wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2024 – 01:00 pm BST

PDB ID	:	1GT8
Title	:	DIHYDROPYRIMIDINE DEHYDROGENASE (DPD) FROM PIG, TERNARY COMPLEX WITH NADPH AND URACIL-4-ACETIC ACID
Authors	:	Dobritzsch, D.; Ricagno, S.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on	:	2002-01-14
Resolution	:	3.30 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:

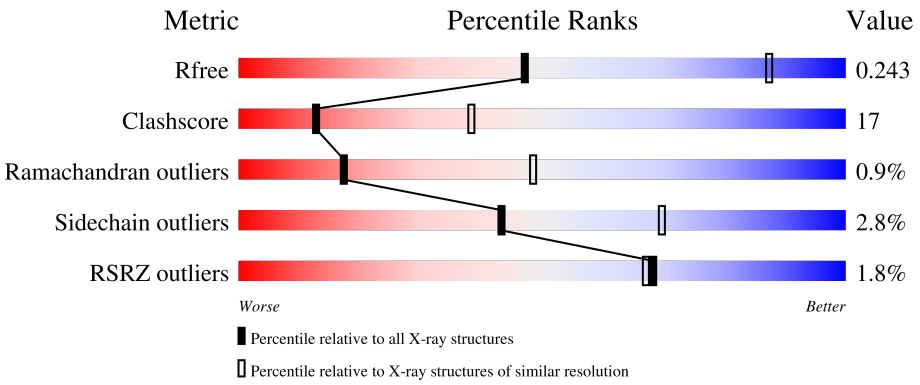
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	1025	% 70% 28% ••
1	B	1025	% 68% 29% ••
1	C	1025	2% 66% 31% ••
1	D	1025	2% 64% 34% ••

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
2	SF4	A	1027	-	-	X	-
2	SF4	A	1028	-	-	X	-
2	SF4	B	1026	-	-	X	-
2	SF4	B	1027	-	-	X	-
2	SF4	B	1028	-	-	X	-
2	SF4	B	1029	-	-	X	-
2	SF4	C	1027	-	-	X	-
2	SF4	C	1028	-	-	X	-
2	SF4	D	1027	-	-	X	-
2	SF4	D	1028	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31588 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.

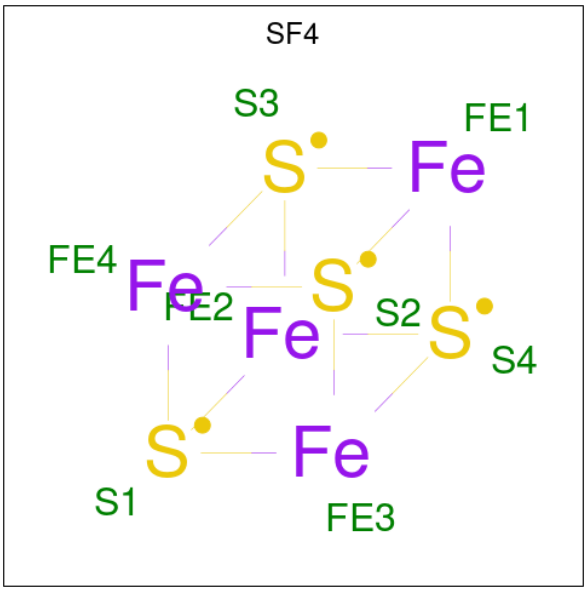
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1017	7755	4919	1312	1468	56	0	0	0
1	B	1010	7703	4885	1304	1458	56	0	0	0
1	C	1010	7708	4892	1303	1459	54	0	0	0
1	D	1012	7718	4894	1307	1461	56	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0
			Total	Fe	S		
2	A	1	8	4	4	0	0
			Total	Fe	S		
2	A	1	8	4	4	0	0
			Total	Fe	S		
2	A	1	8	4	4	0	0
			Total	Fe	S		
2	B	1	8	4	4	0	0
			Total	Fe	S		
2	B	1	8	4	4	0	0
			Total	Fe	S		
2	B	1	8	4	4	0	0
			Total	Fe	S		
2	B	1	8	4	4	0	0
			Total	Fe	S		
2	C	1	8	4	4	0	0
			Total	Fe	S		
2	C	1	8	4	4	0	0
			Total	Fe	S		
2	C	1	8	4	4	0	0
			Total	Fe	S		
2	C	1	8	4	4	0	0
			Total	Fe	S		
2	D	1	8	4	4	0	0
			Total	Fe	S		
2	D	1	8	4	4	0	0

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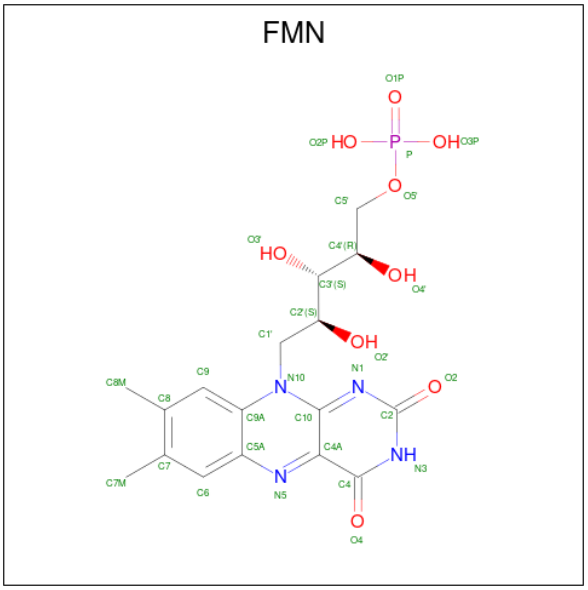
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	D	1	8	4	4	0	0
			Total	Fe	S		
2	D	1	8	4	4	0	0

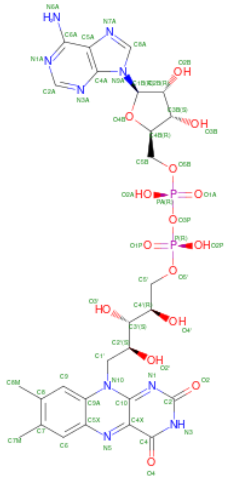
- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
3	B	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
3	C	1	31	17	4	9	1	0	0
			Total	C	N	O	P		
3	D	1	31	17	4	9	1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

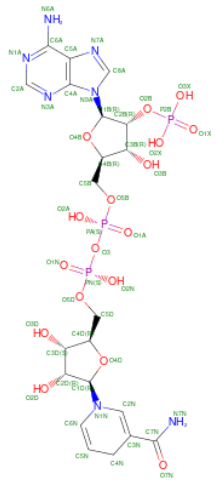
FAD



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

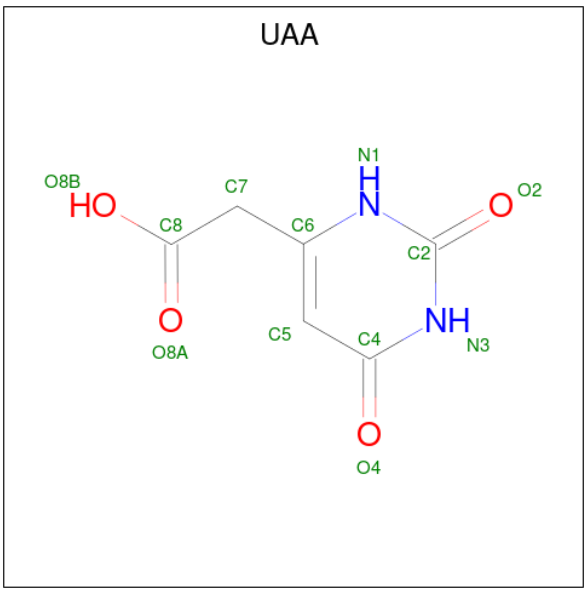
- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

NDP



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

- Molecule 6 is URACIL-6-ACETIC ACID (three-letter code: UAA) (formula: $C_6H_6N_2O_4$).



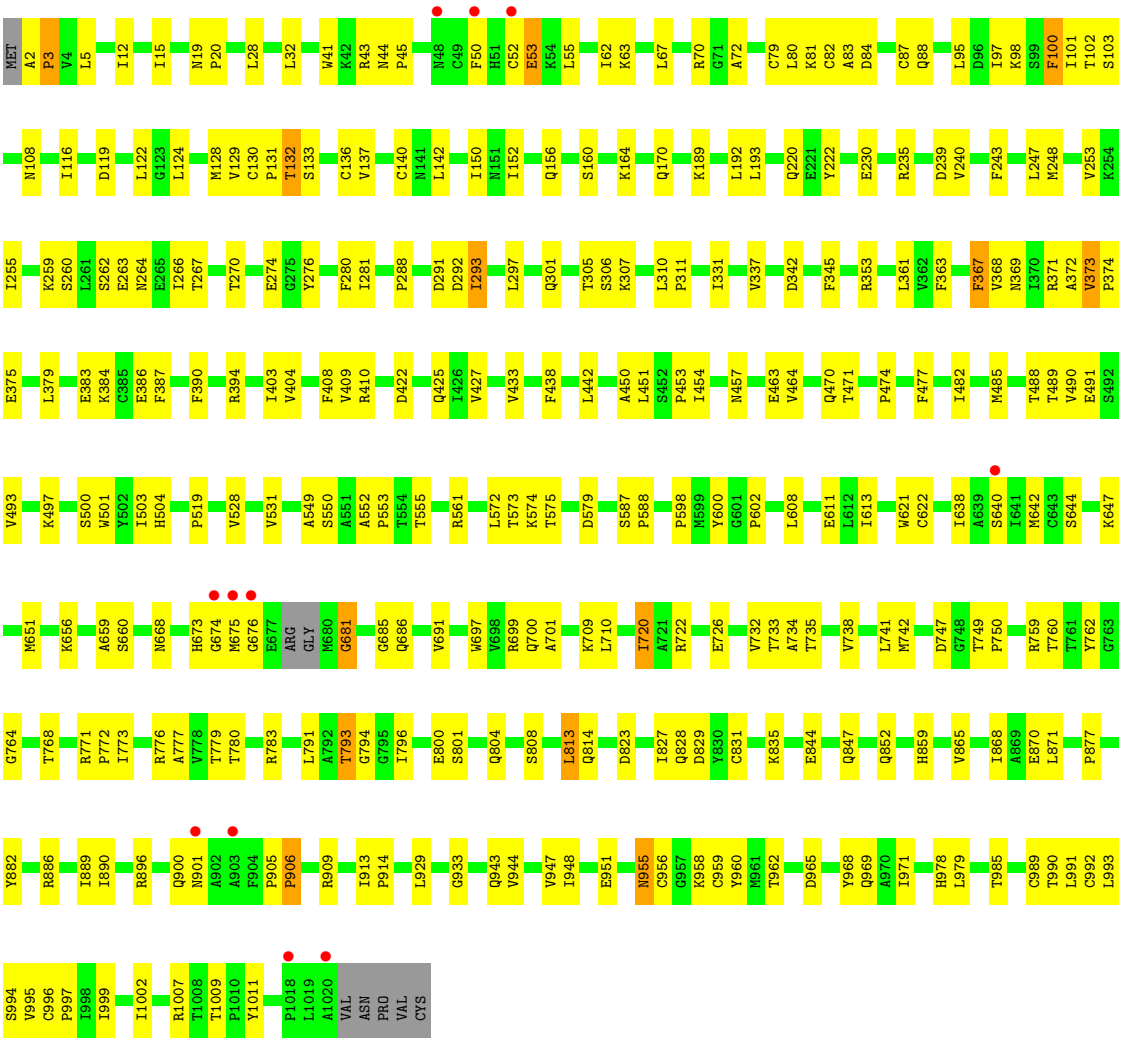
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	12	6	2	4	0	0
6	B	1	12	6	2	4	0	0
6	C	1	12	6	2	4	0	0
6	D	1	12	6	2	4	0	0

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.

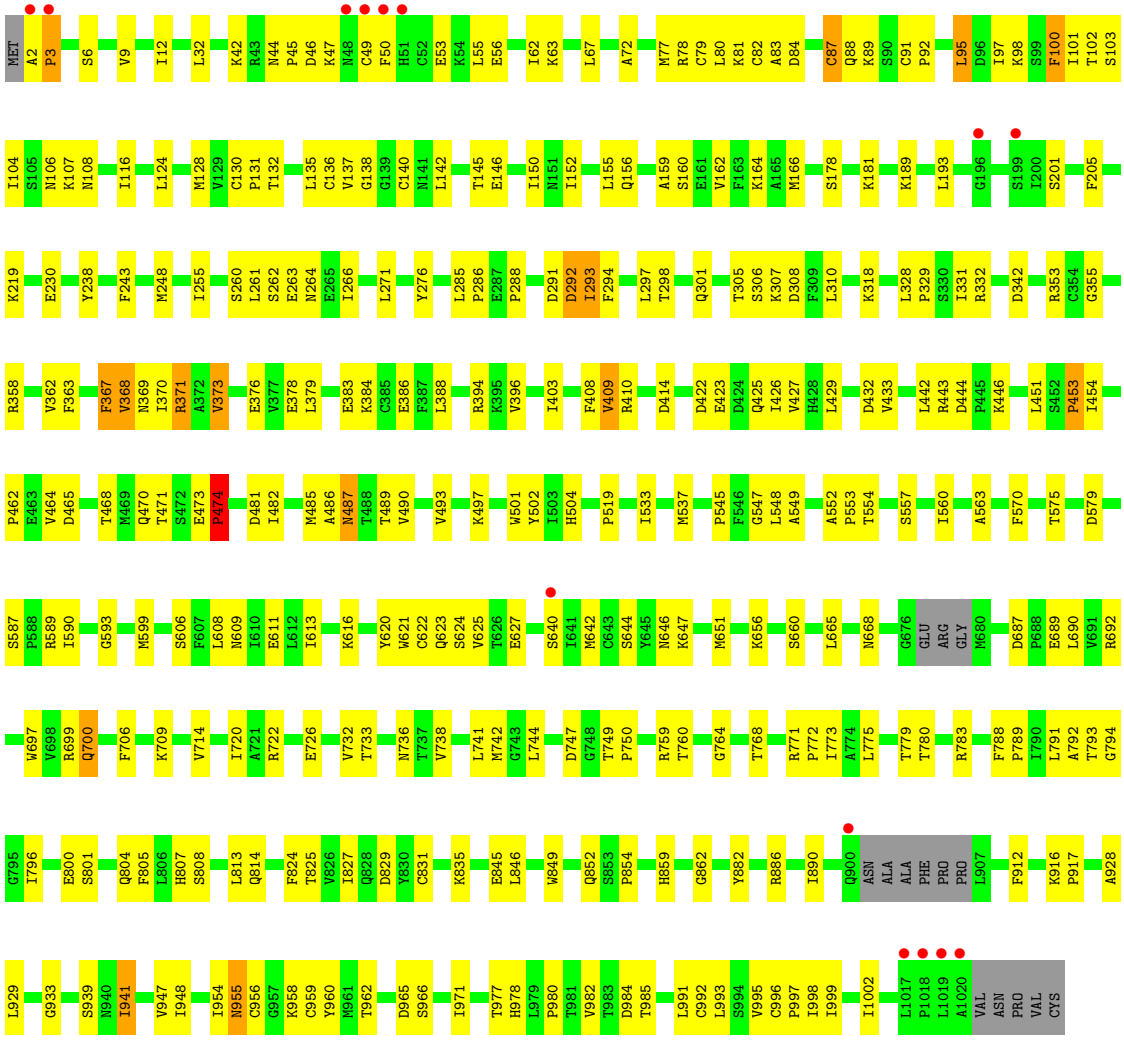
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain A:



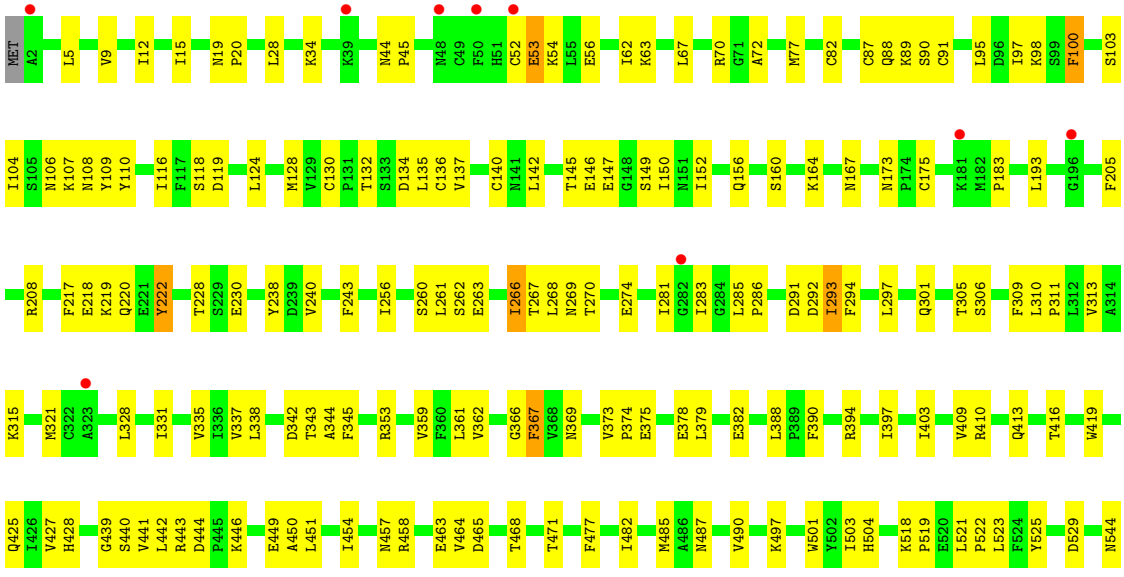
• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

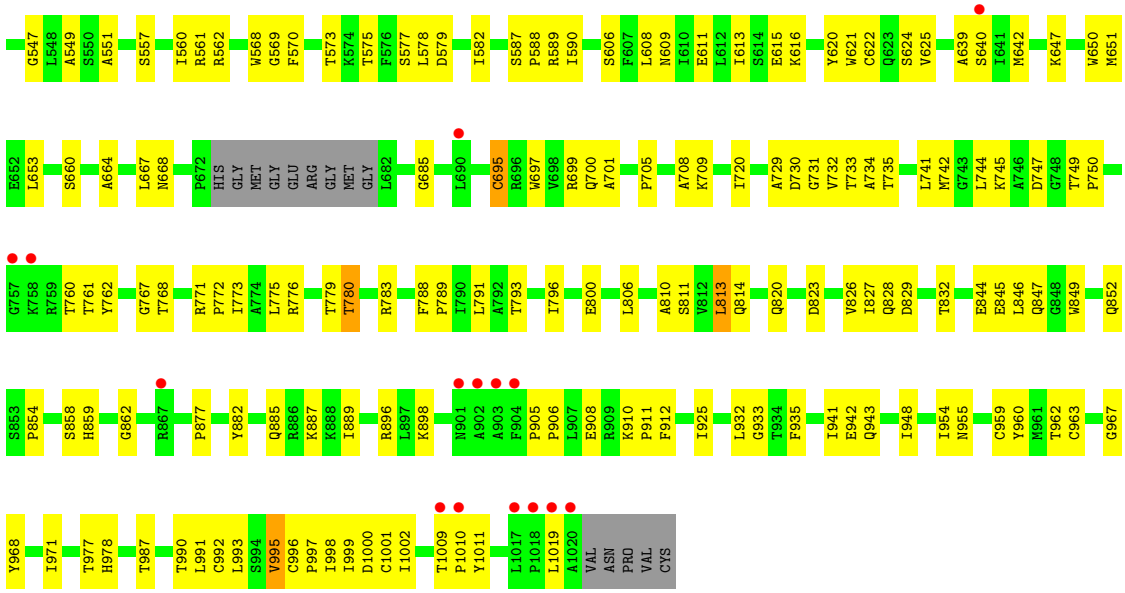
Chain B:



• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

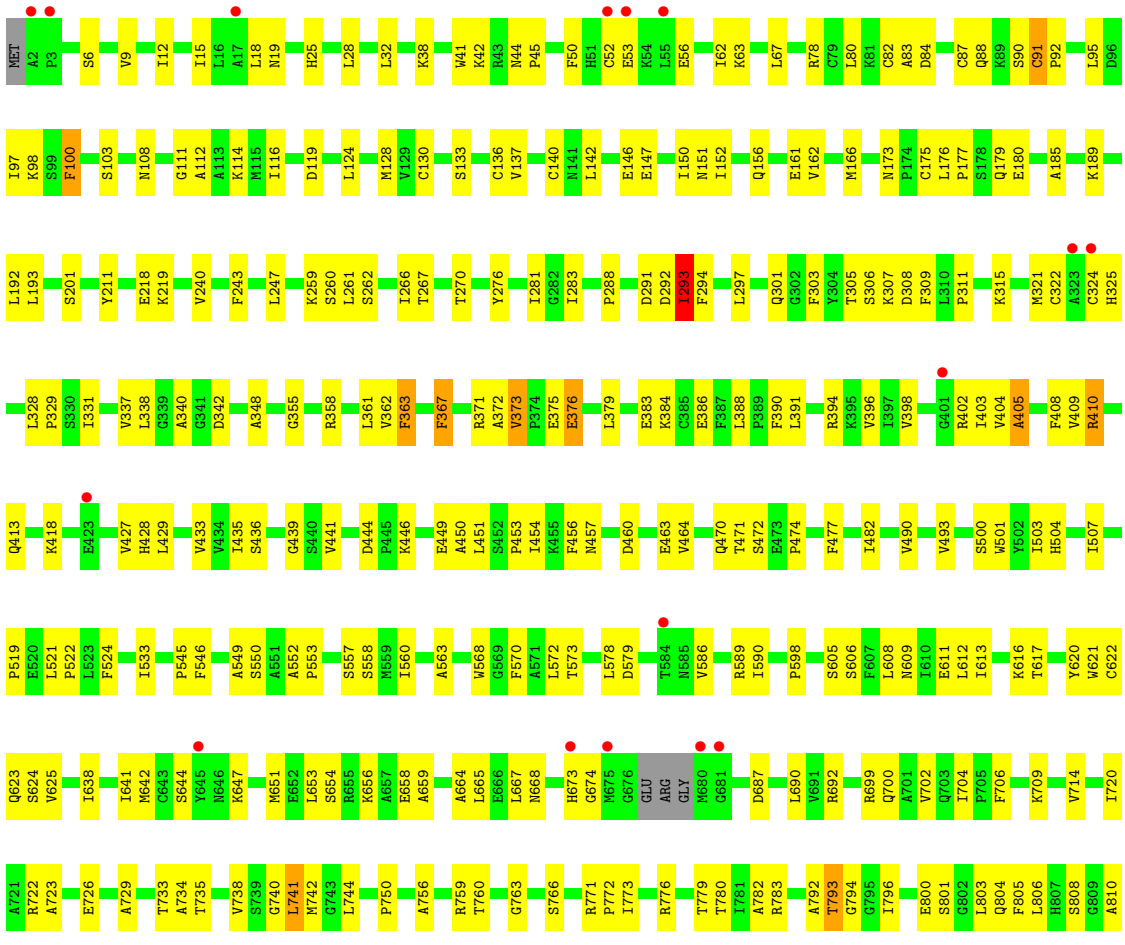
Chain C:

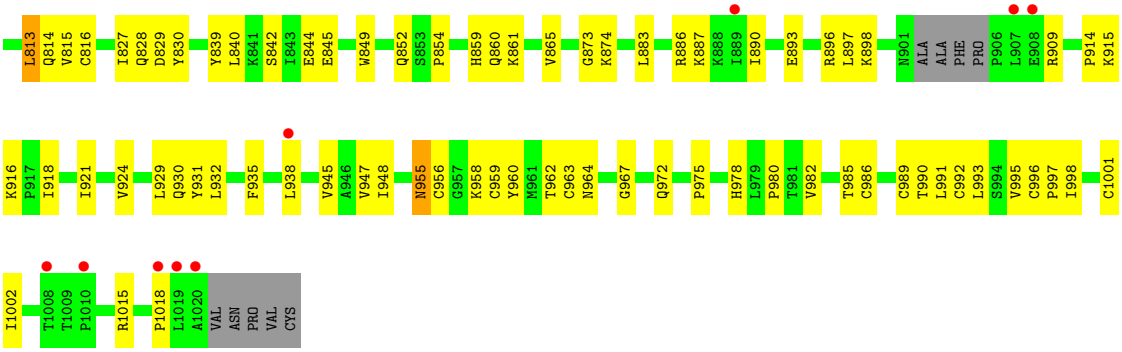




- Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain D:




L813
Q814
V815
C816
I827
Q828
D829
Y830
Y839
L840
K841
S842
I843
E844
E845
W849
Q852
S853
P854
H859
Q860
K861
V865
G873
K874
L883
R886
K887
K888
I889
I890
E893
R896
L897
K898
N901
ALA
ALA
PHE
PRO
P906
L907
E908
R909
P914
K915
K916
P917
I918
I921
V924
L929
Q930
Y931
L932
F935
L938
V945
A946
V947
I948
N955
C956
G957
K958
C959
Y960
M961
T962
C963
N964
G967
Q972
P975
H978
L979
P980
T981
V982
T985
C986
C989
T990
L991
C992
L993
S994
W995
C996
P997
I998
C1001
I1002
T1008
T1009
P1010
R1015
P1018
L1019
A1020
VAL
ASN
PRO
VAL
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.03Å 159.53Å 166.02Å 90.00° 97.16° 90.00°	Depositor
Resolution (Å)	29.75 – 3.30 29.75 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.75-3.30) 98.5 (29.75-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.269 0.195 , 0.243	Depositor DCC
R_{free} test set	1247 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	71.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31588	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: UAA, FAD, FMN, SF4, NDP

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	0.45	0/7916	0.65	0/10729
1	B	0.45	1/7860 (0.0%)	0.65	0/10649
1	C	0.44	0/7868	0.64	0/10667
1	D	0.43	0/7876	0.64	0/10671
All	All	0.44	1/31520 (0.0%)	0.65	0/42716

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	CYS	CB-SG	-5.12	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7755	0	7781	262	0
1	B	7703	0	7735	274	0
1	C	7708	0	7743	307	0
1	D	7718	0	7750	313	0
2	A	32	0	0	6	0
2	B	32	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	32	0	0	6	0
2	D	32	0	0	8	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	C	31	0	19	0	0
3	D	31	0	19	1	0
4	A	53	0	31	0	0
4	B	53	0	31	0	0
4	C	53	0	31	2	0
4	D	53	0	31	3	0
5	A	48	0	26	6	0
5	B	48	0	26	5	0
5	C	48	0	26	6	0
5	D	48	0	26	6	0
6	A	12	0	5	1	0
6	B	12	0	5	1	0
6	C	12	0	5	1	0
6	D	12	0	5	0	0
All	All	31588	0	31333	1044	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 17.

The worst 5 of 1044 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:136:CYS:SG	1:C:137:VAL:HG23	2.02	1.00
1:C:116:ILE:HD13	1:C:156:GLN:HG3	1.43	0.99
1:C:410:ARG:NH1	1:D:427:VAL:HG13	1.84	0.92
1:C:776:ARG:O	1:C:780:THR:HG22	1.71	0.90
1:C:173:ASN:HD21	1:C:175:CYS:HB2	1.36	0.90

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	1013/1025 (99%)	927 (92%)	72 (7%)	14 (1%)	11	38
1	B	1004/1025 (98%)	920 (92%)	77 (8%)	7 (1%)	22	54
1	C	1006/1025 (98%)	926 (92%)	74 (7%)	6 (1%)	25	57
1	D	1006/1025 (98%)	924 (92%)	73 (7%)	9 (1%)	17	48
All	All	4029/4100 (98%)	3697 (92%)	296 (7%)	36 (1%)	17	48

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	GLY
1	A	676	GLY
1	A	906	PRO
1	C	613	ILE
1	A	3	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	847/854 (99%)	829 (98%)	18 (2%)	53	75
1	B	842/854 (99%)	815 (97%)	27 (3%)	39	67
1	C	843/854 (99%)	824 (98%)	19 (2%)	50	73
1	D	844/854 (99%)	813 (96%)	31 (4%)	34	63
All	All	3376/3416 (99%)	3281 (97%)	95 (3%)	43	70

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	780	THR
1	D	322	CYS
1	C	800	GLU

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Mol	Chain	Res	Type
1	D	53	GLU
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	807	HIS
1	D	693	ASN
1	C	170	GLN
1	D	943	GLN
1	D	220	GLN

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)

32 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	SF4	D	1027	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMN	A	1030	-	33,33,33	1.84	9 (27%)	48,50,50	1.91	13 (27%)
6	UAA	D	1035	-	12,12,12	1.13	2 (16%)	12,16,16	1.56	3 (25%)
2	SF4	A	1027	-	0,12,12	-	-	-		
5	NDP	A	1032	-	45,52,52	1.67	8 (17%)	53,80,80	1.74	9 (16%)
2	SF4	C	1027	1	0,12,12	-	-	-		
4	FAD	C	1031	-	53,58,58	1.93	21 (39%)	68,89,89	1.21	8 (11%)
2	SF4	D	1028	1	0,12,12	-	-	-		
2	SF4	B	1027	1	0,12,12	-	-	-		
2	SF4	B	1026	1	0,12,12	-	-	-		
3	FMN	C	1030	-	33,33,33	1.98	7 (21%)	48,50,50	1.92	13 (27%)
3	FMN	D	1030	-	33,33,33	1.86	8 (24%)	48,50,50	1.95	14 (29%)
2	SF4	B	1029	1	0,12,12	-	-	-		
4	FAD	B	1031	-	53,58,58	1.88	17 (32%)	68,89,89	1.23	7 (10%)
2	SF4	C	1029	1	0,12,12	-	-	-		
6	UAA	C	1035	-	12,12,12	0.87	0	12,16,16	1.71	4 (33%)
6	UAA	B	1035	-	12,12,12	0.88	0	12,16,16	1.66	5 (41%)
2	SF4	B	1028	1	0,12,12	-	-	-		
5	NDP	B	1032	-	45,52,52	1.71	6 (13%)	53,80,80	1.60	7 (13%)
2	SF4	C	1028	1	0,12,12	-	-	-		
5	NDP	C	1032	-	45,52,52	1.65	7 (15%)	53,80,80	1.59	7 (13%)
5	NDP	D	1032	-	45,52,52	1.72	9 (20%)	53,80,80	1.59	12 (22%)
3	FMN	B	1030	-	33,33,33	1.91	7 (21%)	48,50,50	1.98	14 (29%)
2	SF4	C	1026	1	0,12,12	-	-	-		
4	FAD	A	1031	-	53,58,58	1.85	18 (33%)	68,89,89	1.20	7 (10%)
2	SF4	D	1029	1	0,12,12	-	-	-		
2	SF4	A	1028	1	0,12,12	-	-	-		
2	SF4	A	1029	1	0,12,12	-	-	-		
4	FAD	D	1031	-	53,58,58	1.92	19 (35%)	68,89,89	1.27	8 (11%)
6	UAA	A	1035	-	12,12,12	0.98	0	12,16,16	1.55	2 (16%)
2	SF4	A	1026	-	0,12,12	-	-	-		
2	SF4	D	1026	1	0,12,12	-	-	-		

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	SF4	D	1027	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
6	UAA	D	1035	-	-	0/4/4/4	0/1/1/1
2	SF4	A	1027	-	-	-	0/6/5/5
5	NDP	A	1032	-	-	5/30/77/77	0/5/5/5
2	SF4	C	1027	1	-	-	0/6/5/5
4	FAD	C	1031	-	-	3/30/50/50	0/6/6/6
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	B	1027	1	-	-	0/6/5/5
2	SF4	B	1026	1	-	-	0/6/5/5
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
4	FAD	B	1031	-	-	6/30/50/50	0/6/6/6
2	SF4	B	1029	1	-	-	0/6/5/5
2	SF4	C	1029	1	-	-	0/6/5/5
6	UAA	C	1035	-	-	0/4/4/4	0/1/1/1
6	UAA	B	1035	-	-	0/4/4/4	0/1/1/1
2	SF4	B	1028	1	-	-	0/6/5/5
5	NDP	B	1032	-	-	5/30/77/77	0/5/5/5
2	SF4	C	1028	1	-	-	0/6/5/5
5	NDP	C	1032	-	-	6/30/77/77	0/5/5/5
5	NDP	D	1032	-	-	5/30/77/77	0/5/5/5
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	C	1026	1	-	-	0/6/5/5
4	FAD	A	1031	-	-	4/30/50/50	0/6/6/6
2	SF4	D	1029	1	-	-	0/6/5/5
2	SF4	A	1028	1	-	-	0/6/5/5
2	SF4	A	1029	1	-	-	0/6/5/5
4	FAD	D	1031	-	-	3/30/50/50	0/6/6/6
6	UAA	A	1035	-	-	0/4/4/4	0/1/1/1
2	SF4	A	1026	-	-	-	0/6/5/5
2	SF4	D	1026	1	-	-	0/6/5/5

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1030	FMN	C4A-N5	5.46	1.41	1.30
5	A	1032	NDP	C4N-C3N	-5.24	1.39	1.49
4	C	1031	FAD	O4B-C1B	5.13	1.48	1.41
5	B	1032	NDP	C4N-C3N	-5.11	1.39	1.49
3	B	1030	FMN	C4A-N5	4.88	1.40	1.30

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1032	NDP	PN-O3-PA	5.80	152.72	132.83
5	B	1032	NDP	PN-O3-PA	5.73	152.49	132.83
5	A	1032	NDP	PN-O3-PA	5.24	150.81	132.83
3	B	1030	FMN	C10-N1-C2	5.11	127.11	116.90
3	A	1030	FMN	C10-N1-C2	4.94	126.78	116.90

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1031	FAD	O4B-C4B-C5B-O5B
5	A	1032	NDP	O4D-C1D-N1N-C2N
5	B	1032	NDP	O4D-C1D-N1N-C2N
5	C	1032	NDP	O4D-C1D-N1N-C2N
5	D	1032	NDP	C3B-C2B-O2B-P2B

There are no ring outliers.

26 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1027	SF4	2	0
2	A	1027	SF4	2	0
5	A	1032	NDP	6	0
2	C	1027	SF4	2	0
4	C	1031	FAD	2	0
2	D	1028	SF4	4	0
2	B	1027	SF4	2	0
2	B	1026	SF4	2	0
3	D	1030	FMN	1	0
2	B	1029	SF4	2	0
2	C	1029	SF4	1	0
6	C	1035	UAA	1	0
6	B	1035	UAA	1	0
2	B	1028	SF4	2	0
5	B	1032	NDP	5	0
2	C	1028	SF4	2	0
5	C	1032	NDP	6	0
5	D	1032	NDP	6	0
2	C	1026	SF4	1	0
2	D	1029	SF4	1	0
2	A	1028	SF4	2	0

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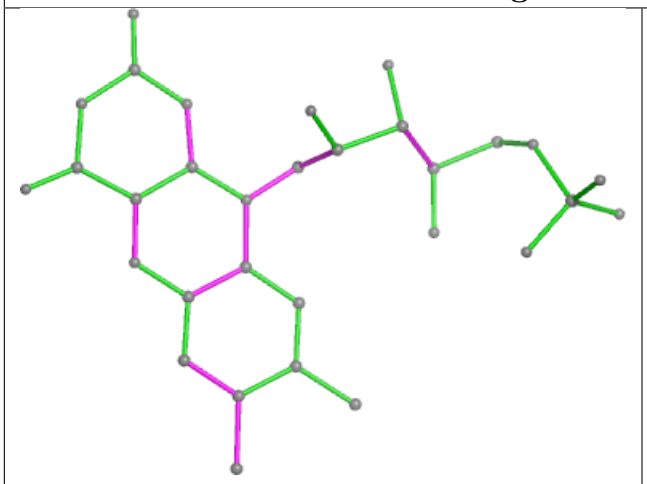
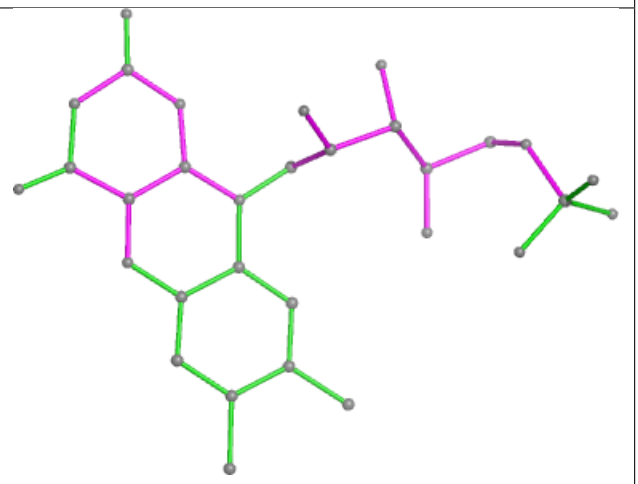
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1029	SF4	1	0
4	D	1031	FAD	3	0
6	A	1035	UAA	1	0
2	A	1026	SF4	1	0
2	D	1026	SF4	1	0

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.

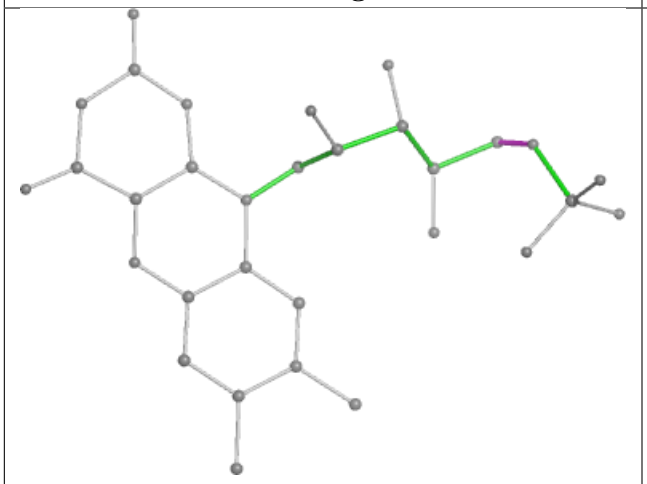
Ligand FMN A 1030



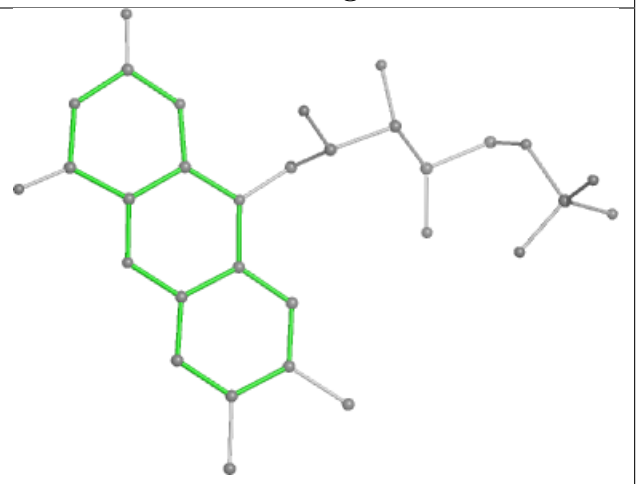
Bond lengths



Bond angles

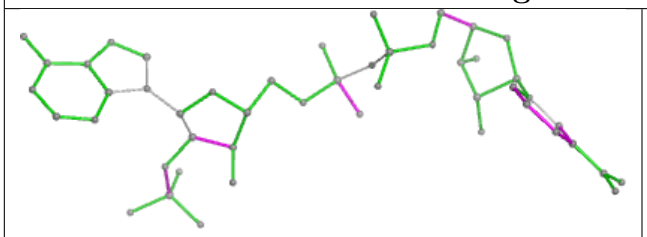


Torsions



Rings

Ligand NDP A 1032



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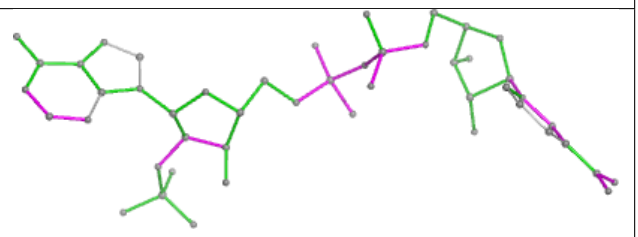

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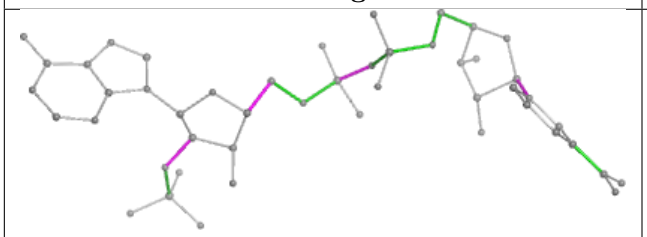
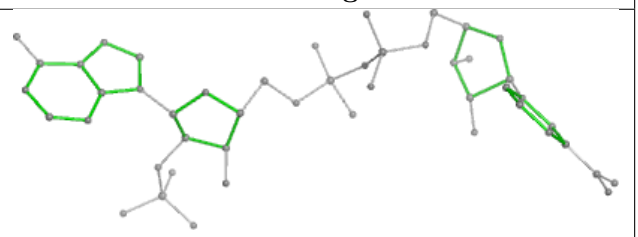
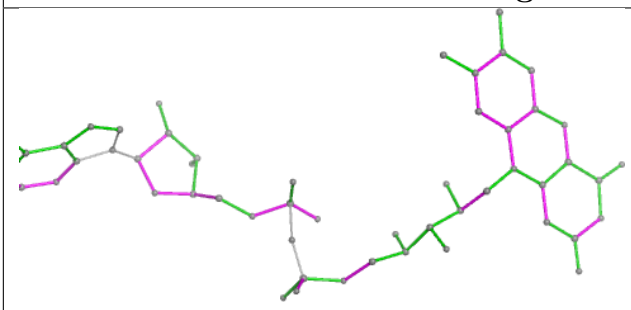
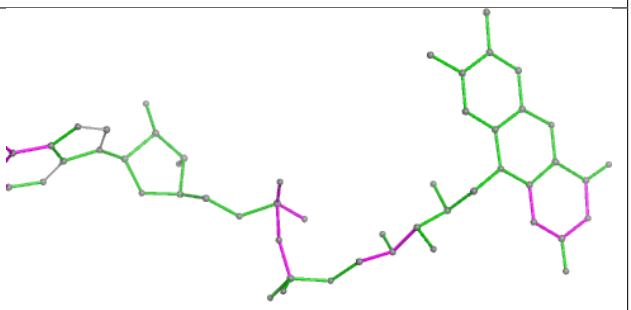
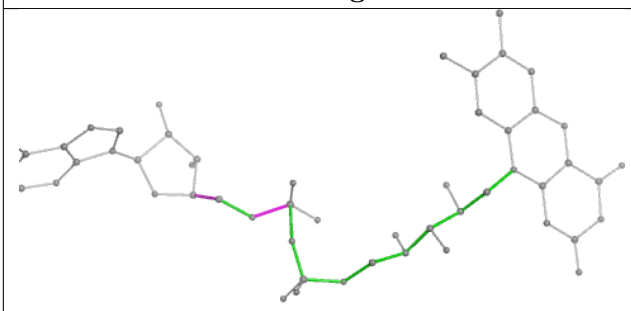
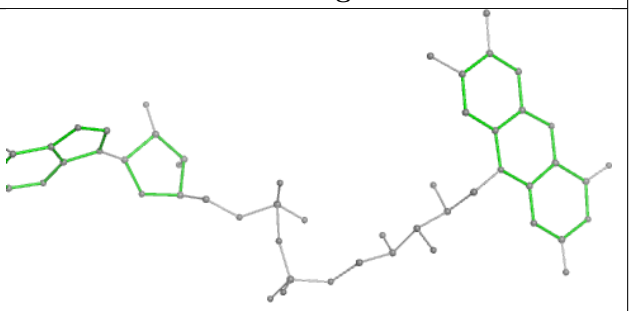


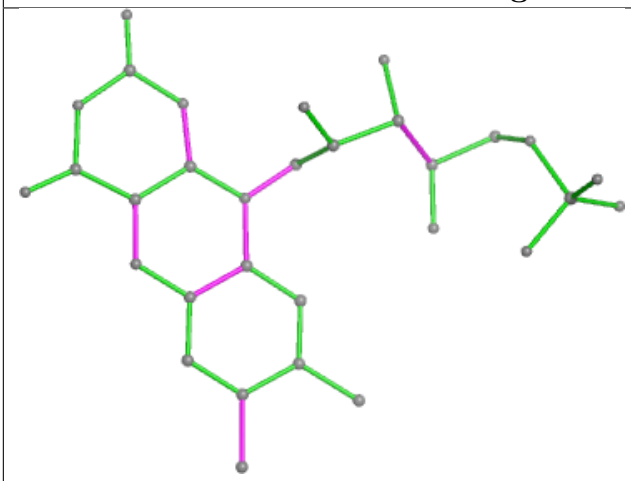
Torsions



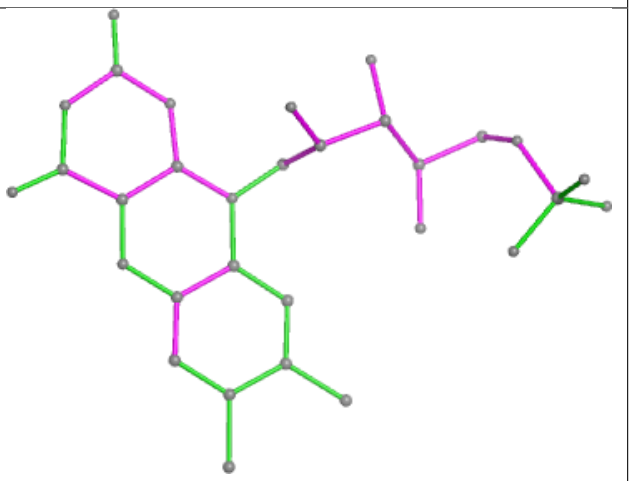
Rings

Ligand FAD C 1031	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FMN C 1030



Bond lengths



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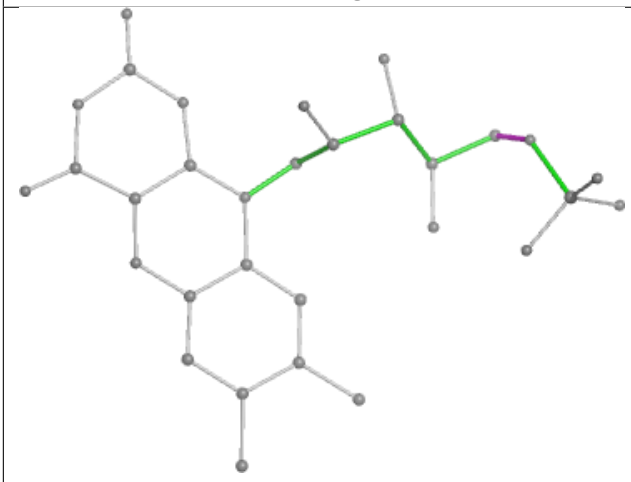
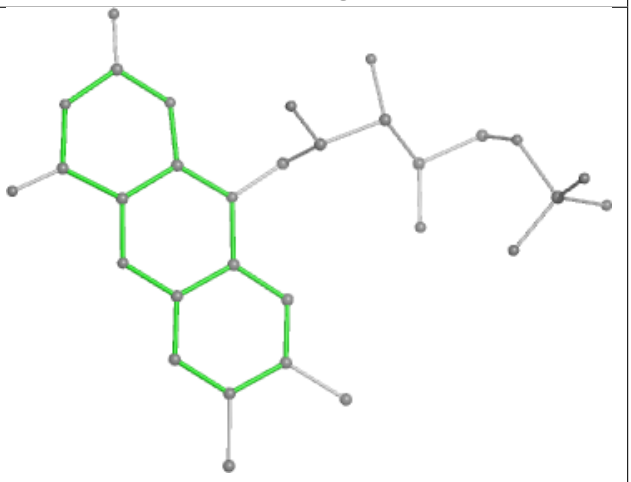
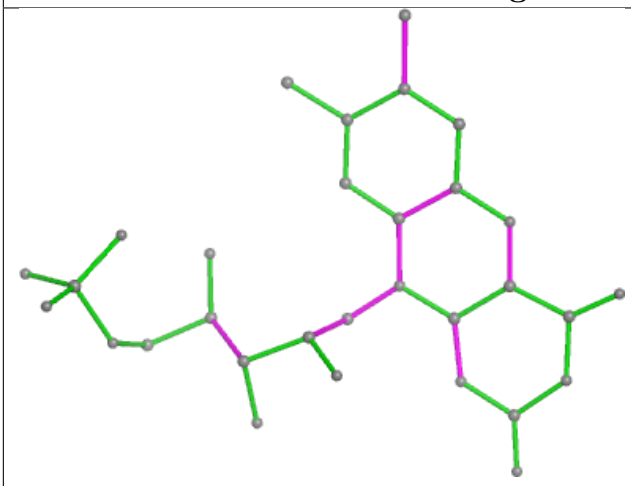


Torsions



Rings

Ligand FMN D 1030



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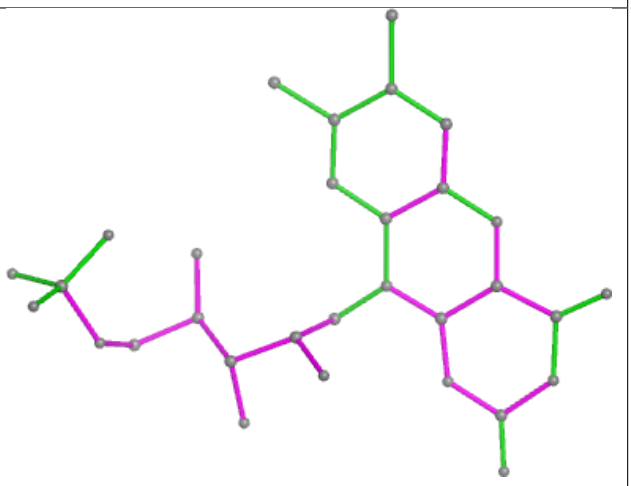

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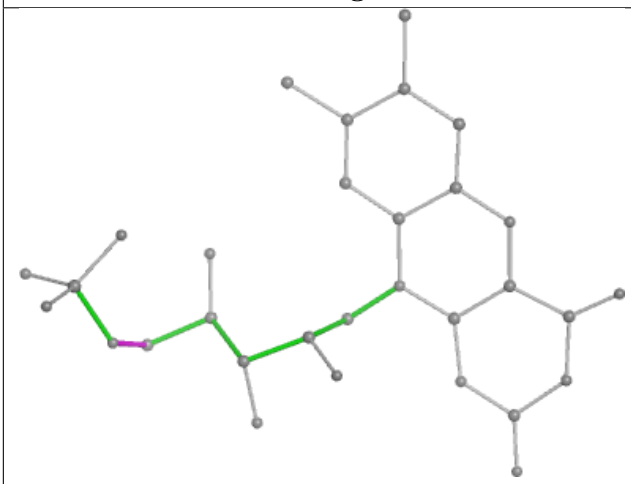

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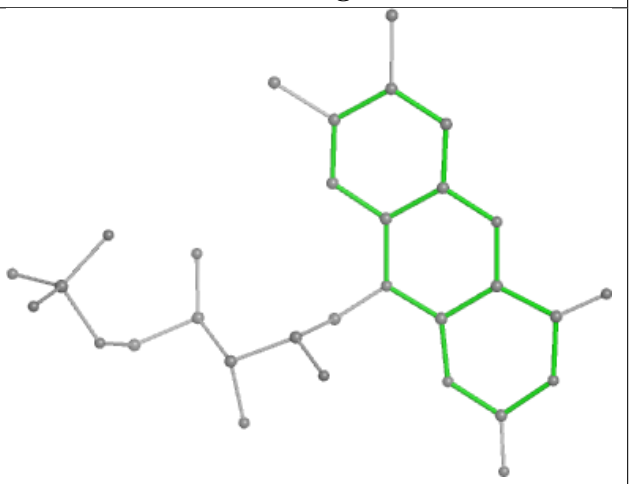
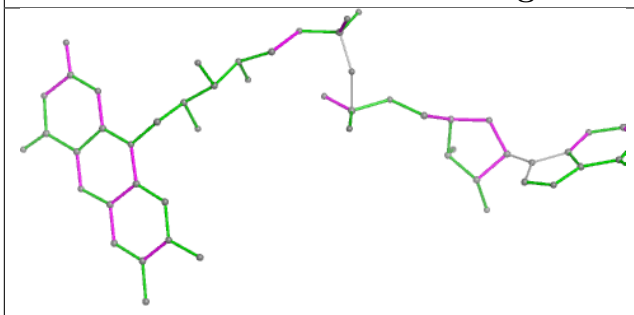


Rings

Ligand FAD B 1031



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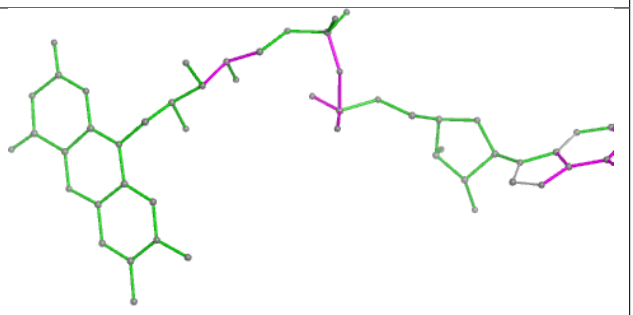

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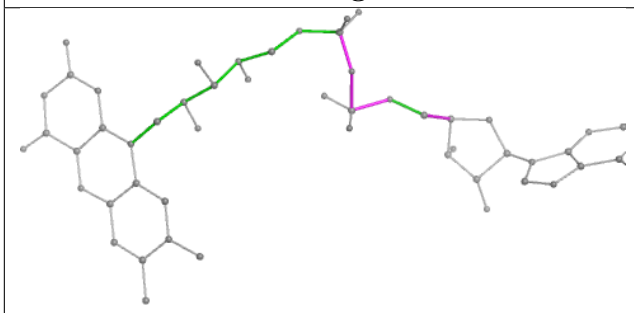

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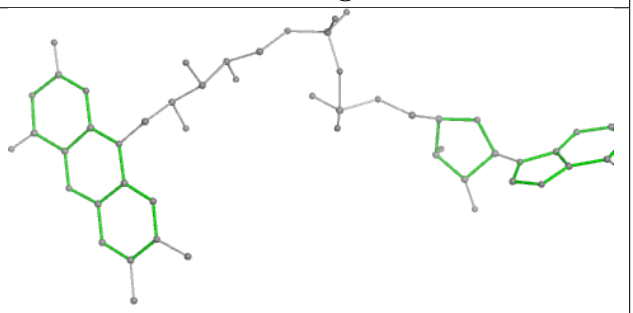
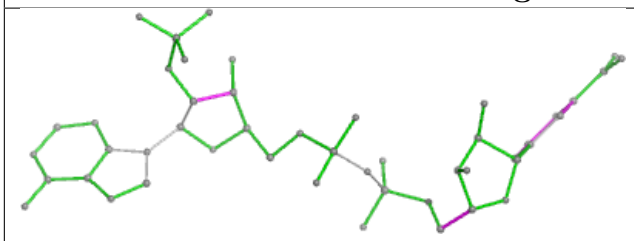


Rings

Ligand NDP B 1032



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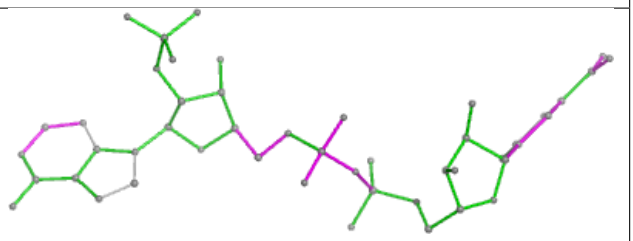

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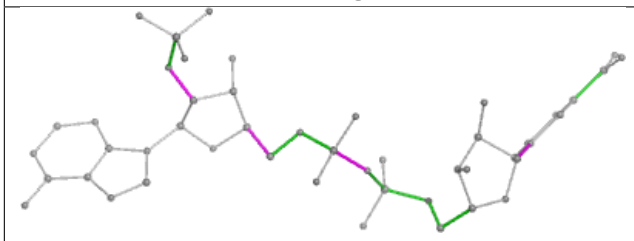

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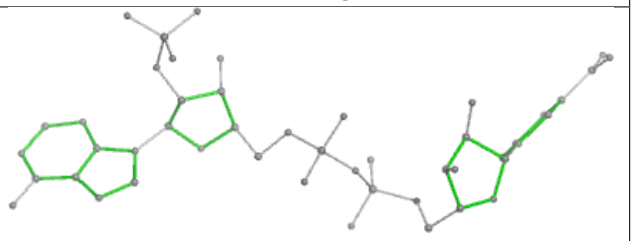
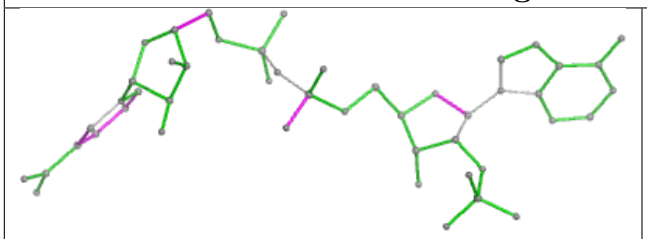


Rings

Ligand NDP C 1032



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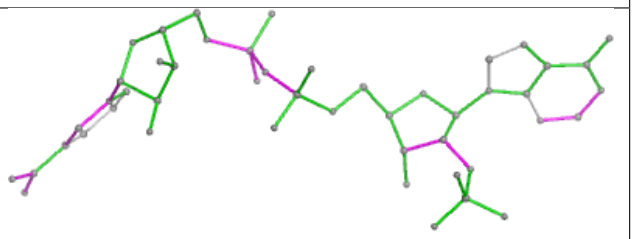
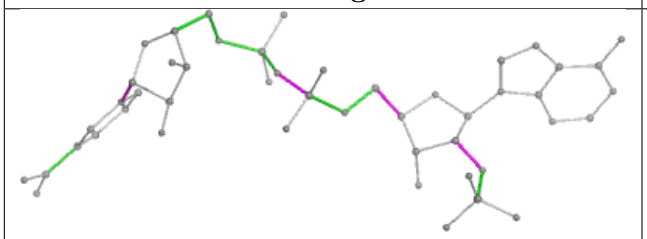
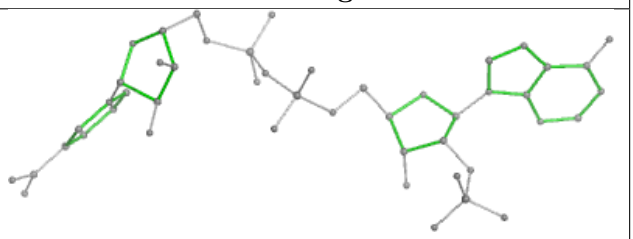


Bond angles

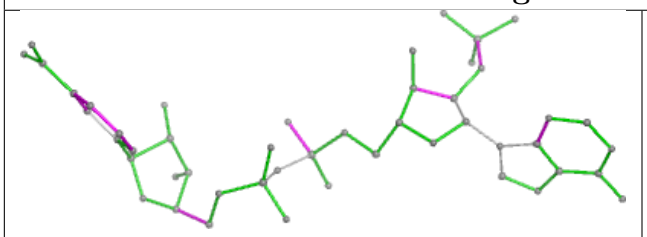


Torsions

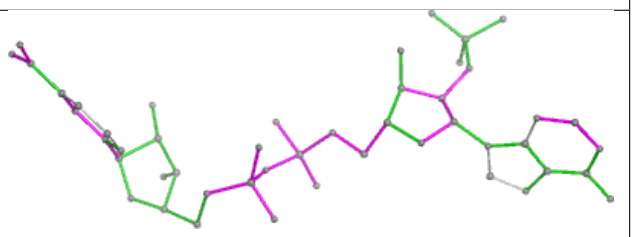


Rings

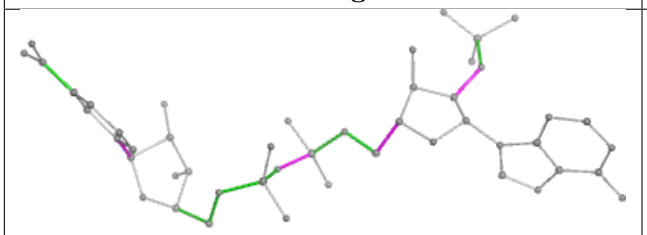
Ligand NDP D 1032



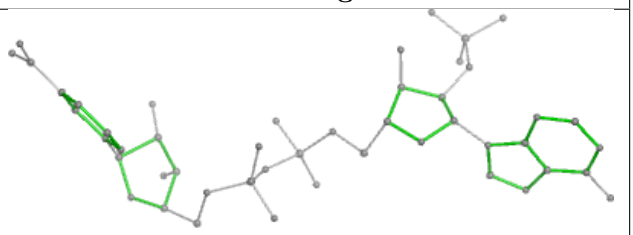
Bond lengths



Bond angles

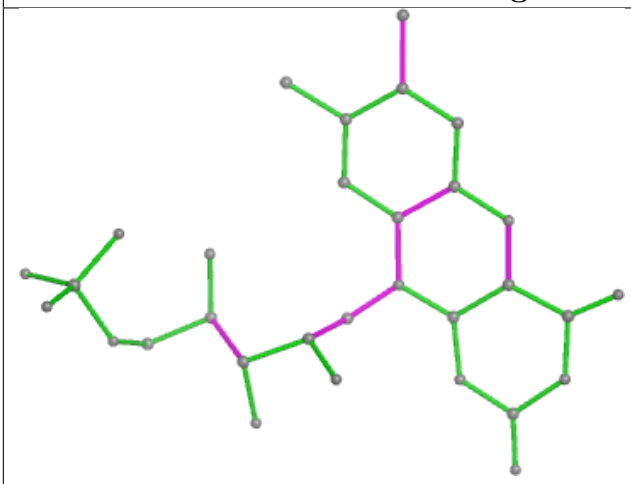


Torsions

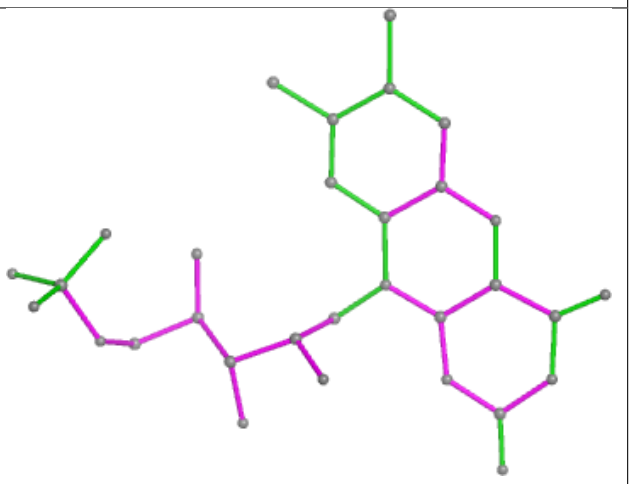


Rings

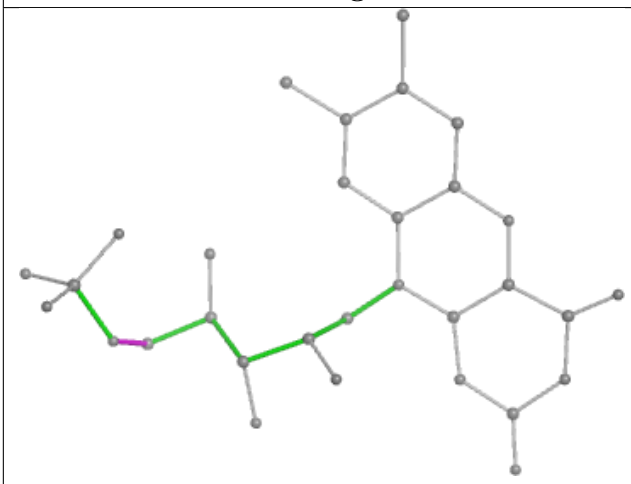
Ligand FMN B 1030



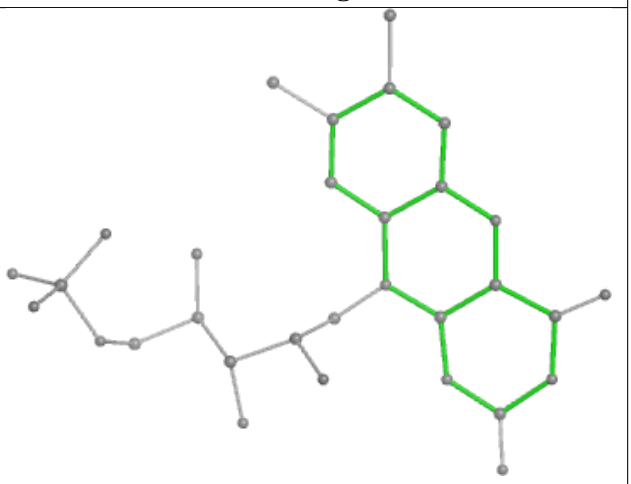
Bond lengths



Bond angles

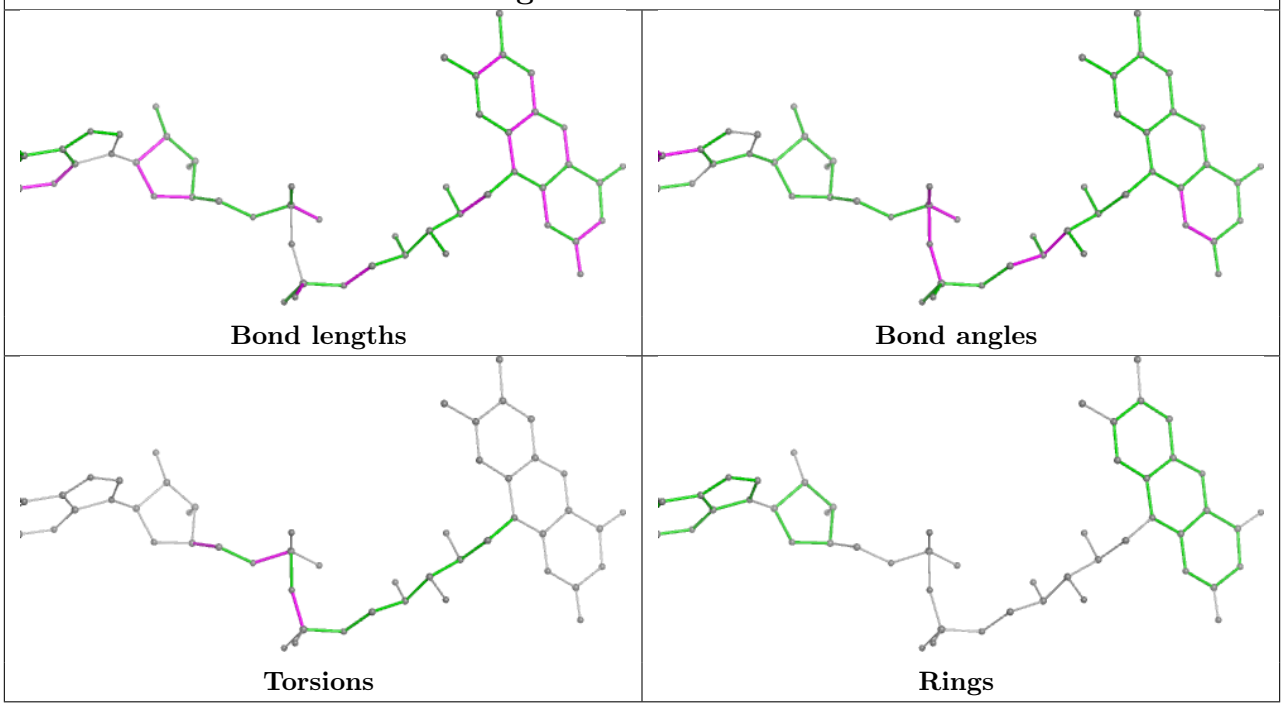


Torsions

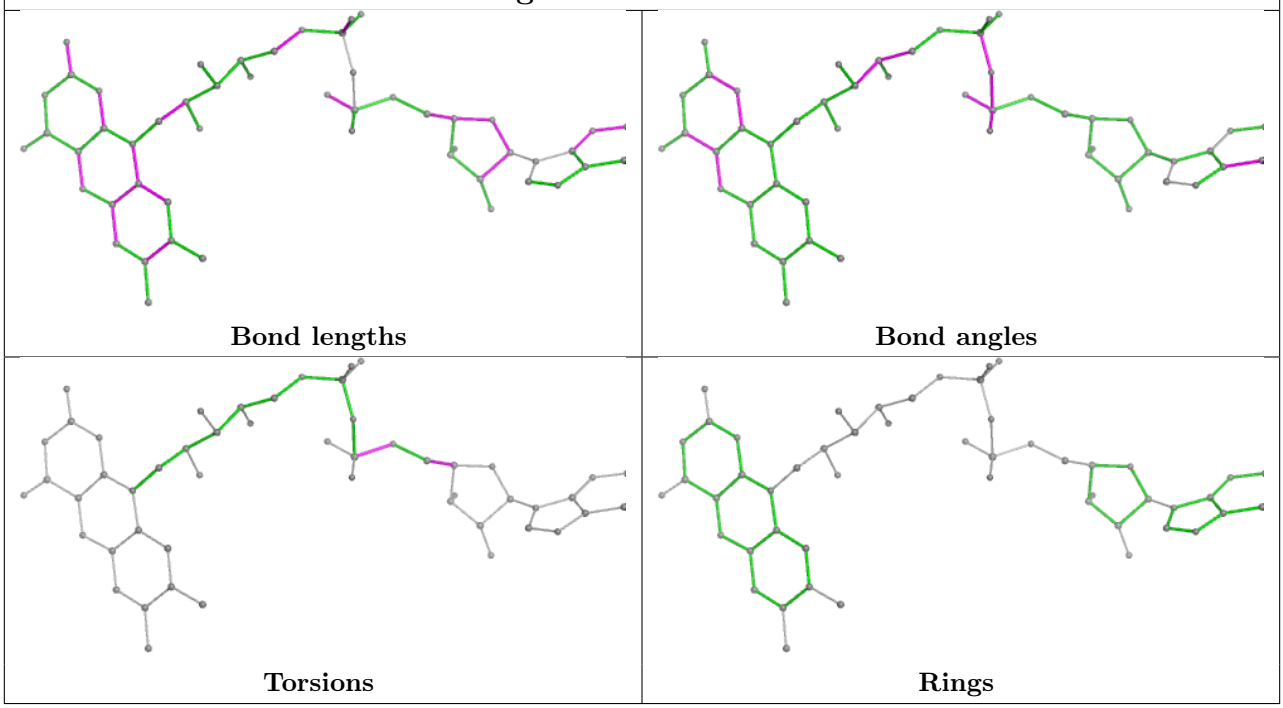


Rings

Ligand FAD A 1031



Ligand FAD D 1031



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	1017/1025 (99%)	-0.42	11 (1%)	80	81	7, 39, 93, 147	0
1	B	1010/1025 (98%)	-0.37	14 (1%)	75	75	7, 40, 96, 141	0
1	C	1010/1025 (98%)	-0.19	24 (2%)	59	56	14, 54, 106, 140	0
1	D	1012/1025 (98%)	-0.12	25 (2%)	57	54	14, 57, 107, 162	0
All	All	4049/4100 (98%)	-0.28	74 (1%)	68	67	7, 47, 102, 162	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1019	LEU	7.4
1	D	2	ALA	7.1
1	C	1020	ALA	5.9
1	C	1018	PRO	5.8
1	B	2	ALA	5.6

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)

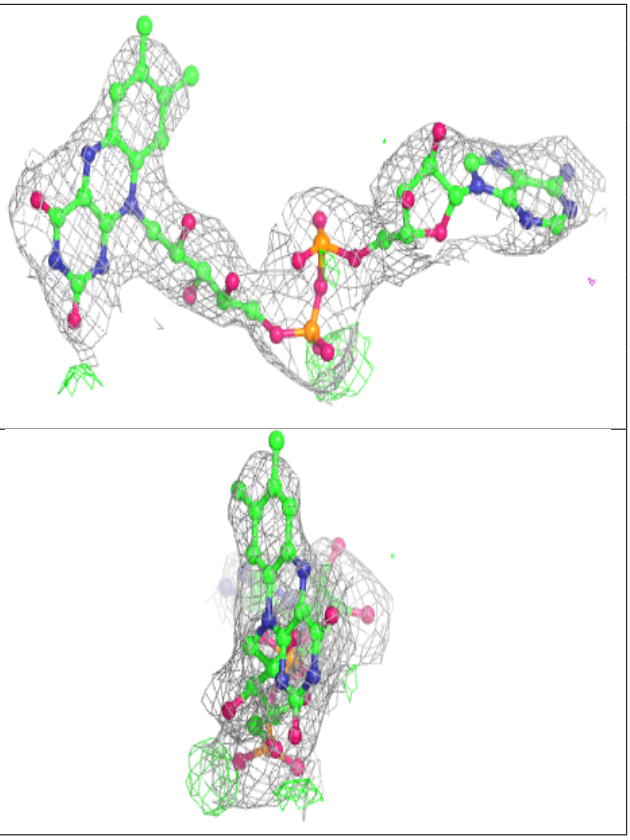
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

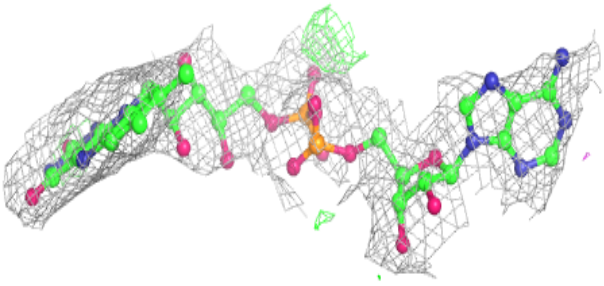
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	UAA	C	1035	12/12	0.78	0.38	138,140,144,144	0
6	UAA	D	1035	12/12	0.82	0.36	107,108,108,109	0
6	UAA	A	1035	12/12	0.86	0.26	111,112,113,113	0
6	UAA	B	1035	12/12	0.88	0.27	146,147,148,148	0
4	FAD	D	1031	53/53	0.91	0.24	40,46,60,60	0
5	NDP	C	1032	48/48	0.93	0.18	53,57,86,88	0
3	FMN	C	1030	31/31	0.94	0.21	45,48,52,55	0
5	NDP	D	1032	48/48	0.94	0.19	57,60,89,92	0
4	FAD	A	1031	53/53	0.94	0.20	20,23,37,38	0
4	FAD	B	1031	53/53	0.94	0.20	19,25,35,37	0
4	FAD	C	1031	53/53	0.94	0.19	29,36,49,50	0
3	FMN	A	1030	31/31	0.94	0.20	31,37,42,45	0
5	NDP	A	1032	48/48	0.95	0.15	42,47,76,78	0
5	NDP	B	1032	48/48	0.95	0.15	42,46,77,81	0
3	FMN	B	1030	31/31	0.95	0.22	28,33,34,38	0
3	FMN	D	1030	31/31	0.95	0.20	48,52,56,59	0
2	SF4	A	1026	8/8	0.99	0.13	18,21,24,24	0
2	SF4	A	1027	8/8	0.99	0.10	6,10,11,12	0
2	SF4	A	1028	8/8	0.99	0.12	9,11,13,14	0
2	SF4	A	1029	8/8	0.99	0.15	18,21,23,24	0
2	SF4	B	1026	8/8	0.99	0.14	7,10,10,12	0
2	SF4	B	1027	8/8	0.99	0.12	4,4,4,4	0
2	SF4	B	1028	8/8	0.99	0.13	21,23,24,25	0
2	SF4	B	1029	8/8	0.99	0.09	13,15,16,18	0
2	SF4	C	1026	8/8	0.99	0.10	22,24,26,27	0
2	SF4	C	1027	8/8	0.99	0.09	25,26,27,28	0
2	SF4	C	1028	8/8	0.99	0.08	29,31,33,33	0
2	SF4	C	1029	8/8	0.99	0.07	34,35,37,37	0
2	SF4	D	1026	8/8	0.99	0.13	26,27,28,28	0
2	SF4	D	1027	8/8	0.99	0.09	28,30,32,32	0
2	SF4	D	1028	8/8	0.99	0.10	34,35,37,38	0
2	SF4	D	1029	8/8	0.99	0.08	39,40,41,42	0

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

Electron density around FAD D 1031:

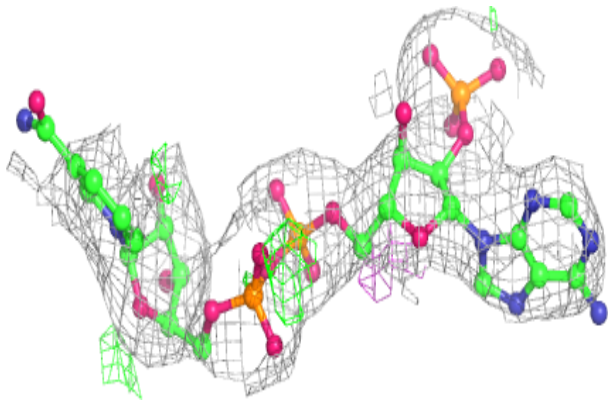
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

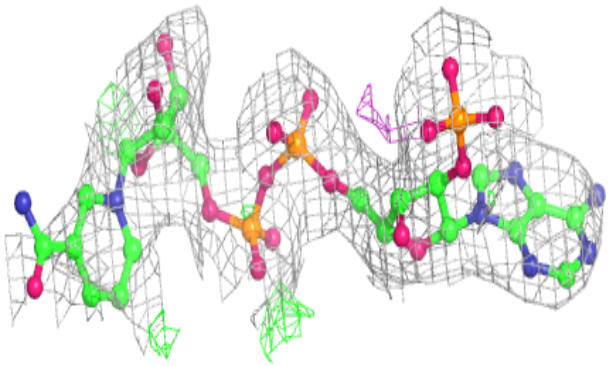


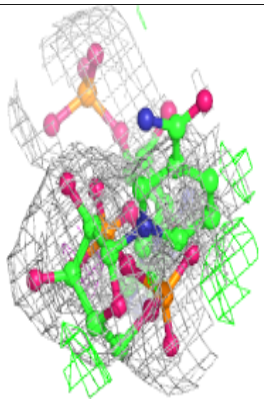


Electron density around NDP C 1032:

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







Electron density around FMN C 1030:

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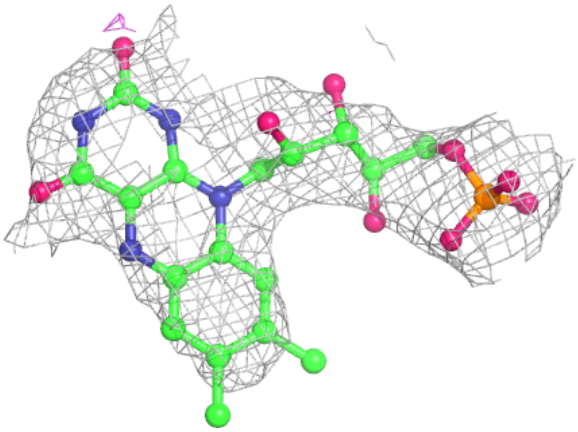
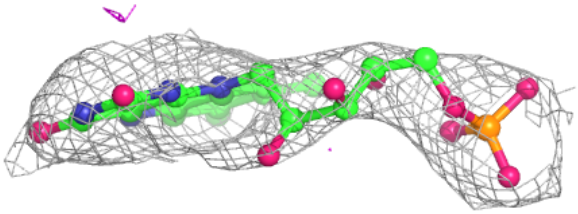
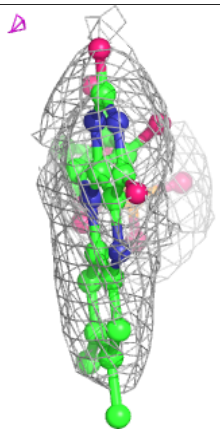
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NDP D 1032:

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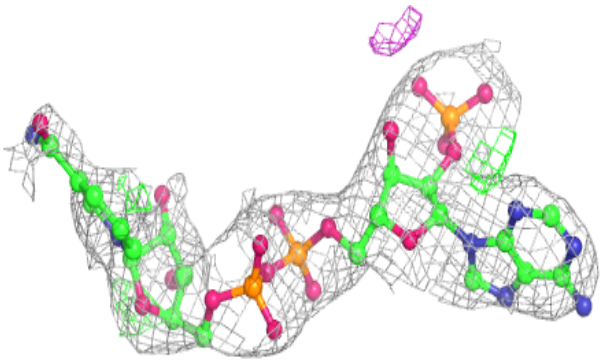
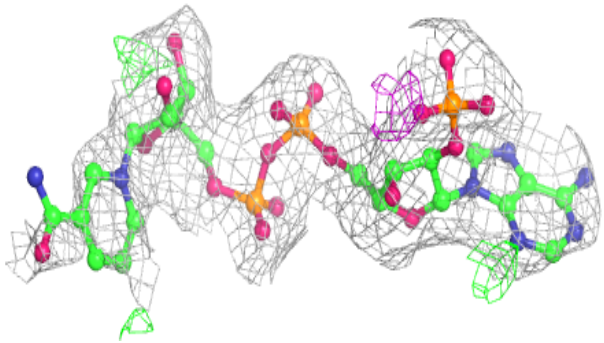
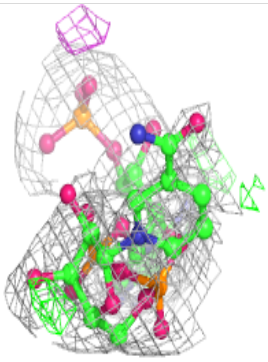
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

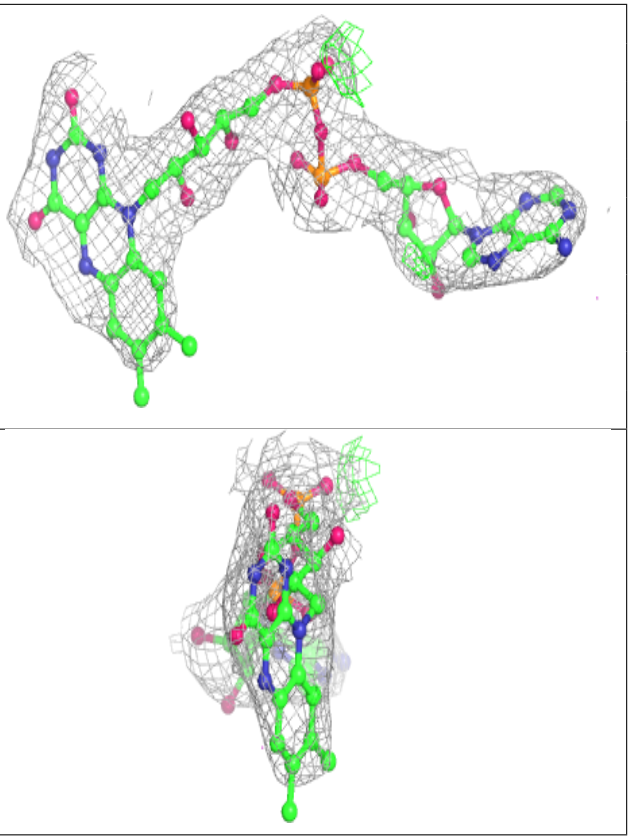






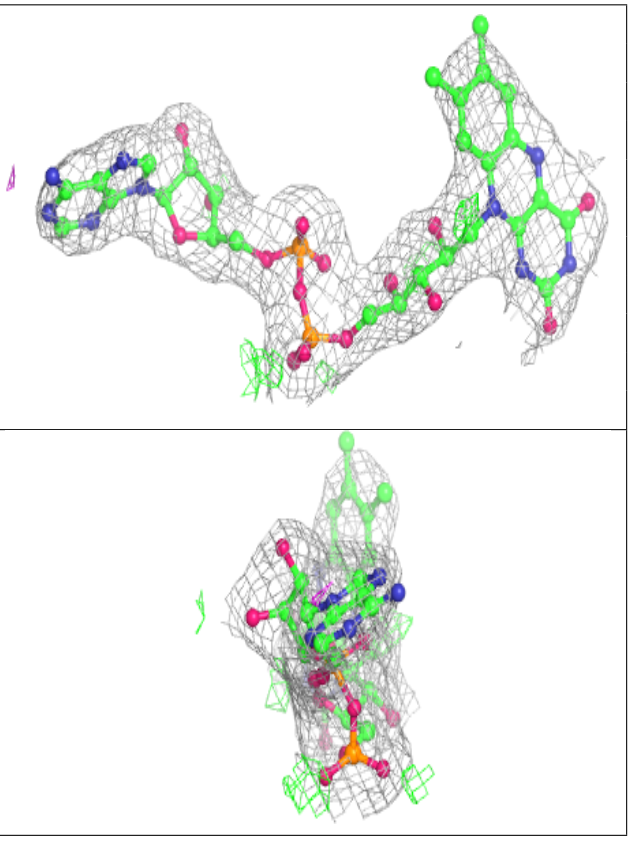
Electron density around FAD A 1031:

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



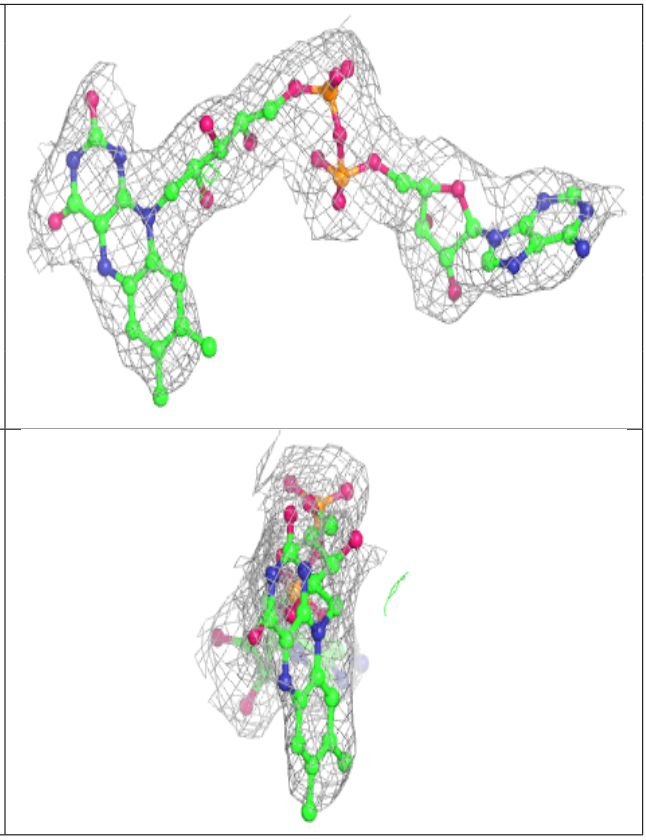
Electron density around FAD B 1031:

$2mF_o$-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 1031:

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



Electron density around FMN A 1030:

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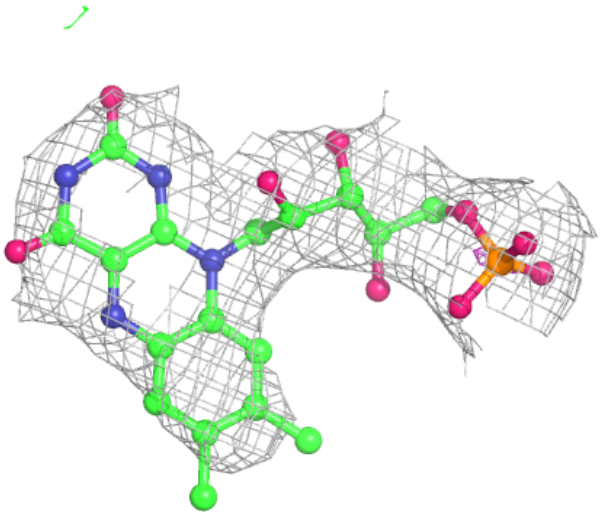
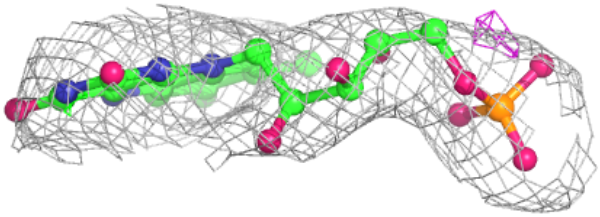
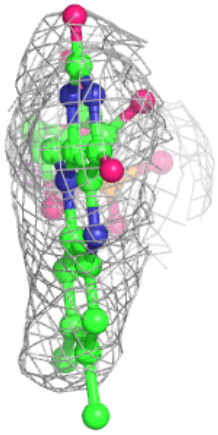
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NDP A 1032:

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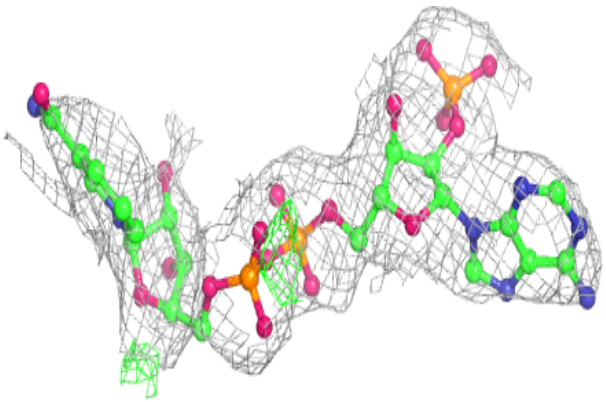
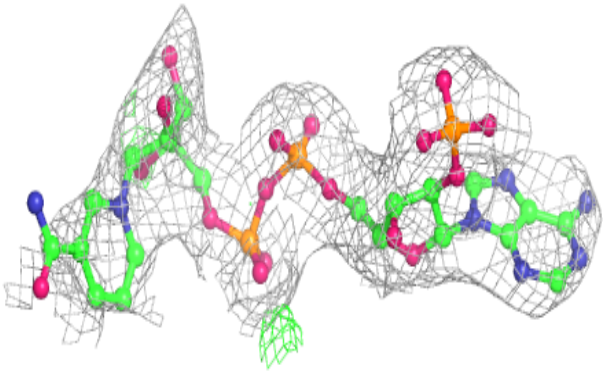
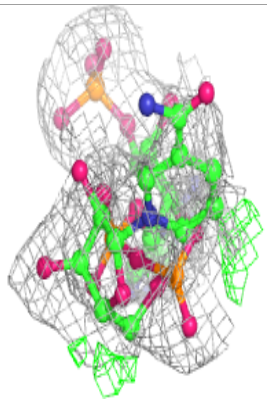
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NDP B 1032:

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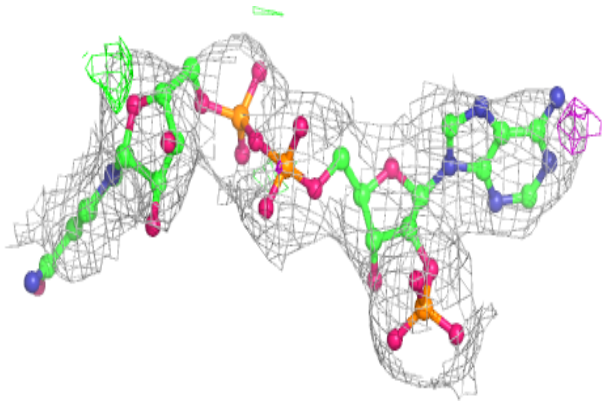
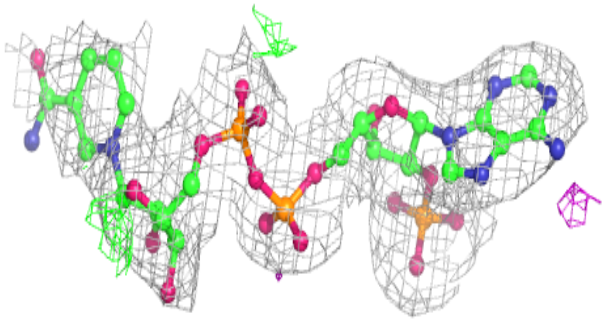
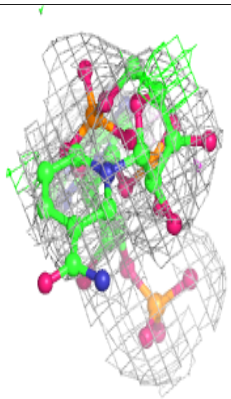
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around FMN B 1030:

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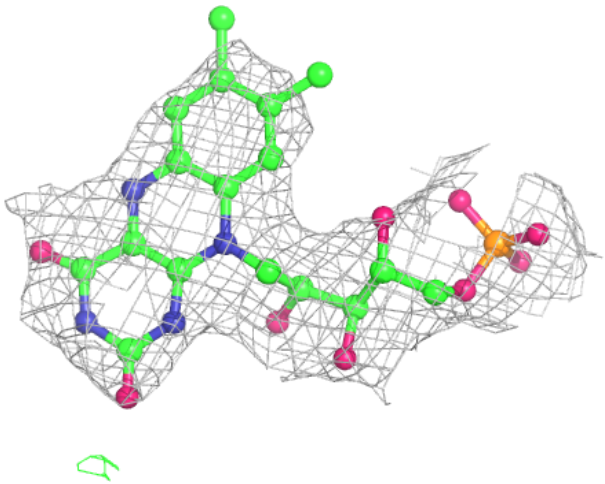
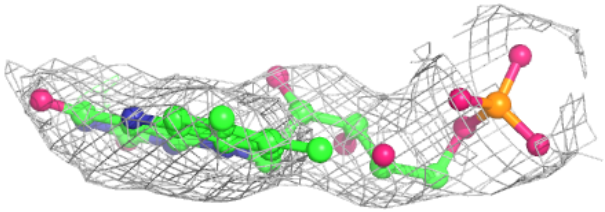
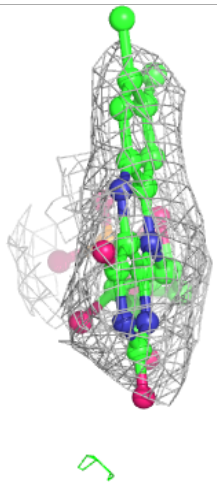
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

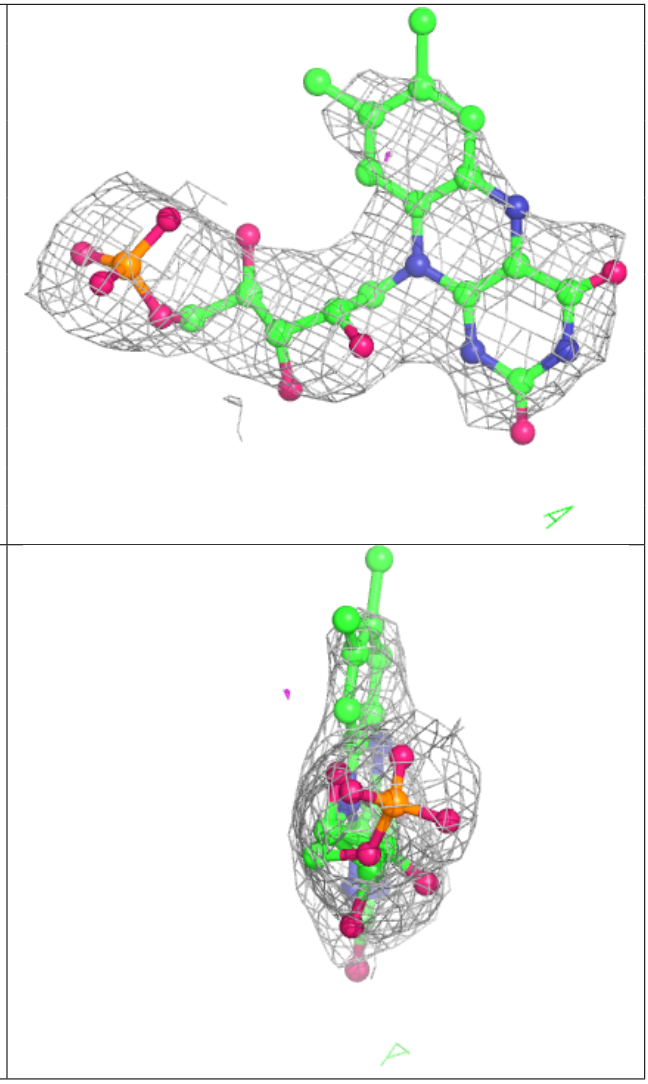






Electron density around FMN D 1030:

$2mF_o$-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.