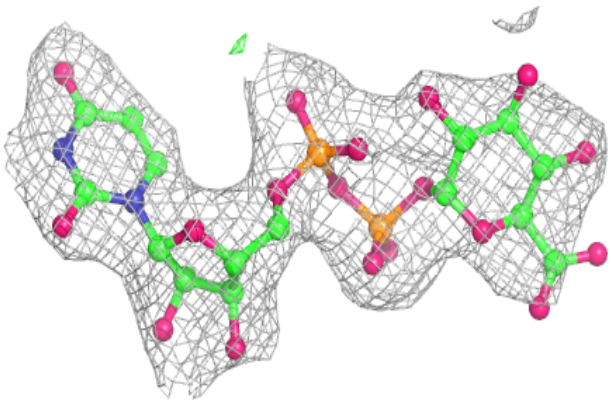
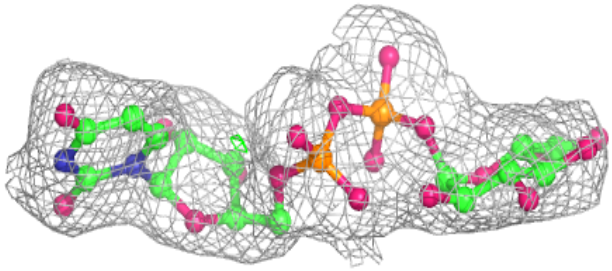
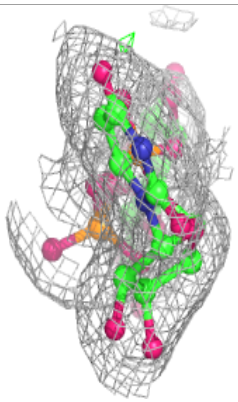
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAD D 501:

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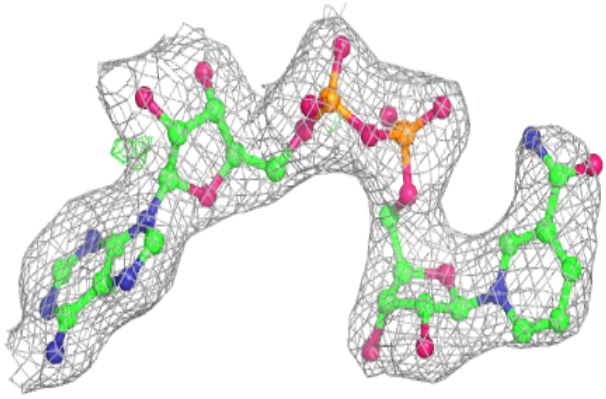
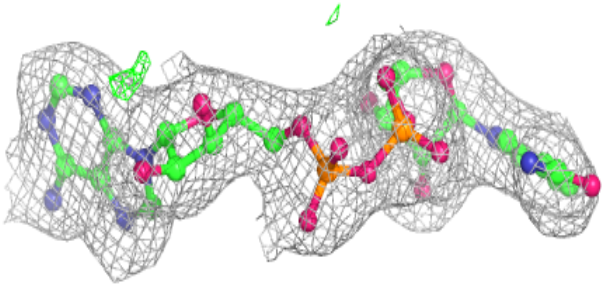
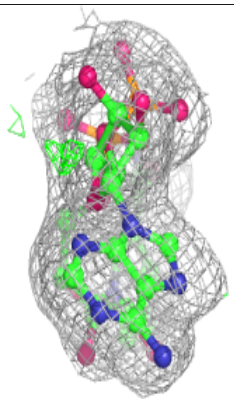
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

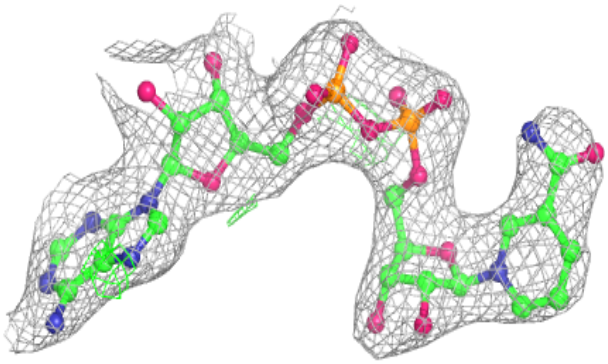


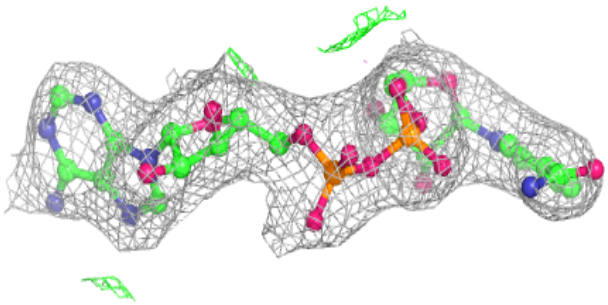


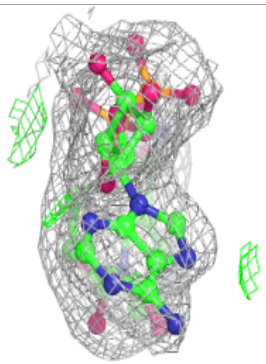


Electron density around NAD A 501:

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

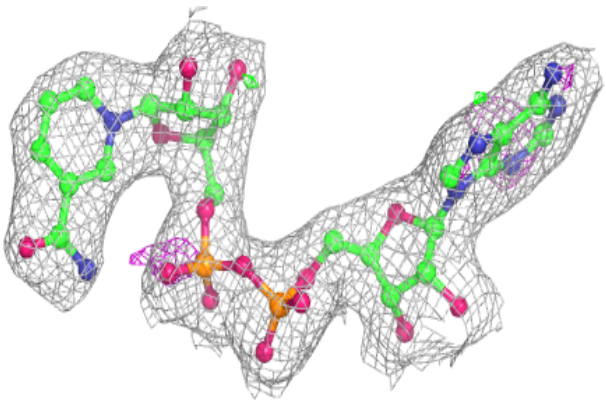


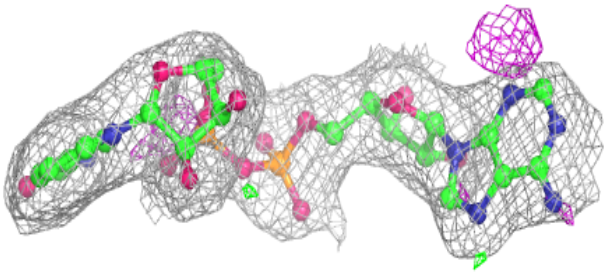


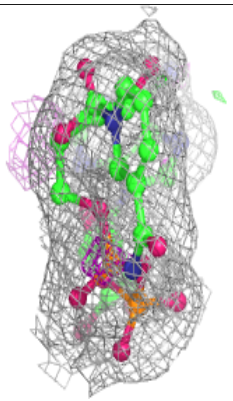


Electron density around NAD C 501:

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

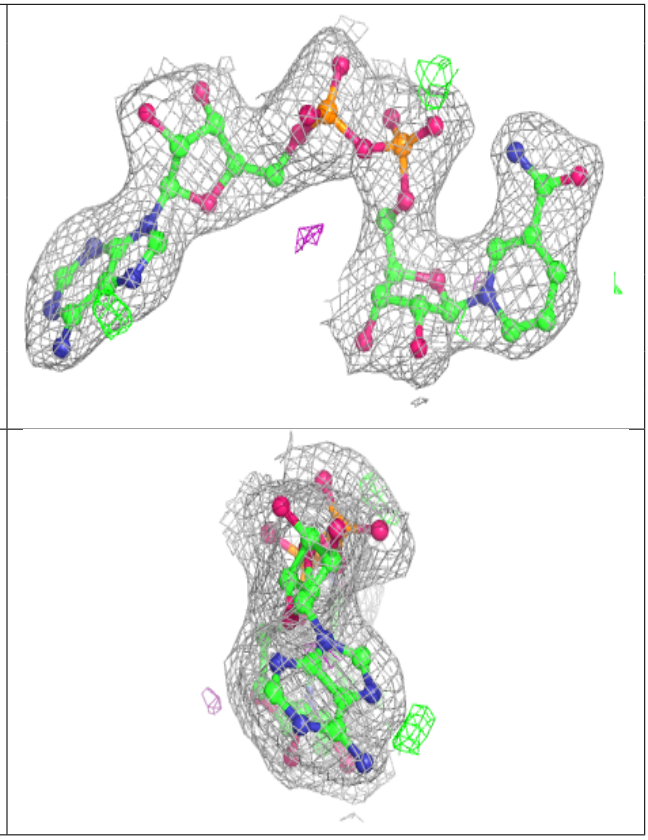






Electron density around NAD B 501:

$2mF_o$-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.