Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:21 pm BST

PDB ID	:	5IFL
Title	:	Crystal structure of B. pseudomallei FabI in complex with NAD and triclosan
Authors	:	Hirschbeck, M.W.; Eltschkner, S.; Tonge, P.J.; Kisker, C.
Deposited on	:	2016-02-26
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

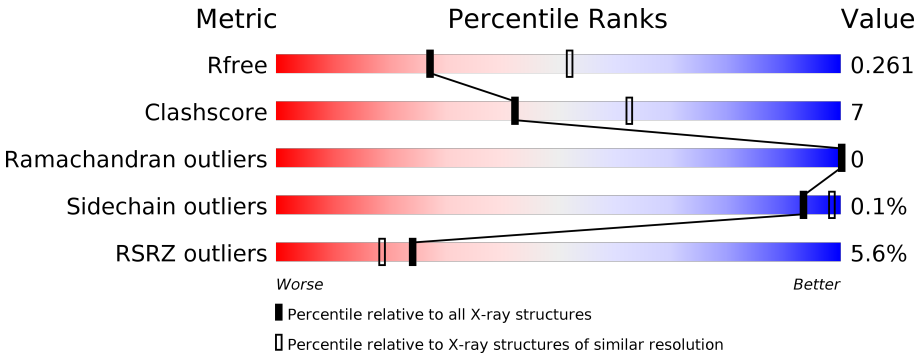
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	276	82% 11% 8%
1	B	276	% 82% 11% 8%
1	C	276	2% 82% 11% 8%
1	D	276	82% 11% 8%
1	E	276	82% 10% 8%
1	F	276	3% 80% 12% 8%

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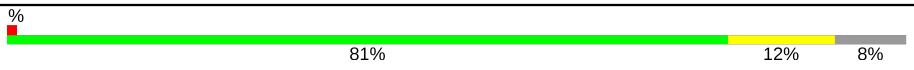
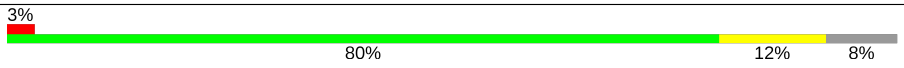
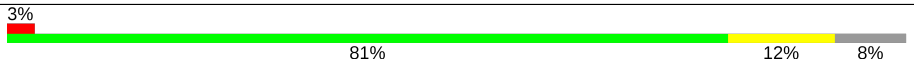
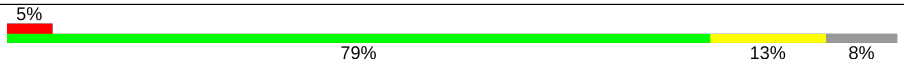
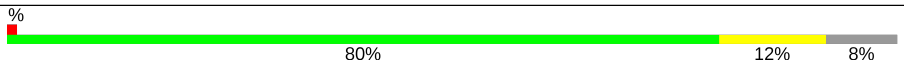
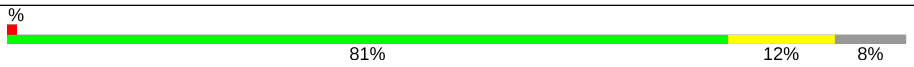
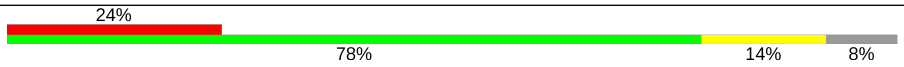
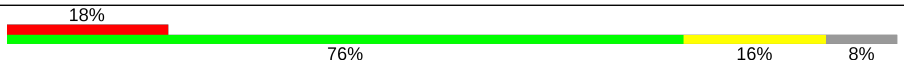
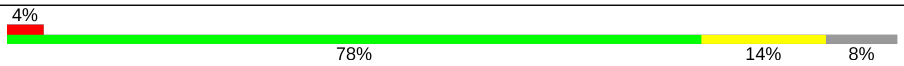
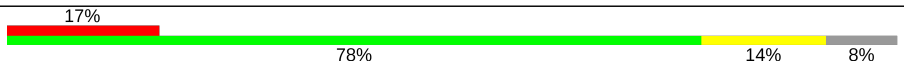
Mol	Chain	Length	Quality of chain
1	G	276	
1	H	276	
1	I	276	
1	J	276	
1	K	276	
1	L	276	
1	M	276	
1	N	276	
1	O	276	
1	P	276	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32377 atoms, of which 432 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	A	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	C	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	D	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	E	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	F	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	G	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	H	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	I	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	J	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	K	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	L	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	M	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	N	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	O	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			
1	P	255	Total	C	N	O	S	0	0	0
			1900	1211	323	361	5			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	LYS	-	expression tag	UNP A0A069B9A4
B	265	LEU	-	expression tag	UNP A0A069B9A4
B	266	ALA	-	expression tag	UNP A0A069B9A4
B	267	ALA	-	expression tag	UNP A0A069B9A4
B	268	ALA	-	expression tag	UNP A0A069B9A4
B	269	LEU	-	expression tag	UNP A0A069B9A4
B	270	GLU	-	expression tag	UNP A0A069B9A4
B	271	HIS	-	expression tag	UNP A0A069B9A4
B	272	HIS	-	expression tag	UNP A0A069B9A4
B	273	HIS	-	expression tag	UNP A0A069B9A4
B	274	HIS	-	expression tag	UNP A0A069B9A4
B	275	HIS	-	expression tag	UNP A0A069B9A4
B	276	HIS	-	expression tag	UNP A0A069B9A4
A	264	LYS	-	expression tag	UNP A0A069B9A4
A	265	LEU	-	expression tag	UNP A0A069B9A4
A	266	ALA	-	expression tag	UNP A0A069B9A4
A	267	ALA	-	expression tag	UNP A0A069B9A4
A	268	ALA	-	expression tag	UNP A0A069B9A4
A	269	LEU	-	expression tag	UNP A0A069B9A4
A	270	GLU	-	expression tag	UNP A0A069B9A4
A	271	HIS	-	expression tag	UNP A0A069B9A4
A	272	HIS	-	expression tag	UNP A0A069B9A4
A	273	HIS	-	expression tag	UNP A0A069B9A4
A	274	HIS	-	expression tag	UNP A0A069B9A4
A	275	HIS	-	expression tag	UNP A0A069B9A4
A	276	HIS	-	expression tag	UNP A0A069B9A4
C	264	LYS	-	expression tag	UNP A0A069B9A4
C	265	LEU	-	expression tag	UNP A0A069B9A4
C	266	ALA	-	expression tag	UNP A0A069B9A4
C	267	ALA	-	expression tag	UNP A0A069B9A4
C	268	ALA	-	expression tag	UNP A0A069B9A4
C	269	LEU	-	expression tag	UNP A0A069B9A4
C	270	GLU	-	expression tag	UNP A0A069B9A4
C	271	HIS	-	expression tag	UNP A0A069B9A4
C	272	HIS	-	expression tag	UNP A0A069B9A4
C	273	HIS	-	expression tag	UNP A0A069B9A4
C	274	HIS	-	expression tag	UNP A0A069B9A4
C	275	HIS	-	expression tag	UNP A0A069B9A4
C	276	HIS	-	expression tag	UNP A0A069B9A4
D	264	LYS	-	expression tag	UNP A0A069B9A4
D	265	LEU	-	expression tag	UNP A0A069B9A4
D	266	ALA	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	267	ALA	-	expression tag	UNP A0A069B9A4
D	268	ALA	-	expression tag	UNP A0A069B9A4
D	269	LEU	-	expression tag	UNP A0A069B9A4
D	270	GLU	-	expression tag	UNP A0A069B9A4
D	271	HIS	-	expression tag	UNP A0A069B9A4
D	272	HIS	-	expression tag	UNP A0A069B9A4
D	273	HIS	-	expression tag	UNP A0A069B9A4
D	274	HIS	-	expression tag	UNP A0A069B9A4
D	275	HIS	-	expression tag	UNP A0A069B9A4
D	276	HIS	-	expression tag	UNP A0A069B9A4
E	264	LYS	-	expression tag	UNP A0A069B9A4
E	265	LEU	-	expression tag	UNP A0A069B9A4
E	266	ALA	-	expression tag	UNP A0A069B9A4
E	267	ALA	-	expression tag	UNP A0A069B9A4
E	268	ALA	-	expression tag	UNP A0A069B9A4
E	269	LEU	-	expression tag	UNP A0A069B9A4
E	270	GLU	-	expression tag	UNP A0A069B9A4
E	271	HIS	-	expression tag	UNP A0A069B9A4
E	272	HIS	-	expression tag	UNP A0A069B9A4
E	273	HIS	-	expression tag	UNP A0A069B9A4
E	274	HIS	-	expression tag	UNP A0A069B9A4
E	275	HIS	-	expression tag	UNP A0A069B9A4
E	276	HIS	-	expression tag	UNP A0A069B9A4
F	264	LYS	-	expression tag	UNP A0A069B9A4
F	265	LEU	-	expression tag	UNP A0A069B9A4
F	266	ALA	-	expression tag	UNP A0A069B9A4
F	267	ALA	-	expression tag	UNP A0A069B9A4
F	268	ALA	-	expression tag	UNP A0A069B9A4
F	269	LEU	-	expression tag	UNP A0A069B9A4
F	270	GLU	-	expression tag	UNP A0A069B9A4
F	271	HIS	-	expression tag	UNP A0A069B9A4
F	272	HIS	-	expression tag	UNP A0A069B9A4
F	273	HIS	-	expression tag	UNP A0A069B9A4
F	274	HIS	-	expression tag	UNP A0A069B9A4
F	275	HIS	-	expression tag	UNP A0A069B9A4
F	276	HIS	-	expression tag	UNP A0A069B9A4
G	264	LYS	-	expression tag	UNP A0A069B9A4
G	265	LEU	-	expression tag	UNP A0A069B9A4
G	266	ALA	-	expression tag	UNP A0A069B9A4
G	267	ALA	-	expression tag	UNP A0A069B9A4
G	268	ALA	-	expression tag	UNP A0A069B9A4
G	269	LEU	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	270	GLU	-	expression tag	UNP A0A069B9A4
G	271	HIS	-	expression tag	UNP A0A069B9A4
G	272	HIS	-	expression tag	UNP A0A069B9A4
G	273	HIS	-	expression tag	UNP A0A069B9A4
G	274	HIS	-	expression tag	UNP A0A069B9A4
G	275	HIS	-	expression tag	UNP A0A069B9A4
G	276	HIS	-	expression tag	UNP A0A069B9A4
H	264	LYS	-	expression tag	UNP A0A069B9A4
H	265	LEU	-	expression tag	UNP A0A069B9A4
H	266	ALA	-	expression tag	UNP A0A069B9A4
H	267	ALA	-	expression tag	UNP A0A069B9A4
H	268	ALA	-	expression tag	UNP A0A069B9A4
H	269	LEU	-	expression tag	UNP A0A069B9A4
H	270	GLU	-	expression tag	UNP A0A069B9A4
H	271	HIS	-	expression tag	UNP A0A069B9A4
H	272	HIS	-	expression tag	UNP A0A069B9A4
H	273	HIS	-	expression tag	UNP A0A069B9A4
H	274	HIS	-	expression tag	UNP A0A069B9A4
H	275	HIS	-	expression tag	UNP A0A069B9A4
H	276	HIS	-	expression tag	UNP A0A069B9A4
I	264	LYS	-	expression tag	UNP A0A069B9A4
I	265	LEU	-	expression tag	UNP A0A069B9A4
I	266	ALA	-	expression tag	UNP A0A069B9A4
I	267	ALA	-	expression tag	UNP A0A069B9A4
I	268	ALA	-	expression tag	UNP A0A069B9A4
I	269	LEU	-	expression tag	UNP A0A069B9A4
I	270	GLU	-	expression tag	UNP A0A069B9A4
I	271	HIS	-	expression tag	UNP A0A069B9A4
I	272	HIS	-	expression tag	UNP A0A069B9A4
I	273	HIS	-	expression tag	UNP A0A069B9A4
I	274	HIS	-	expression tag	UNP A0A069B9A4
I	275	HIS	-	expression tag	UNP A0A069B9A4
I	276	HIS	-	expression tag	UNP A0A069B9A4
J	264	LYS	-	expression tag	UNP A0A069B9A4
J	265	LEU	-	expression tag	UNP A0A069B9A4
J	266	ALA	-	expression tag	UNP A0A069B9A4
J	267	ALA	-	expression tag	UNP A0A069B9A4
J	268	ALA	-	expression tag	UNP A0A069B9A4
J	269	LEU	-	expression tag	UNP A0A069B9A4
J	270	GLU	-	expression tag	UNP A0A069B9A4
J	271	HIS	-	expression tag	UNP A0A069B9A4
J	272	HIS	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	273	HIS	-	expression tag	UNP A0A069B9A4
J	274	HIS	-	expression tag	UNP A0A069B9A4
J	275	HIS	-	expression tag	UNP A0A069B9A4
J	276	HIS	-	expression tag	UNP A0A069B9A4
K	264	LYS	-	expression tag	UNP A0A069B9A4
K	265	LEU	-	expression tag	UNP A0A069B9A4
K	266	ALA	-	expression tag	UNP A0A069B9A4
K	267	ALA	-	expression tag	UNP A0A069B9A4
K	268	ALA	-	expression tag	UNP A0A069B9A4
K	269	LEU	-	expression tag	UNP A0A069B9A4
K	270	GLU	-	expression tag	UNP A0A069B9A4
K	271	HIS	-	expression tag	UNP A0A069B9A4
K	272	HIS	-	expression tag	UNP A0A069B9A4
K	273	HIS	-	expression tag	UNP A0A069B9A4
K	274	HIS	-	expression tag	UNP A0A069B9A4
K	275	HIS	-	expression tag	UNP A0A069B9A4
K	276	HIS	-	expression tag	UNP A0A069B9A4
L	264	LYS	-	expression tag	UNP A0A069B9A4
L	265	LEU	-	expression tag	UNP A0A069B9A4
L	266	ALA	-	expression tag	UNP A0A069B9A4
L	267	ALA	-	expression tag	UNP A0A069B9A4
L	268	ALA	-	expression tag	UNP A0A069B9A4
L	269	LEU	-	expression tag	UNP A0A069B9A4
L	270	GLU	-	expression tag	UNP A0A069B9A4
L	271	HIS	-	expression tag	UNP A0A069B9A4
L	272	HIS	-	expression tag	UNP A0A069B9A4
L	273	HIS	-	expression tag	UNP A0A069B9A4
L	274	HIS	-	expression tag	UNP A0A069B9A4
L	275	HIS	-	expression tag	UNP A0A069B9A4
L	276	HIS	-	expression tag	UNP A0A069B9A4
M	264	LYS	-	expression tag	UNP A0A069B9A4
M	265	LEU	-	expression tag	UNP A0A069B9A4
M	266	ALA	-	expression tag	UNP A0A069B9A4
M	267	ALA	-	expression tag	UNP A0A069B9A4
M	268	ALA	-	expression tag	UNP A0A069B9A4
M	269	LEU	-	expression tag	UNP A0A069B9A4
M	270	GLU	-	expression tag	UNP A0A069B9A4
M	271	HIS	-	expression tag	UNP A0A069B9A4
M	272	HIS	-	expression tag	UNP A0A069B9A4
M	273	HIS	-	expression tag	UNP A0A069B9A4
M	274	HIS	-	expression tag	UNP A0A069B9A4
M	275	HIS	-	expression tag	UNP A0A069B9A4

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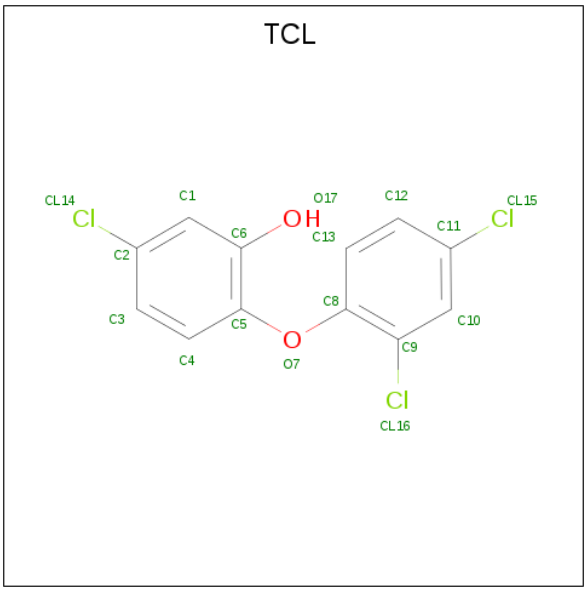
Chain	Residue	Modelled	Actual	Comment	Reference
M	276	HIS	-	expression tag	UNP A0A069B9A4
N	264	LYS	-	expression tag	UNP A0A069B9A4
N	265	LEU	-	expression tag	UNP A0A069B9A4
N	266	ALA	-	expression tag	UNP A0A069B9A4
N	267	ALA	-	expression tag	UNP A0A069B9A4
N	268	ALA	-	expression tag	UNP A0A069B9A4
N	269	LEU	-	expression tag	UNP A0A069B9A4
N	270	GLU	-	expression tag	UNP A0A069B9A4
N	271	HIS	-	expression tag	UNP A0A069B9A4
N	272	HIS	-	expression tag	UNP A0A069B9A4
N	273	HIS	-	expression tag	UNP A0A069B9A4
N	274	HIS	-	expression tag	UNP A0A069B9A4
N	275	HIS	-	expression tag	UNP A0A069B9A4
N	276	HIS	-	expression tag	UNP A0A069B9A4
O	264	LYS	-	expression tag	UNP A0A069B9A4
O	265	LEU	-	expression tag	UNP A0A069B9A4
O	266	ALA	-	expression tag	UNP A0A069B9A4
O	267	ALA	-	expression tag	UNP A0A069B9A4
O	268	ALA	-	expression tag	UNP A0A069B9A4
O	269	LEU	-	expression tag	UNP A0A069B9A4
O	270	GLU	-	expression tag	UNP A0A069B9A4
O	271	HIS	-	expression tag	UNP A0A069B9A4
O	272	HIS	-	expression tag	UNP A0A069B9A4
O	273	HIS	-	expression tag	UNP A0A069B9A4
O	274	HIS	-	expression tag	UNP A0A069B9A4
O	275	HIS	-	expression tag	UNP A0A069B9A4
O	276	HIS	-	expression tag	UNP A0A069B9A4
P	264	LYS	-	expression tag	UNP A0A069B9A4
P	265	LEU	-	expression tag	UNP A0A069B9A4
P	266	ALA	-	expression tag	UNP A0A069B9A4
P	267	ALA	-	expression tag	UNP A0A069B9A4
P	268	ALA	-	expression tag	UNP A0A069B9A4
P	269	LEU	-	expression tag	UNP A0A069B9A4
P	270	GLU	-	expression tag	UNP A0A069B9A4
P	271	HIS	-	expression tag	UNP A0A069B9A4
P	272	HIS	-	expression tag	UNP A0A069B9A4
P	273	HIS	-	expression tag	UNP A0A069B9A4
P	274	HIS	-	expression tag	UNP A0A069B9A4
P	275	HIS	-	expression tag	UNP A0A069B9A4
P	276	HIS	-	expression tag	UNP A0A069B9A4

- Molecule 2 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	D	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	E	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	F	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	G	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	H	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	I	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	J	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	K	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	L	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	M	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	N	1	Total	C	Cl	O	0	0
			17	12	3	2		

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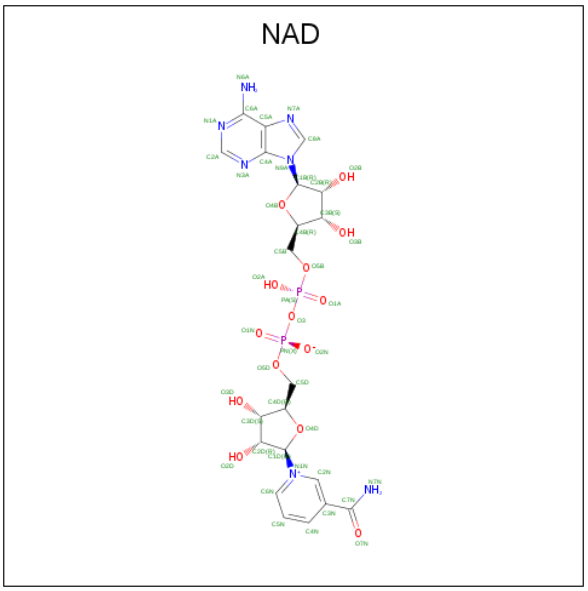
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	O	1	Total C Cl O 17 12 3 2	0	0
2	P	1	Total C Cl O 17 12 3 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C H N O P 71 21 27 7 14 2	0	0
3	A	1	Total C H N O P 71 21 27 7 14 2	0	0
3	C	1	Total C H N O P 71 21 27 7 14 2	0	0
3	D	1	Total C H N O P 71 21 27 7 14 2	0	0
3	E	1	Total C H N O P 71 21 27 7 14 2	0	0
3	F	1	Total C H N O P 71 21 27 7 14 2	0	0
3	G	1	Total C H N O P 71 21 27 7 14 2	0	0
3	H	1	Total C H N O P 71 21 27 7 14 2	0	0
3	I	1	Total C H N O P 71 21 27 7 14 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	J	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	K	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	L	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	M	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	N	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	O	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	P	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	60	Total	O	0	0
			60	60		
4	A	44	Total	O	0	0
			44	44		
4	C	35	Total	O	0	0
			35	35		
4	D	45	Total	O	0	0
			45	45		
4	E	47	Total	O	0	0
			47	47		
4	F	28	Total	O	0	0
			28	28		
4	G	36	Total	O	0	0
			36	36		
4	H	23	Total	O	0	0
			23	23		
4	I	36	Total	O	0	0
			36	36		
4	J	29	Total	O	0	0
			29	29		
4	K	46	Total	O	0	0
			46	46		
4	L	29	Total	O	0	0
			29	29		

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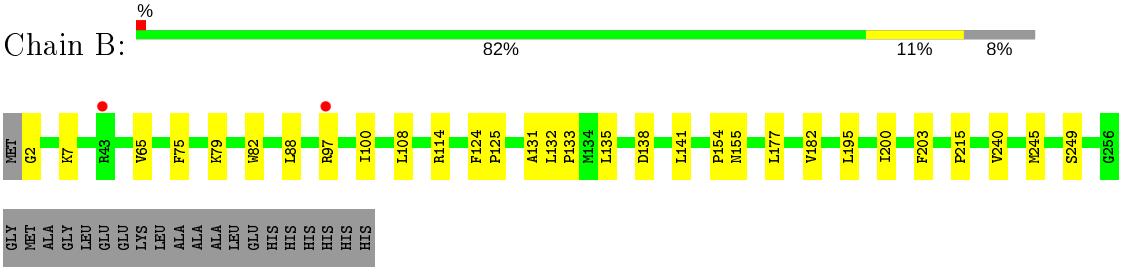
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	21	Total O 21 21	0	0
4	N	26	Total O 26 26	0	0
4	O	39	Total O 39 39	0	0
4	P	25	Total O 25 25	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

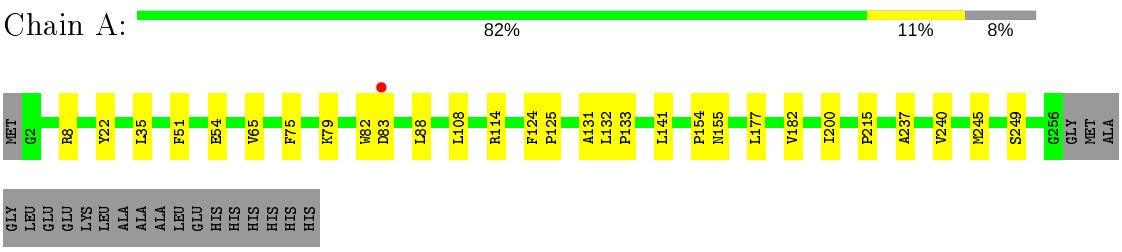
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain B:



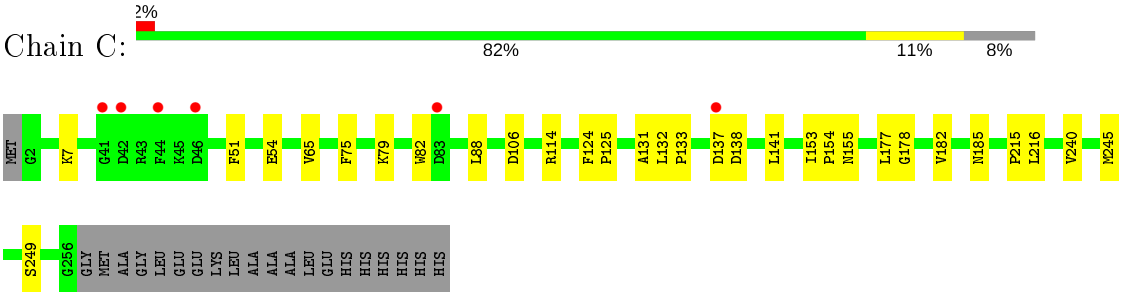
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



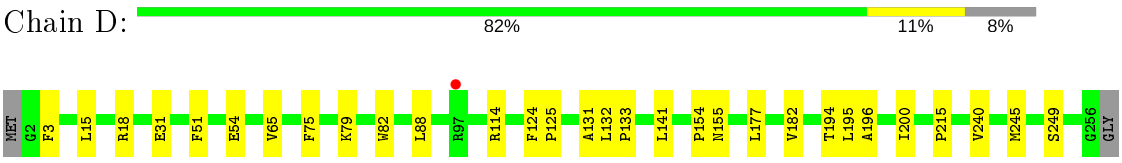
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain C:



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:

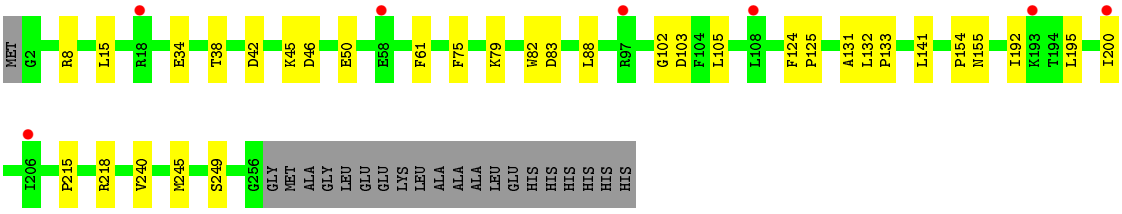


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain E:

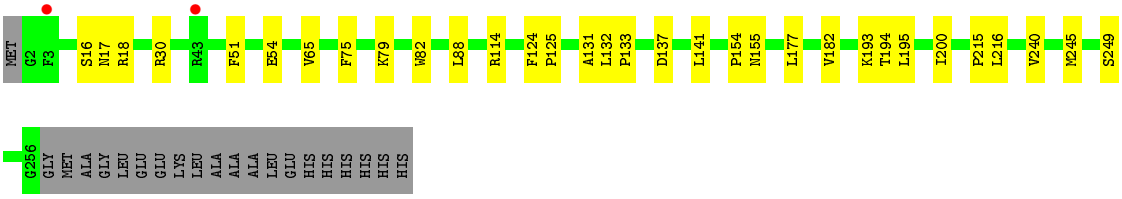
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain F:



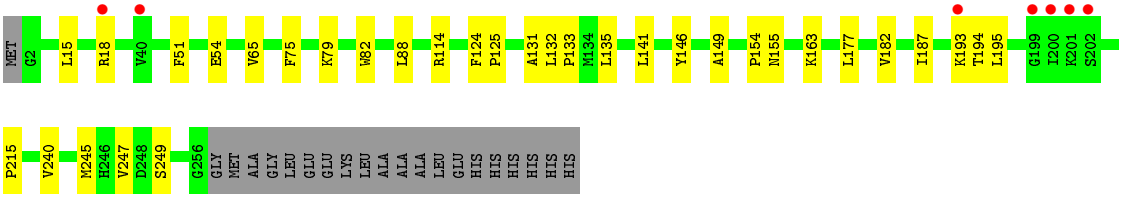
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain G:



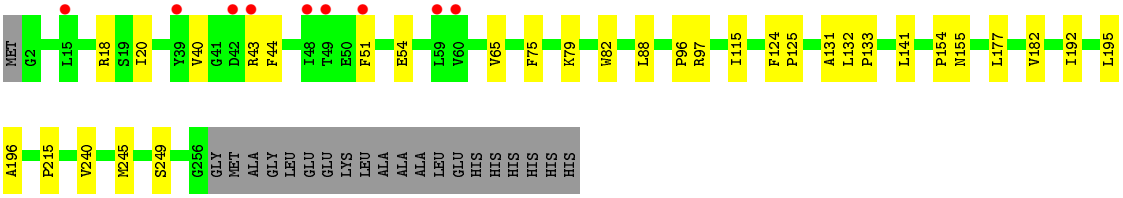
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain H:

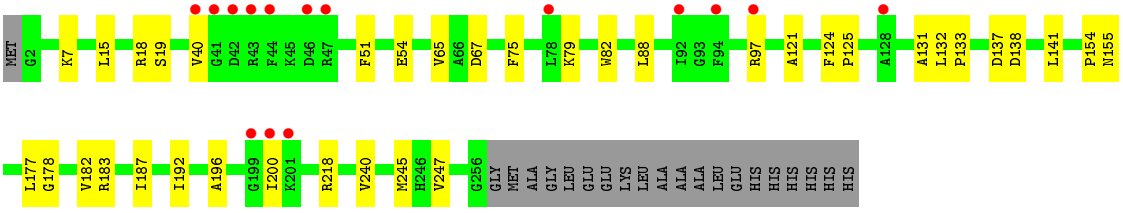


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

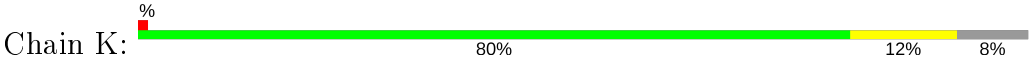
Chain I:

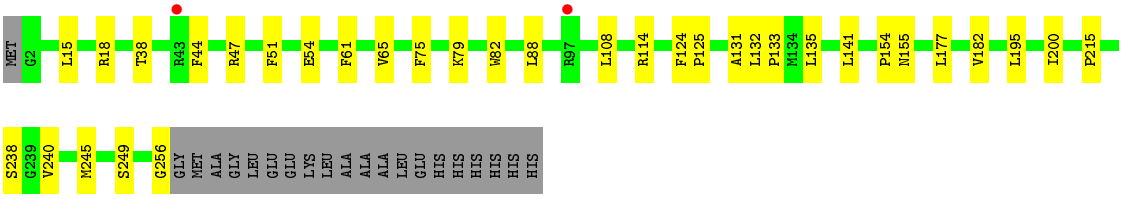


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

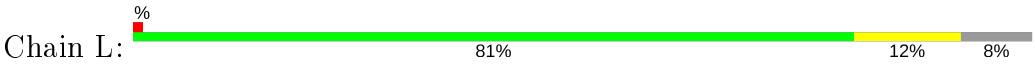


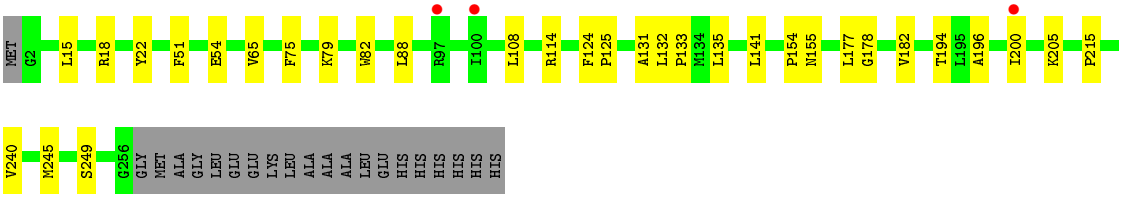
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



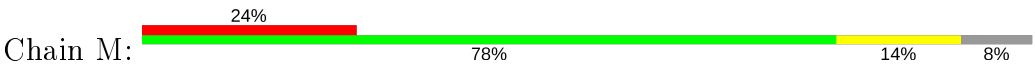


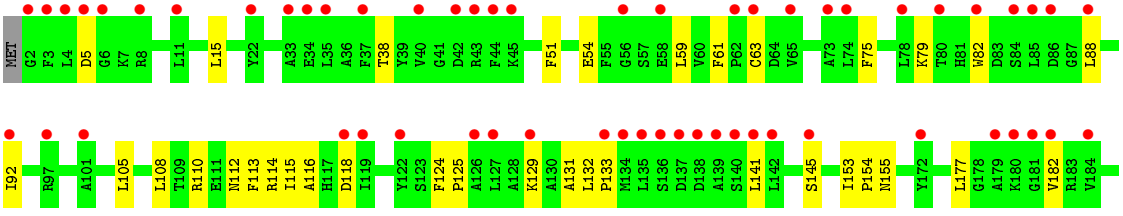
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

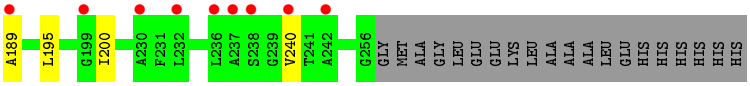




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

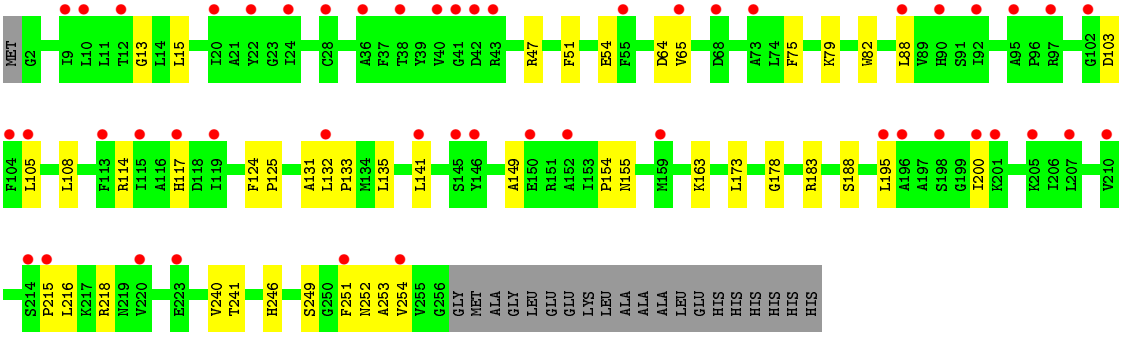






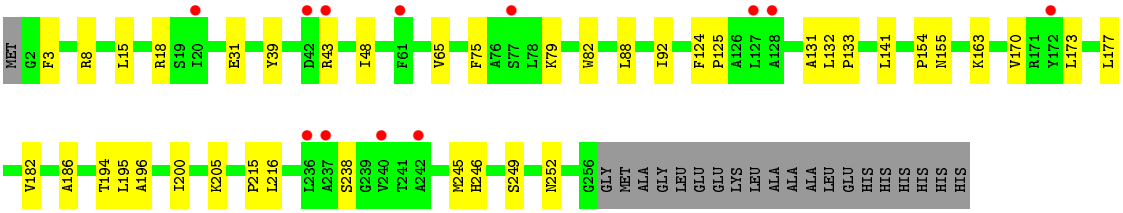
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain N:



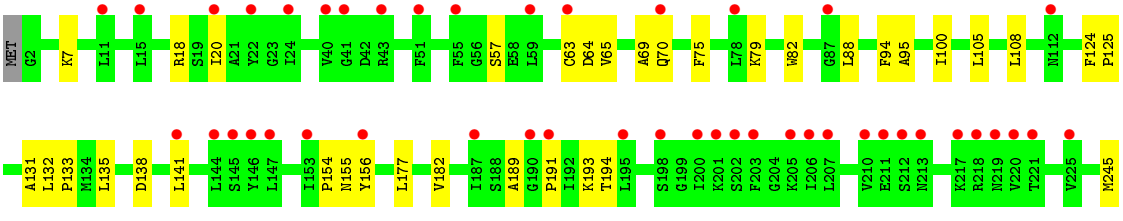
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain O:



• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.36Å 99.92Å 139.86Å 82.87° 89.20° 78.13°	Depositor
Resolution (Å)	48.58 – 2.60 68.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.58-2.60) 98.5 (68.85-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.262 0.222 , 0.261	Depositor DCC
R_{free} test set	5631 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TCL, NAD

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	0.22	0/1933	0.40	0/2616
1	B	0.22	0/1933	0.40	0/2616
1	C	0.22	0/1933	0.40	0/2616
1	D	0.22	0/1933	0.40	0/2616
1	E	0.22	0/1933	0.40	0/2616
1	F	0.22	0/1933	0.40	0/2616
1	G	0.22	0/1933	0.41	0/2616
1	H	0.22	0/1933	0.42	0/2616
1	I	0.22	0/1933	0.40	0/2616
1	J	0.24	0/1933	0.43	1/2616 (0.0%)
1	K	0.22	0/1933	0.40	0/2616
1	L	0.22	0/1933	0.40	0/2616
1	M	0.22	0/1933	0.41	0/2616
1	N	0.23	0/1933	0.41	0/2616
1	O	0.22	0/1933	0.40	0/2616
1	P	0.22	0/1933	0.41	0/2616
All	All	0.22	0/30928	0.41	1/41856 (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	J	18	ARG	NE-CZ-NH2	5.91	123.26	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1900	0	1907	29	1
1	B	1900	0	1907	29	0
1	C	1900	0	1907	23	2
1	D	1900	0	1907	24	0
1	E	1900	0	1907	22	0
1	F	1900	0	1907	34	0
1	G	1900	0	1907	29	0
1	H	1900	0	1907	32	0
1	I	1900	0	1907	35	0
1	J	1900	0	1907	28	2
1	K	1900	0	1907	28	0
1	L	1900	0	1907	27	1
1	M	1900	0	1907	40	0
1	N	1900	0	1907	40	0
1	O	1900	0	1907	36	0
1	P	1900	0	1907	37	0
2	A	17	0	7	2	0
2	B	17	0	7	3	0
2	C	17	0	7	0	0
2	D	17	0	7	2	0
2	E	17	0	7	0	0
2	F	17	0	7	1	0
2	G	17	0	7	1	0
2	H	17	0	7	0	0
2	I	17	0	7	0	0
2	J	17	0	7	2	0
2	K	17	0	7	1	0
2	L	17	0	7	1	0
2	M	17	0	7	3	0
2	N	17	0	7	2	0
2	O	17	0	7	2	0
2	P	17	0	7	4	0
3	A	44	27	26	2	0
3	B	44	27	26	1	0
3	C	44	27	26	1	0
3	D	44	27	26	3	0
3	E	44	27	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	44	27	26	1	0
3	G	44	27	26	1	0
3	H	44	27	26	4	0
3	I	44	27	26	4	0
3	J	44	27	26	4	0
3	K	44	27	26	2	0
3	L	44	27	26	3	0
3	M	44	27	26	8	0
3	N	44	27	26	4	0
3	O	44	27	26	3	0
3	P	44	27	26	6	0
4	A	44	0	0	1	0
4	B	60	0	0	1	0
4	C	35	0	0	1	0
4	D	45	0	0	2	0
4	E	47	0	0	5	0
4	F	28	0	0	3	0
4	G	36	0	0	3	0
4	H	23	0	0	1	0
4	I	36	0	0	3	0
4	J	29	0	0	2	0
4	K	46	0	0	2	0
4	L	29	0	0	2	0
4	M	21	0	0	6	0
4	N	26	0	0	3	0
4	O	39	0	0	3	0
4	P	25	0	0	5	0
All	All	31945	432	31040	428	3

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 7.

All (428) 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:50:GLU:OE2	1:I:97:ARG:NH1	2.14	0.81
1:P:191:PRO:HA	3:P:302:NAD:O7N	1.80	0.80
1:M:15:LEU:HD23	1:M:195:LEU:HD22	1.63	0.80
1:P:18:ARG:NH1	1:P:193:LYS:O	2.15	0.79
1:B:200:ILE:HD11	2:B:301:TCL:H131	1.64	0.79
1:M:114:ARG:HG3	1:N:114:ARG:HG3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:116:ALA:N	4:M:401:HOH:O	2.15	0.78
1:H:193:LYS:HZ1	1:P:69:ALA:HA	1.50	0.76
1:M:112:ASN:O	4:M:401:HOH:O	2.04	0.74
1:F:15:LEU:HD23	1:F:195:LEU:HD22	1.70	0.73
1:H:65:VAL:HG22	3:H:302:NAD:N1A	2.03	0.72
1:N:252:ASN:OD1	1:N:253:ALA:N	2.22	0.71
1:N:252:ASN:HA	4:N:415:HOH:O	1.91	0.71
1:P:95:ALA:N	2:P:301:TCL:CL15	2.61	0.70
1:L:205:LYS:NZ	4:L:401:HOH:O	2.19	0.70
1:F:103:ASP:OD2	4:F:401:HOH:O	2.10	0.70
1:E:240:VAL:HG21	1:H:245:MET:HE2	1.74	0.69
1:O:43:ARG:NH2	4:O:401:HOH:O	2.26	0.69
1:K:18:ARG:NH1	4:K:402:HOH:O	2.25	0.69
1:N:200:ILE:HD11	2:N:301:TCL:H131	1.75	0.68
1:L:88:LEU:HB3	1:L:141:LEU:HD22	1.75	0.68
1:P:189:ALA:HB3	3:P:302:NAD:C5N	2.24	0.68
1:F:88:LEU:HB3	1:F:141:LEU:HD22	1.77	0.67
1:B:97:ARG:NH1	1:F:218:ARG:HD2	2.09	0.67
1:B:88:LEU:HB3	1:B:141:LEU:HD22	1.77	0.67
1:G:18:ARG:NH1	1:G:194:THR:HA	2.08	0.67
1:D:88:LEU:HB3	1:D:141:LEU:HD22	1.77	0.66
1:P:251:PHE:O	1:P:254:VAL:HG22	1.96	0.66
1:J:88:LEU:HB3	1:J:141:LEU:HD22	1.77	0.65
1:P:65:VAL:N	4:P:401:HOH:O	2.29	0.65
1:H:75:PHE:CE1	1:H:131:ALA:HB2	2.32	0.65
1:I:75:PHE:CE1	1:I:131:ALA:HB2	2.32	0.65
1:K:200:ILE:HD11	2:K:301:TCL:H131	1.78	0.64
1:K:88:LEU:HB3	1:K:141:LEU:HD22	1.79	0.64
1:O:18:ARG:NH2	1:O:195:LEU:HD22	2.11	0.64
1:K:75:PHE:CE1	1:K:131:ALA:HB2	2.32	0.64
1:C:75:PHE:CE1	1:C:131:ALA:HB2	2.33	0.63
1:F:45:LYS:HZ3	1:I:115:ILE:HD12	1.61	0.63
1:I:132:LEU:HB3	1:I:133:PRO:HD3	1.80	0.63
1:B:97:ARG:HH11	1:F:218:ARG:HD2	1.63	0.63
1:J:75:PHE:CE1	1:J:131:ALA:HB2	2.34	0.63
1:D:18:ARG:HH22	1:D:195:LEU:HD13	1.63	0.63
1:K:132:LEU:HB3	1:K:133:PRO:HD3	1.81	0.63
1:P:194:THR:OG1	3:P:302:NAD:O1N	2.16	0.63
1:G:18:ARG:HH12	1:G:194:THR:HA	1.63	0.63
1:B:75:PHE:CE1	1:B:131:ALA:HB2	2.34	0.63
1:N:132:LEU:HB3	1:N:133:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:75:PHE:CE1	1:N:131:ALA:HB2	2.34	0.63
3:D:302:NAD:O1N	3:D:302:NAD:N7N	2.28	0.62
1:M:75:PHE:CE1	1:M:131:ALA:HB2	2.34	0.62
1:D:132:LEU:HB3	1:D:133:PRO:HD3	1.82	0.62
1:I:88:LEU:HB3	1:I:141:LEU:HD22	1.80	0.62
1:A:79:LYS:HA	1:A:82:TRP:O	2.00	0.61
1:G:75:PHE:CE1	1:G:131:ALA:HB2	2.34	0.61
1:J:132:LEU:HB3	1:J:133:PRO:HD3	1.82	0.61
1:E:132:LEU:HB3	1:E:133:PRO:HD3	1.81	0.61
1:F:8:ARG:NE	1:F:34:GLU:OE1	2.28	0.61
1:G:65:VAL:HG22	3:G:302:NAD:N1A	2.16	0.61
1:D:75:PHE:CE1	1:D:131:ALA:HB2	2.35	0.61
1:F:192:ILE:N	3:F:302:NAD:O7N	2.34	0.61
1:M:15:LEU:CD2	1:M:195:LEU:HD22	2.31	0.61
1:O:15:LEU:HB2	3:O:302:NAD:O3B	2.01	0.61
1:F:15:LEU:CD2	1:F:195:LEU:HD22	2.30	0.60
1:K:65:VAL:HG22	3:K:302:NAD:N1A	2.17	0.60
1:M:132:LEU:HB3	1:M:133:PRO:HD3	1.83	0.60
1:A:75:PHE:CE1	1:A:131:ALA:HB2	2.35	0.60
1:E:75:PHE:CE1	1:E:131:ALA:HB2	2.37	0.60
1:H:132:LEU:HB3	1:H:133:PRO:HD3	1.83	0.60
1:C:132:LEU:HB3	1:C:133:PRO:HD3	1.83	0.60
1:A:245:MET:HE2	1:D:240:VAL:HG21	1.83	0.60
1:L:132:LEU:HB3	1:L:133:PRO:HD3	1.83	0.60
1:G:30:ARG:NH1	4:G:403:HOH:O	2.23	0.60
1:N:246:HIS:CG	1:N:252:ASN:ND2	2.70	0.60
1:A:245:MET:CE	1:D:240:VAL:HG21	2.32	0.59
1:G:88:LEU:HB3	1:G:141:LEU:HD22	1.83	0.59
1:P:132:LEU:HB3	1:P:133:PRO:HD3	1.83	0.59
1:B:195:LEU:HD12	1:G:137:ASP:OD2	2.02	0.59
1:D:15:LEU:HB2	3:D:302:NAD:O3B	2.02	0.59
3:E:302:NAD:O1A	4:E:401:HOH:O	2.16	0.59
1:M:115:ILE:O	1:M:118:ASP:HB3	2.02	0.59
1:M:59:LEU:HG	4:M:411:HOH:O	2.02	0.59
1:P:88:LEU:HB3	1:P:141:LEU:HD22	1.84	0.59
1:O:75:PHE:CE1	1:O:131:ALA:HB2	2.37	0.59
1:P:94:PHE:HA	2:P:301:TCL:H101	1.83	0.59
1:L:75:PHE:CE1	1:L:131:ALA:HB2	2.37	0.59
1:M:15:LEU:HD22	3:M:302:NAD:H51A	1.85	0.59
1:F:75:PHE:CE1	1:F:131:ALA:HB2	2.38	0.58
1:M:92:ILE:HG23	3:M:302:NAD:N3A	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:LEU:HB3	1:E:141:LEU:HD22	1.84	0.58
1:M:200:ILE:HD12	2:M:301:TCL:C3	2.34	0.58
1:F:79:LYS:HA	1:F:82:TRP:O	2.03	0.58
1:M:88:LEU:HB3	1:M:141:LEU:HD22	1.85	0.58
1:B:245:MET:CE	1:C:240:VAL:HG21	2.33	0.57
1:E:240:VAL:HG21	1:H:245:MET:CE	2.33	0.57
1:O:65:VAL:HG22	3:O:302:NAD:N1A	2.18	0.57
1:P:75:PHE:CE1	1:P:131:ALA:HB2	2.40	0.57
1:I:192:ILE:N	3:I:302:NAD:O7N	2.30	0.57
1:J:196:ALA:HB1	2:J:301:TCL:C9	2.35	0.57
1:A:132:LEU:HB3	1:A:133:PRO:HD3	1.86	0.57
1:A:200:ILE:HD11	2:A:301:TCL:H131	1.87	0.57
1:D:65:VAL:HG22	3:D:302:NAD:N1A	2.20	0.57
1:I:124:PHE:HB3	1:I:125:PRO:CD	2.35	0.56
1:O:18:ARG:NH1	1:O:194:THR:HA	2.20	0.56
1:L:205:LYS:NZ	4:L:402:HOH:O	2.32	0.56
1:O:132:LEU:HB3	1:O:133:PRO:HD3	1.87	0.56
1:G:18:ARG:HH12	1:G:194:THR:CA	2.17	0.56
1:J:124:PHE:HB3	1:J:125:PRO:CD	2.35	0.56
1:F:132:LEU:HB3	1:F:133:PRO:HD3	1.88	0.56
1:K:124:PHE:HB3	1:K:125:PRO:CD	2.35	0.56
1:M:92:ILE:HD13	3:M:302:NAD:H2A	1.86	0.56
1:C:88:LEU:HB3	1:C:141:LEU:HD22	1.86	0.56
1:B:132:LEU:HB3	1:B:133:PRO:HD3	1.87	0.56
1:N:88:LEU:HB3	1:N:141:LEU:HD22	1.86	0.56
1:A:240:VAL:HG21	1:D:245:MET:HE2	1.88	0.56
1:M:108:LEU:HD22	1:N:125:PRO:HB2	1.87	0.56
1:P:64:ASP:OD1	4:P:401:HOH:O	2.18	0.56
1:G:132:LEU:HB3	1:G:133:PRO:HD3	1.87	0.55
1:N:15:LEU:HD23	1:N:195:LEU:HD22	1.87	0.55
1:A:83:ASP:CG	1:I:195:LEU:HD21	2.26	0.55
1:A:124:PHE:HB3	1:A:125:PRO:CD	2.36	0.55
1:L:124:PHE:HB3	1:L:125:PRO:CD	2.36	0.55
1:N:13:GLY:HA2	3:N:302:NAD:O2B	2.06	0.55
1:H:79:LYS:HA	1:H:82:TRP:O	2.06	0.55
1:I:240:VAL:HG21	1:L:245:MET:HE2	1.87	0.55
1:P:124:PHE:HB3	1:P:125:PRO:CD	2.37	0.55
1:E:43:ARG:HG2	4:E:447:HOH:O	2.07	0.55
1:J:79:LYS:HA	1:J:82:TRP:O	2.07	0.54
1:P:246:HIS:CG	1:P:252:ASN:HD21	2.25	0.54
1:A:83:ASP:OD2	1:I:195:LEU:HD21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:PHE:HB3	1:C:125:PRO:CD	2.37	0.54
1:N:124:PHE:HB3	1:N:125:PRO:CD	2.37	0.54
1:O:200:ILE:HD11	2:O:301:TCL:H131	1.88	0.54
1:O:88:LEU:HB3	1:O:141:LEU:HD22	1.88	0.54
1:F:240:VAL:HG21	1:G:245:MET:HE2	1.88	0.54
1:E:124:PHE:HB3	1:E:125:PRO:CD	2.38	0.54
1:O:124:PHE:HB3	1:O:125:PRO:CD	2.37	0.54
1:L:79:LYS:HA	1:L:82:TRP:O	2.06	0.54
1:G:79:LYS:HA	1:G:82:TRP:O	2.07	0.54
1:I:79:LYS:HA	1:I:82:TRP:O	2.08	0.54
1:K:124:PHE:HB3	1:K:125:PRO:HD3	1.90	0.54
1:K:79:LYS:HA	1:K:82:TRP:O	2.08	0.54
1:H:124:PHE:HB3	1:H:125:PRO:CD	2.37	0.54
1:N:79:LYS:HA	1:N:82:TRP:O	2.07	0.54
1:A:124:PHE:HB3	1:A:125:PRO:HD3	1.90	0.53
1:F:8:ARG:HG2	1:F:34:GLU:HB2	1.90	0.53
1:N:178:GLY:HA3	1:O:215:PRO:O	2.08	0.53
1:B:124:PHE:HB3	1:B:125:PRO:CD	2.38	0.53
1:C:124:PHE:HB3	1:C:125:PRO:HD3	1.91	0.53
1:I:124:PHE:HB3	1:I:125:PRO:HD3	1.89	0.53
1:N:75:PHE:CZ	1:N:131:ALA:HB2	2.43	0.53
1:N:218:ARG:NH2	1:O:238:SER:O	2.41	0.53
1:I:75:PHE:CZ	1:I:131:ALA:HB2	2.44	0.53
1:B:240:VAL:HG21	1:C:245:MET:HE2	1.90	0.53
1:G:124:PHE:HB3	1:G:125:PRO:CD	2.38	0.53
1:K:114:ARG:HG3	1:L:114:ARG:HG3	1.90	0.53
1:L:124:PHE:HB3	1:L:125:PRO:HD3	1.91	0.53
1:M:79:LYS:HA	1:M:82:TRP:O	2.08	0.52
1:J:124:PHE:HB3	1:J:125:PRO:HD3	1.92	0.52
1:P:70:GLN:O	4:P:402:HOH:O	2.19	0.52
1:D:124:PHE:HB3	1:D:125:PRO:CD	2.38	0.52
1:O:18:ARG:HH12	1:O:194:THR:HA	1.74	0.52
1:M:195:LEU:HB2	3:M:302:NAD:O1A	2.09	0.52
1:D:79:LYS:HA	1:D:82:TRP:O	2.10	0.52
1:C:79:LYS:HA	1:C:82:TRP:O	2.09	0.52
1:O:124:PHE:HB3	1:O:125:PRO:HD3	1.91	0.52
1:E:195:LEU:HD23	4:E:401:HOH:O	2.09	0.51
1:H:124:PHE:HB3	1:H:125:PRO:HD3	1.92	0.51
1:M:129:LYS:HB2	1:N:105:LEU:HD22	1.92	0.51
1:A:51:PHE:O	1:A:54:GLU:HB3	2.10	0.51
1:B:245:MET:HE2	1:C:240:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:PHE:O	4:D:401:HOH:O	2.18	0.51
1:E:124:PHE:HB3	1:E:125:PRO:HD3	1.92	0.51
1:N:124:PHE:HB3	1:N:125:PRO:HD3	1.92	0.51
1:N:47:ARG:HG3	4:N:410:HOH:O	2.10	0.51
1:C:75:PHE:CZ	1:C:131:ALA:HB2	2.46	0.51
1:P:124:PHE:HB3	1:P:125:PRO:HD3	1.91	0.51
1:F:124:PHE:HB3	1:F:125:PRO:CD	2.41	0.50
1:H:88:LEU:HB3	1:H:141:LEU:HD22	1.92	0.50
1:P:194:THR:HG21	3:P:302:NAD:O2N	2.11	0.50
1:M:108:LEU:CD2	1:N:125:PRO:HB2	2.42	0.50
1:N:64:ASP:HA	3:N:302:NAD:N1A	2.27	0.50
1:F:45:LYS:NZ	1:I:115:ILE:HD12	2.27	0.50
1:O:79:LYS:HA	1:O:82:TRP:O	2.10	0.50
1:B:124:PHE:HB3	1:B:125:PRO:HD3	1.93	0.50
1:B:79:LYS:HA	1:B:82:TRP:O	2.12	0.50
1:E:79:LYS:HA	1:E:82:TRP:O	2.10	0.50
1:M:124:PHE:HB3	1:M:125:PRO:CD	2.41	0.50
1:L:177:LEU:HB3	1:L:182:VAL:HB	1.94	0.50
1:J:75:PHE:CZ	1:J:131:ALA:HB2	2.47	0.50
1:N:246:HIS:CG	1:N:252:ASN:HD22	2.29	0.50
1:B:75:PHE:CZ	1:B:131:ALA:HB2	2.47	0.50
1:M:75:PHE:CZ	1:M:131:ALA:HB2	2.47	0.50
1:P:79:LYS:HA	1:P:82:TRP:O	2.11	0.50
1:B:65:VAL:HG22	3:B:302:NAD:N1A	2.28	0.49
1:M:92:ILE:HG12	3:M:302:NAD:HO2A	1.77	0.49
1:O:8:ARG:HB3	1:O:82:TRP:CZ3	2.47	0.49
1:H:75:PHE:CZ	1:H:131:ALA:HB2	2.47	0.49
1:K:75:PHE:CZ	1:K:131:ALA:HB2	2.48	0.49
1:L:51:PHE:O	1:L:54:GLU:HB3	2.12	0.49
1:C:65:VAL:HG22	3:C:302:NAD:N1A	2.27	0.49
1:H:177:LEU:HB3	1:H:182:VAL:HB	1.95	0.49
1:I:65:VAL:HG22	3:I:302:NAD:N1A	2.28	0.49
1:F:46:ASP:CG	1:I:97:ARG:H	2.15	0.49
1:A:83:ASP:OD2	1:I:195:LEU:HD11	2.13	0.49
1:N:241:THR:HG21	1:O:216:LEU:HG	1.95	0.49
1:E:75:PHE:CZ	1:E:131:ALA:HB2	2.48	0.49
1:I:240:VAL:HG21	1:L:245:MET:CE	2.42	0.49
1:H:154:PRO:O	1:H:155:ASN:HB2	2.13	0.49
1:G:124:PHE:HB3	1:G:125:PRO:HD3	1.93	0.49
1:D:124:PHE:HB3	1:D:125:PRO:HD3	1.94	0.48
1:I:154:PRO:O	1:I:155:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:PRO:O	1:M:155:ASN:HB2	2.13	0.48
1:O:154:PRO:O	1:O:155:ASN:HB2	2.13	0.48
1:A:88:LEU:HB3	1:A:141:LEU:HD22	1.95	0.48
1:D:75:PHE:CZ	1:D:131:ALA:HB2	2.48	0.48
1:J:15:LEU:HB2	3:J:302:NAD:H3B	1.95	0.48
1:L:154:PRO:O	1:L:155:ASN:HB2	2.13	0.48
1:L:200:ILE:HD11	2:L:301:TCL:H131	1.96	0.48
1:E:154:PRO:O	1:E:155:ASN:HB2	2.12	0.48
1:J:192:ILE:N	3:J:302:NAD:O7N	2.39	0.48
1:K:154:PRO:O	1:K:155:ASN:HB2	2.14	0.48
1:D:200:ILE:HD11	2:D:301:TCL:H131	1.95	0.48
1:F:124:PHE:HB3	1:F:125:PRO:HD3	1.95	0.48
1:G:154:PRO:O	1:G:155:ASN:HB2	2.13	0.48
1:J:154:PRO:O	1:J:155:ASN:HB2	2.14	0.48
1:P:75:PHE:CZ	1:P:131:ALA:HB2	2.49	0.48
1:L:132:LEU:HA	1:L:135:LEU:HD12	1.96	0.48
1:J:200:ILE:HD11	2:J:301:TCL:H131	1.94	0.48
1:O:215:PRO:HD2	1:O:249:SER:O	2.13	0.48
1:P:154:PRO:O	1:P:155:ASN:HB2	2.13	0.48
1:E:245:MET:CE	1:H:240:VAL:HG21	2.44	0.48
1:O:177:LEU:HB3	1:O:182:VAL:HB	1.96	0.48
1:O:92:ILE:HG23	3:O:302:NAD:C4A	2.43	0.48
1:H:193:LYS:NZ	1:P:69:ALA:CB	2.77	0.48
2:N:301:TCL:CL16	3:N:302:NAD:H3D	2.51	0.48
1:O:163:LYS:NZ	4:O:404:HOH:O	2.27	0.48
1:C:7:LYS:NZ	1:C:138:ASP:OD2	2.47	0.47
1:B:154:PRO:O	1:B:155:ASN:HB2	2.14	0.47
1:D:154:PRO:O	1:D:155:ASN:HB2	2.14	0.47
1:J:245:MET:HE2	1:K:240:VAL:HG21	1.95	0.47
1:A:83:ASP:OD1	1:I:195:LEU:HD11	2.14	0.47
1:M:105:LEU:HD21	1:N:173:LEU:HD21	1.96	0.47
1:O:18:ARG:HH12	1:O:194:THR:CA	2.28	0.47
1:B:177:LEU:HB3	1:B:182:VAL:HB	1.97	0.47
1:C:154:PRO:O	1:C:155:ASN:HB2	2.15	0.47
1:A:240:VAL:HG21	1:D:245:MET:CE	2.44	0.47
1:M:124:PHE:HB3	1:M:125:PRO:HD3	1.95	0.47
1:N:246:HIS:CD2	1:N:252:ASN:HD22	2.32	0.47
1:E:219:ASN:HB3	4:E:425:HOH:O	2.13	0.47
1:M:189:ALA:HB3	3:M:302:NAD:C5N	2.45	0.47
2:M:301:TCL:C4	2:M:301:TCL:H131	2.44	0.47
1:A:75:PHE:CZ	1:A:131:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:PHE:CE1	2:B:301:TCL:H31	2.49	0.47
1:A:154:PRO:O	1:A:155:ASN:HB2	2.14	0.47
1:O:205:LYS:NZ	4:O:406:HOH:O	2.31	0.47
1:O:75:PHE:CZ	1:O:131:ALA:HB2	2.50	0.47
1:H:132:LEU:HA	1:H:135:LEU:HD12	1.96	0.47
1:A:8:ARG:CZ	1:I:18:ARG:HH11	2.28	0.46
1:C:216:LEU:HB2	1:C:249:SER:HB3	1.97	0.46
1:E:215:PRO:HD2	1:E:249:SER:O	2.15	0.46
1:F:154:PRO:O	1:F:155:ASN:HB2	2.15	0.46
1:G:75:PHE:CZ	1:G:131:ALA:HB2	2.50	0.46
1:I:40:VAL:HG21	3:I:302:NAD:N3A	2.30	0.46
1:M:63:CYS:O	4:M:402:HOH:O	2.21	0.46
1:H:193:LYS:HZ3	1:P:69:ALA:CB	2.29	0.46
1:C:114:ARG:HG3	1:D:114:ARG:HG3	1.97	0.46
1:D:177:LEU:HB3	1:D:182:VAL:HB	1.96	0.46
1:H:15:LEU:HB2	3:H:302:NAD:O3B	2.16	0.46
1:I:43:ARG:O	4:I:401:HOH:O	2.20	0.46
1:M:110:ARG:NH2	1:N:65:VAL:O	2.35	0.46
1:G:200:ILE:HD11	2:G:301:TCL:H131	1.96	0.46
1:P:20:ILE:HG13	3:P:302:NAD:O2N	2.16	0.46
1:H:18:ARG:O	1:H:194:THR:HG22	2.16	0.46
1:M:145:SER:O	3:M:302:NAD:H5N	2.16	0.46
1:N:154:PRO:O	1:N:155:ASN:HB2	2.14	0.46
1:D:196:ALA:HB1	2:D:301:TCL:C9	2.46	0.46
1:F:75:PHE:CZ	1:F:131:ALA:HB2	2.50	0.46
1:H:15:LEU:HD23	1:H:195:LEU:HD22	1.96	0.46
1:I:196:ALA:HB2	3:I:302:NAD:O2A	2.15	0.46
1:N:15:LEU:HB2	3:N:302:NAD:O3B	2.16	0.46
1:F:8:ARG:HB3	1:F:82:TRP:CZ3	2.51	0.45
1:G:18:ARG:NH1	1:G:193:LYS:O	2.50	0.45
1:F:245:MET:HE2	1:G:240:VAL:HG21	1.97	0.45
1:J:240:VAL:HG21	1:K:245:MET:CE	2.46	0.45
1:B:2:GLY:N	4:B:409:HOH:O	2.49	0.45
1:C:185:ASN:HB2	4:C:426:HOH:O	2.16	0.45
1:D:194:THR:HB	4:D:407:HOH:O	2.16	0.45
1:E:245:MET:HE2	1:H:240:VAL:HG21	1.99	0.45
1:K:125:PRO:HB2	1:L:108:LEU:HD22	1.97	0.45
3:P:302:NAD:PA	3:P:302:NAD:HO3A	2.39	0.45
1:K:177:LEU:HB3	1:K:182:VAL:HB	1.98	0.45
1:K:15:LEU:HB2	3:K:302:NAD:O3B	2.17	0.45
1:M:115:ILE:HB	4:M:401:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:188:SER:HB3	1:N:246:HIS:CD2	2.51	0.45
1:P:7:LYS:NZ	1:P:138:ASP:OD2	2.50	0.45
1:E:38:THR:HA	1:E:61:PHE:O	2.17	0.45
1:M:114:ARG:O	1:M:118:ASP:HB2	2.16	0.45
1:I:245:MET:HE2	1:L:240:VAL:HG21	1.97	0.45
1:P:100:ILE:HD13	2:P:301:TCL:H121	1.98	0.45
1:B:215:PRO:O	1:C:178:GLY:HA3	2.16	0.45
1:I:51:PHE:O	1:I:54:GLU:HB3	2.17	0.45
1:M:240:VAL:HG21	1:P:245:MET:HE2	1.98	0.45
1:M:92:ILE:HG12	3:M:302:NAD:O2B	2.17	0.44
1:N:251:PHE:O	1:N:254:VAL:HG22	2.16	0.44
1:H:146:TYR:HB2	3:H:302:NAD:H5N	1.98	0.44
1:M:5:ASP:HB2	4:M:418:HOH:O	2.17	0.44
1:G:18:ARG:HG3	4:G:401:HOH:O	2.16	0.44
1:K:215:PRO:HD2	1:K:249:SER:O	2.18	0.44
1:K:51:PHE:O	1:K:54:GLU:HB3	2.17	0.44
1:K:38:THR:HA	1:K:61:PHE:O	2.18	0.44
1:A:83:ASP:CG	1:I:195:LEU:HD11	2.38	0.44
1:B:100:ILE:HD13	2:B:301:TCL:CL15	2.54	0.44
1:I:215:PRO:HD2	1:I:249:SER:O	2.18	0.44
1:J:65:VAL:HG22	3:J:302:NAD:N1A	2.33	0.44
1:N:103:ASP:HA	4:N:412:HOH:O	2.17	0.44
1:M:125:PRO:HB2	1:N:108:LEU:HD22	1.98	0.44
1:O:125:PRO:HB2	1:P:108:LEU:CD2	2.48	0.44
1:P:132:LEU:HA	1:P:135:LEU:HD12	1.99	0.44
1:D:215:PRO:HD2	1:D:249:SER:O	2.18	0.44
1:F:102:GLY:HA2	4:F:425:HOH:O	2.18	0.44
1:J:19:SER:HB3	4:J:414:HOH:O	2.18	0.44
1:J:40:VAL:HG21	3:J:302:NAD:N3A	2.33	0.44
1:L:15:LEU:HB2	3:L:302:NAD:O3B	2.17	0.44
1:J:178:GLY:HA3	1:K:215:PRO:O	2.18	0.43
1:L:75:PHE:CZ	1:L:131:ALA:HB2	2.53	0.43
1:H:187:ILE:HG23	1:H:247:VAL:HG23	2.00	0.43
1:I:20:ILE:N	4:I:406:HOH:O	2.50	0.43
1:H:193:LYS:NZ	1:P:69:ALA:HA	2.28	0.43
1:O:216:LEU:HB2	1:O:249:SER:HB3	2.01	0.43
3:E:302:NAD:O1N	3:E:302:NAD:H2N	2.18	0.43
1:K:132:LEU:HA	1:K:135:LEU:HD12	2.00	0.43
1:A:237:ALA:HA	4:A:412:HOH:O	2.18	0.43
1:P:177:LEU:HB3	1:P:182:VAL:HB	2.00	0.43
1:P:246:HIS:CG	1:P:252:ASN:ND2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:VAL:HG21	1:G:245:MET:CE	2.48	0.43
1:G:177:LEU:HB3	1:G:182:VAL:HB	2.01	0.43
1:M:113:PHE:HE1	1:N:117:HIS:HB3	1.84	0.43
1:E:177:LEU:HB3	1:E:182:VAL:HB	2.01	0.43
1:F:245:MET:CE	1:G:240:VAL:HG21	2.49	0.43
1:G:51:PHE:O	1:G:54:GLU:HB3	2.19	0.43
1:H:215:PRO:HD2	1:H:249:SER:O	2.18	0.43
1:B:7:LYS:NZ	1:B:138:ASP:OD2	2.51	0.43
1:E:231:PHE:HE2	1:H:245:MET:HE3	1.84	0.43
1:C:51:PHE:O	1:C:54:GLU:HB3	2.19	0.43
1:C:215:PRO:HD2	1:C:249:SER:O	2.18	0.42
1:H:163:LYS:NZ	3:H:302:NAD:O2D	2.49	0.42
1:O:196:ALA:HB1	2:O:301:TCL:C9	2.48	0.42
1:P:63:CYS:HA	4:P:402:HOH:O	2.18	0.42
1:I:177:LEU:HB3	1:I:182:VAL:HB	2.00	0.42
1:I:215:PRO:O	1:L:178:GLY:HA3	2.19	0.42
1:I:44:PHE:HA	4:I:422:HOH:O	2.19	0.42
1:G:16:SER:HB3	1:G:195:LEU:HD21	2.00	0.42
1:J:177:LEU:HB3	1:J:182:VAL:HB	1.99	0.42
1:F:45:LYS:NZ	1:I:96:PRO:HG2	2.34	0.42
1:I:245:MET:CE	1:L:240:VAL:HG21	2.48	0.42
1:N:240:VAL:HG21	1:O:245:MET:HE2	2.02	0.42
1:C:177:LEU:HB3	1:C:182:VAL:HB	2.00	0.42
1:J:187:ILE:HG23	1:J:247:VAL:HG23	2.01	0.42
1:J:218:ARG:NH2	1:K:238:SER:O	2.50	0.42
1:M:51:PHE:O	1:M:54:GLU:HB3	2.19	0.42
1:A:65:VAL:HG22	3:A:302:NAD:N1A	2.35	0.42
1:H:51:PHE:O	1:H:54:GLU:HB3	2.20	0.42
1:M:38:THR:HA	1:M:61:PHE:O	2.20	0.42
1:M:177:LEU:HB3	1:M:182:VAL:HB	2.01	0.42
1:O:3:PHE:CZ	1:O:31:GLU:HG3	2.55	0.42
1:A:215:PRO:HD2	1:A:249:SER:O	2.20	0.42
2:M:301:TCL:C4	2:M:301:TCL:C13	2.95	0.42
1:B:114:ARG:HG3	1:A:114:ARG:HG3	2.01	0.42
1:O:8:ARG:HB3	1:O:82:TRP:CH2	2.55	0.42
1:G:216:LEU:HB2	1:G:249:SER:HB3	2.02	0.42
1:B:215:PRO:HD2	1:B:249:SER:O	2.20	0.41
1:G:17:ASN:OD1	4:G:401:HOH:O	2.21	0.41
1:H:54:GLU:HB2	4:H:411:HOH:O	2.18	0.41
1:N:51:PHE:O	1:N:54:GLU:HB3	2.20	0.41
2:A:301:TCL:CL16	3:A:302:NAD:H3D	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:VAL:HG22	3:L:302:NAD:N1A	2.35	0.41
1:P:156:TYR:CE1	2:P:301:TCL:H11	2.55	0.41
1:B:125:PRO:HB2	1:A:108:LEU:HD22	2.01	0.41
1:B:240:VAL:HG21	1:C:245:MET:CE	2.50	0.41
1:D:3:PHE:CZ	1:D:31:GLU:HG3	2.55	0.41
1:F:105:LEU:N	4:F:401:HOH:O	2.52	0.41
1:G:215:PRO:HD2	1:G:249:SER:O	2.20	0.41
1:N:149:ALA:HB2	1:N:163:LYS:HB3	2.02	0.41
1:A:79:LYS:HD2	1:A:83:ASP:HA	2.01	0.41
1:E:18:ARG:NH2	1:E:195:LEU:HD22	2.35	0.41
1:J:240:VAL:HG21	1:K:245:MET:HE2	2.03	0.41
1:L:196:ALA:HB2	3:L:302:NAD:O2A	2.20	0.41
1:F:200:ILE:HD11	2:F:301:TCL:H131	2.02	0.41
1:J:7:LYS:NZ	1:J:138:ASP:OD2	2.54	0.41
1:J:245:MET:CE	1:K:240:VAL:HG21	2.50	0.41
1:N:215:PRO:HD2	1:N:249:SER:O	2.21	0.41
1:O:39:TYR:CD1	1:O:48:ILE:HG21	2.55	0.41
1:B:108:LEU:CD2	1:A:125:PRO:HB2	2.51	0.41
1:D:51:PHE:O	1:D:54:GLU:HB3	2.21	0.41
1:F:42:ASP:OD1	1:I:115:ILE:HD13	2.20	0.41
1:K:108:LEU:HD22	1:L:125:PRO:HB2	2.03	0.41
1:K:44:PHE:HE1	1:K:47:ARG:NH1	2.17	0.41
1:L:215:PRO:HD2	1:L:249:SER:O	2.21	0.41
1:A:177:LEU:HB3	1:A:182:VAL:HB	2.02	0.41
1:O:173:LEU:CD2	1:P:105:LEU:HD21	2.51	0.41
1:J:121:ALA:O	1:J:125:PRO:HD2	2.21	0.41
1:J:51:PHE:O	1:J:54:GLU:HB3	2.21	0.41
1:N:132:LEU:HA	1:N:135:LEU:HD12	2.03	0.41
1:B:125:PRO:HB2	1:A:108:LEU:CD2	2.51	0.41
1:H:149:ALA:HB2	1:H:163:LYS:HB3	2.02	0.41
1:M:153:ILE:HA	1:M:154:PRO:HD3	1.98	0.41
1:P:57:SER:HA	4:P:409:HOH:O	2.21	0.41
1:B:132:LEU:HA	1:B:135:LEU:HD12	2.03	0.40
1:E:2:GLY:N	4:E:413:HOH:O	2.54	0.40
1:F:79:LYS:HD2	1:F:83:ASP:HA	2.03	0.40
1:G:18:ARG:NH2	1:G:195:LEU:HD22	2.36	0.40
1:H:193:LYS:HZ1	1:P:69:ALA:CA	2.27	0.40
1:K:256:GLY:O	4:K:401:HOH:O	2.22	0.40
1:N:183:ARG:HD2	1:N:240:VAL:O	2.21	0.40
1:C:216:LEU:HD12	1:C:249:SER:HA	2.03	0.40
1:F:38:THR:HA	1:F:61:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:ASP:HA	4:J:406:HOH:O	2.21	0.40
1:O:170:VAL:HG21	1:O:186:ALA:HB2	2.03	0.40
1:O:246:HIS:CG	1:O:252:ASN:ND2	2.89	0.40
1:O:8:ARG:NH1	1:O:82:TRP:CD1	2.89	0.40
1:E:51:PHE:O	1:E:54:GLU:HB3	2.21	0.40
1:F:215:PRO:HD2	1:F:249:SER:O	2.20	0.40
1:F:8:ARG:NH1	1:F:82:TRP:CD1	2.88	0.40
1:G:114:ARG:HG3	1:H:114:ARG:HG3	2.04	0.40
1:L:18:ARG:O	1:L:194:THR:HG22	2.22	0.40
1:N:216:LEU:HB2	1:N:249:SER:HB3	2.03	0.40
1:C:153:ILE:HA	1:C:154:PRO:HD3	1.98	0.40
1:J:183:ARG:HD2	1:J:240:VAL:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:OH	1:C:137:ASP:OD2[1_655]	1.92	0.28
1:C:106:ASP:O	1:J:97:ARG:NH1[1_545]	2.05	0.15
1:J:137:ASP:OD2	1:L:22:TYR:OH[1_455]	2.10	0.10

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	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	B	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	C	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	D	253/276 (92%)	242 (96%)	11 (4%)	0	100	100
1	E	253/276 (92%)	242 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	G	253/276 (92%)	242 (96%)	11 (4%)	0	100	100
1	H	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	I	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	J	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	K	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	L	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	M	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	N	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	O	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	P	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
All	All	4048/4416 (92%)	3893 (96%)	155 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	194/209 (93%)	193 (100%)	1 (0%)	88	96
1	B	194/209 (93%)	194 (100%)	0	100	100
1	C	194/209 (93%)	194 (100%)	0	100	100
1	D	194/209 (93%)	194 (100%)	0	100	100
1	E	194/209 (93%)	194 (100%)	0	100	100
1	F	194/209 (93%)	194 (100%)	0	100	100
1	G	194/209 (93%)	194 (100%)	0	100	100
1	H	194/209 (93%)	194 (100%)	0	100	100
1	I	194/209 (93%)	194 (100%)	0	100	100
1	J	194/209 (93%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	194/209 (93%)	193 (100%)	1 (0%)	88 96
1	L	194/209 (93%)	194 (100%)	0	100 100
1	M	194/209 (93%)	194 (100%)	0	100 100
1	N	194/209 (93%)	194 (100%)	0	100 100
1	O	194/209 (93%)	194 (100%)	0	100 100
1	P	194/209 (93%)	194 (100%)	0	100 100
All	All	3104/3344 (93%)	3102 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	K	195	LEU

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

Mol	Chain	Res	Type
1	N	246	HIS
1	P	246	HIS
1	P	252	ASN

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 carbohydrates 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	$\#\|Z\| > 2$
3	NAD	E	302	-	42,48,48	0.89	1 (2%)	50,73,73	1.45	4 (8%)
2	TCL	H	301	-	18,18,18	0.46	0	25,25,25	0.78	1 (4%)
3	NAD	D	302	-	42,48,48	0.85	2 (4%)	50,73,73	1.37	2 (4%)
3	NAD	H	302	-	42,48,48	1.00	2 (4%)	50,73,73	1.51	2 (4%)
3	NAD	J	302	-	42,48,48	0.98	1 (2%)	50,73,73	1.41	3 (6%)
2	TCL	P	301	-	18,18,18	0.48	0	25,25,25	0.89	1 (4%)
3	NAD	L	302	-	42,48,48	0.91	2 (4%)	50,73,73	1.35	3 (6%)
3	NAD	A	302	-	42,48,48	0.89	2 (4%)	50,73,73	1.37	4 (8%)
2	TCL	A	301	-	18,18,18	0.42	0	25,25,25	0.83	1 (4%)
3	NAD	I	302	-	42,48,48	0.92	2 (4%)	50,73,73	1.36	4 (8%)
2	TCL	F	301	-	18,18,18	0.45	0	25,25,25	0.74	0
2	TCL	N	301	-	18,18,18	0.48	0	25,25,25	0.86	0
3	NAD	K	302	-	42,48,48	0.93	2 (4%)	50,73,73	1.50	3 (6%)
3	NAD	M	302	-	42,48,48	0.87	2 (4%)	50,73,73	1.28	2 (4%)
3	NAD	N	302	-	42,48,48	1.00	2 (4%)	50,73,73	1.25	3 (6%)
2	TCL	J	301	-	18,18,18	0.48	0	25,25,25	0.74	1 (4%)
3	NAD	C	302	-	42,48,48	0.93	2 (4%)	50,73,73	1.52	3 (6%)
3	NAD	B	302	-	42,48,48	0.85	2 (4%)	50,73,73	1.37	3 (6%)
3	NAD	G	302	-	42,48,48	0.91	2 (4%)	50,73,73	1.26	3 (6%)
3	NAD	F	302	-	42,48,48	0.97	2 (4%)	50,73,73	1.43	3 (6%)
3	NAD	O	302	-	42,48,48	0.90	2 (4%)	50,73,73	1.34	4 (8%)
2	TCL	O	301	-	18,18,18	0.47	0	25,25,25	0.81	1 (4%)
2	TCL	B	301	-	18,18,18	0.51	0	25,25,25	0.82	1 (4%)
2	TCL	G	301	-	18,18,18	0.45	0	25,25,25	0.78	1 (4%)
2	TCL	E	301	-	18,18,18	0.47	0	25,25,25	0.86	1 (4%)
2	TCL	C	301	-	18,18,18	0.50	0	25,25,25	0.77	1 (4%)
3	NAD	P	302	-	42,48,48	1.10	2 (4%)	50,73,73	1.26	2 (4%)
2	TCL	M	301	-	18,18,18	0.39	0	25,25,25	0.75	1 (4%)
2	TCL	K	301	-	18,18,18	0.50	0	25,25,25	0.85	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TCL	I	301	-	18,18,18	0.48	0	25,25,25	0.72	0
2	TCL	D	301	-	18,18,18	0.48	0	25,25,25	0.63	0
2	TCL	L	301	-	18,18,18	0.44	0	25,25,25	0.78	1 (4%)

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
3	NAD	E	302	-	-	2/26/62/62	0/5/5/5
2	TCL	H	301	-	-	0/4/4/4	0/2/2/2
3	NAD	D	302	-	-	5/26/62/62	0/5/5/5
3	NAD	H	302	-	-	2/26/62/62	0/5/5/5
3	NAD	J	302	-	-	7/26/62/62	0/5/5/5
2	TCL	P	301	-	-	0/4/4/4	0/2/2/2
3	NAD	L	302	-	-	6/26/62/62	0/5/5/5
3	NAD	A	302	-	-	8/26/62/62	0/5/5/5
2	TCL	A	301	-	-	0/4/4/4	0/2/2/2
3	NAD	I	302	-	-	7/26/62/62	0/5/5/5
2	TCL	F	301	-	-	0/4/4/4	0/2/2/2
2	TCL	N	301	-	-	0/4/4/4	0/2/2/2
3	NAD	K	302	-	-	11/26/62/62	0/5/5/5
3	NAD	M	302	-	-	11/26/62/62	0/5/5/5
3	NAD	N	302	-	-	9/26/62/62	0/5/5/5
2	TCL	J	301	-	-	0/4/4/4	0/2/2/2
3	NAD	C	302	-	-	6/26/62/62	0/5/5/5
3	NAD	B	302	-	-	5/26/62/62	0/5/5/5
3	NAD	G	302	-	-	6/26/62/62	0/5/5/5
3	NAD	F	302	-	-	9/26/62/62	0/5/5/5
3	NAD	O	302	-	-	4/26/62/62	0/5/5/5
2	TCL	O	301	-	-	0/4/4/4	0/2/2/2
2	TCL	B	301	-	-	0/4/4/4	0/2/2/2
2	TCL	G	301	-	-	0/4/4/4	0/2/2/2
2	TCL	E	301	-	-	0/4/4/4	0/2/2/2
2	TCL	C	301	-	-	0/4/4/4	0/2/2/2
3	NAD	P	302	-	-	18/26/62/62	0/5/5/5
2	TCL	M	301	-	-	1/4/4/4	0/2/2/2
2	TCL	K	301	-	-	0/4/4/4	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TCL	I	301	-	-	0/4/4/4	0/2/2/2
2	TCL	D	301	-	-	0/4/4/4	0/2/2/2
2	TCL	L	301	-	-	0/4/4/4	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	302	NAD	C2N-N1N	4.88	1.40	1.35
3	H	302	NAD	C2N-N1N	4.70	1.40	1.35
3	F	302	NAD	C2N-N1N	4.65	1.40	1.35
3	P	302	NAD	O4D-C1D	-4.33	1.35	1.41
3	P	302	NAD	C2N-N1N	4.31	1.40	1.35
3	C	302	NAD	C2N-N1N	4.22	1.40	1.35
3	I	302	NAD	C2N-N1N	4.00	1.39	1.35
3	K	302	NAD	C2N-N1N	3.99	1.39	1.35
3	O	302	NAD	C2N-N1N	3.90	1.39	1.35
3	L	302	NAD	C2N-N1N	3.88	1.39	1.35
3	A	302	NAD	C2N-N1N	3.83	1.39	1.35
3	E	302	NAD	C2N-N1N	3.83	1.39	1.35
3	N	302	NAD	O4D-C1D	-3.81	1.35	1.41
3	N	302	NAD	C2N-N1N	3.77	1.39	1.35
3	D	302	NAD	C2N-N1N	3.76	1.39	1.35
3	G	302	NAD	C2N-N1N	3.74	1.39	1.35
3	M	302	NAD	C2N-N1N	3.43	1.39	1.35
3	B	302	NAD	C2N-N1N	3.38	1.39	1.35
3	G	302	NAD	O4D-C1D	-2.96	1.36	1.41
3	L	302	NAD	O4D-C1D	-2.71	1.37	1.41
3	K	302	NAD	O4D-C1D	-2.63	1.37	1.41
3	I	302	NAD	O4D-C1D	-2.62	1.37	1.41
3	B	302	NAD	O4D-C1D	-2.62	1.37	1.41
3	O	302	NAD	O4D-C1D	-2.60	1.37	1.41
3	C	302	NAD	O4D-C1D	-2.53	1.37	1.41
3	H	302	NAD	O4D-C1D	-2.50	1.37	1.41
3	F	302	NAD	O4D-C1D	-2.33	1.37	1.41
3	M	302	NAD	O4D-C1D	-2.30	1.37	1.41
3	A	302	NAD	O4D-C1D	-2.23	1.38	1.41
3	D	302	NAD	O4D-C1D	-2.16	1.38	1.41

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	302	NAD	PN-O3-PA	8.89	163.34	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	302	NAD	PN-O3-PA	8.65	162.51	132.83
3	C	302	NAD	PN-O3-PA	8.60	162.32	132.83
3	D	302	NAD	PN-O3-PA	7.93	160.05	132.83
3	J	302	NAD	PN-O3-PA	7.93	160.04	132.83
3	L	302	NAD	PN-O3-PA	7.72	159.33	132.83
3	B	302	NAD	PN-O3-PA	7.66	159.13	132.83
3	F	302	NAD	PN-O3-PA	7.58	158.83	132.83
3	I	302	NAD	PN-O3-PA	7.51	158.59	132.83
3	E	302	NAD	PN-O3-PA	7.46	158.42	132.83
3	A	302	NAD	PN-O3-PA	7.46	158.42	132.83
3	M	302	NAD	PN-O3-PA	7.19	157.50	132.83
3	O	302	NAD	PN-O3-PA	7.01	156.87	132.83
3	N	302	NAD	PN-O3-PA	6.80	156.18	132.83
3	G	302	NAD	PN-O3-PA	6.80	156.15	132.83
3	P	302	NAD	PN-O3-PA	6.69	155.79	132.83
3	E	302	NAD	C3D-C2D-C1D	-3.80	95.26	100.98
3	F	302	NAD	O4D-C1D-C2D	-3.38	101.99	106.93
3	C	302	NAD	O4D-C1D-C2D	-3.17	102.29	106.93
3	O	302	NAD	O4D-C1D-C2D	-2.91	102.68	106.93
3	J	302	NAD	O4D-C1D-C2D	-2.83	102.78	106.93
2	P	301	TCL	O7-C5-C6	2.76	121.38	116.22
3	K	302	NAD	O4D-C1D-C2D	-2.72	102.95	106.93
3	A	302	NAD	O4D-C1D-C2D	-2.71	102.97	106.93
3	G	302	NAD	O4D-C1D-C2D	-2.50	103.27	106.93
2	K	301	TCL	O7-C5-C6	2.44	120.79	116.22
2	E	301	TCL	O7-C5-C6	2.36	120.63	116.22
2	O	301	TCL	O7-C5-C6	2.34	120.60	116.22
3	I	302	NAD	C5A-C6A-N6A	2.33	123.90	120.35
3	K	302	NAD	C5A-C6A-N6A	2.33	123.90	120.35
3	I	302	NAD	O4D-C1D-C2D	-2.32	103.53	106.93
3	C	302	NAD	C5A-C6A-N6A	2.30	123.84	120.35
3	L	302	NAD	O4D-C1D-C2D	-2.28	103.59	106.93
3	B	302	NAD	C5A-C6A-N6A	2.28	123.81	120.35
2	C	301	TCL	O7-C5-C6	2.27	120.47	116.22
3	H	302	NAD	C5A-C6A-N6A	2.27	123.80	120.35
3	J	302	NAD	C5A-C6A-N6A	2.26	123.79	120.35
3	G	302	NAD	C5A-C6A-N6A	2.26	123.79	120.35
3	B	302	NAD	O4D-C1D-C2D	-2.26	103.63	106.93
3	D	302	NAD	C5A-C6A-N6A	2.25	123.78	120.35
3	O	302	NAD	C5A-C6A-N6A	2.25	123.77	120.35
2	L	301	TCL	O7-C5-C6	2.23	120.39	116.22
3	A	302	NAD	C5A-C6A-N6A	2.23	123.74	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	302	NAD	C5A-C6A-N6A	2.23	123.73	120.35
3	F	302	NAD	C5A-C6A-N6A	2.22	123.72	120.35
3	E	302	NAD	C5A-C6A-N6A	2.22	123.72	120.35
3	M	302	NAD	C5A-C6A-N6A	2.21	123.72	120.35
3	L	302	NAD	C5A-C6A-N6A	2.19	123.69	120.35
2	M	301	TCL	C8-C9-CL16	2.18	121.99	119.43
3	E	302	NAD	O4D-C1D-C2D	-2.17	103.75	106.93
2	G	301	TCL	O7-C5-C6	2.17	120.27	116.22
3	N	302	NAD	O2D-C2D-C1D	-2.15	102.93	110.85
2	A	301	TCL	O7-C5-C6	2.13	120.20	116.22
3	A	302	NAD	C3D-C2D-C1D	-2.12	97.78	100.98
2	H	301	TCL	O7-C5-C6	2.10	120.15	116.22
2	B	301	TCL	O7-C5-C6	2.10	120.14	116.22
2	J	301	TCL	O7-C5-C6	2.07	120.09	116.22
3	P	302	NAD	C5A-C6A-N6A	2.06	123.49	120.35
3	I	302	NAD	O4B-C1B-C2B	-2.03	103.96	106.93
3	O	302	NAD	O4B-C1B-C2B	-2.02	103.98	106.93

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	302	NAD	O4D-C1D-N1N-C2N
3	J	302	NAD	C3B-C4B-C5B-O5B
3	J	302	NAD	PA-O3-PN-O5D
3	J	302	NAD	C5D-O5D-PN-O2N
3	L	302	NAD	C5D-O5D-PN-O1N
3	L	302	NAD	C5D-O5D-PN-O2N
3	L	302	NAD	O4D-C1D-N1N-C2N
3	A	302	NAD	C5D-O5D-PN-O1N
3	A	302	NAD	C5D-O5D-PN-O2N
3	A	302	NAD	O4D-C1D-N1N-C2N
3	I	302	NAD	C5D-O5D-PN-O1N
3	I	302	NAD	C5D-O5D-PN-O2N
3	I	302	NAD	O4D-C1D-N1N-C2N
3	M	302	NAD	C5B-O5B-PA-O1A
3	M	302	NAD	C5D-O5D-PN-O1N
3	M	302	NAD	C5D-O5D-PN-O2N
3	M	302	NAD	O4D-C1D-N1N-C2N
3	M	302	NAD	O4D-C1D-N1N-C6N
3	M	302	NAD	C2D-C1D-N1N-C2N
3	M	302	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	K	302	NAD	C5B-O5B-PA-O1A
3	K	302	NAD	O4B-C4B-C5B-O5B
3	K	302	NAD	C5D-O5D-PN-O1N
3	K	302	NAD	C5D-O5D-PN-O2N
3	K	302	NAD	O4D-C1D-N1N-C2N
3	N	302	NAD	C3B-C4B-C5B-O5B
3	N	302	NAD	C5D-O5D-PN-O2N
3	C	302	NAD	C5D-O5D-PN-O2N
3	B	302	NAD	C5D-O5D-PN-O1N
3	B	302	NAD	C5D-O5D-PN-O2N
3	B	302	NAD	O4D-C1D-N1N-C2N
3	G	302	NAD	C5D-O5D-PN-O1N
3	G	302	NAD	C5D-O5D-PN-O2N
3	G	302	NAD	O4D-C1D-N1N-C2N
3	F	302	NAD	C5B-O5B-PA-O1A
3	F	302	NAD	C5B-O5B-PA-O3
3	F	302	NAD	PN-O3-PA-O5B
3	F	302	NAD	C5D-O5D-PN-O1N
3	F	302	NAD	C5D-O5D-PN-O2N
3	O	302	NAD	C5D-O5D-PN-O1N
3	O	302	NAD	C5D-O5D-PN-O2N
3	P	302	NAD	C5B-O5B-PA-O1A
3	P	302	NAD	C5B-O5B-PA-O2A
3	P	302	NAD	PN-O3-PA-O5B
3	P	302	NAD	O4D-C1D-N1N-C2N
3	P	302	NAD	O4D-C1D-N1N-C6N
3	P	302	NAD	C2D-C1D-N1N-C2N
3	P	302	NAD	C2D-C1D-N1N-C6N
3	J	302	NAD	O4B-C4B-C5B-O5B
3	K	302	NAD	C3B-C4B-C5B-O5B
3	N	302	NAD	O4B-C4B-C5B-O5B
3	F	302	NAD	O4B-C4B-C5B-O5B
3	F	302	NAD	C3B-C4B-C5B-O5B
3	I	302	NAD	PA-O3-PN-O1N
3	J	302	NAD	C4B-C5B-O5B-PA
3	M	302	NAD	C4B-C5B-O5B-PA
3	P	302	NAD	C4B-C5B-O5B-PA
3	N	302	NAD	C4B-C5B-O5B-PA
3	L	302	NAD	PN-O3-PA-O5B
3	N	302	NAD	PN-O3-PA-O5B
3	N	302	NAD	PA-O3-PN-O5D
3	F	302	NAD	PA-O3-PN-O5D

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Mol	Chain	Res	Type	Atoms
3	P	302	NAD	PA-O3-PN-O5D
3	J	302	NAD	C5D-O5D-PN-O3
3	M	302	NAD	C5B-O5B-PA-O3
3	M	302	NAD	C5D-O5D-PN-O3
3	N	302	NAD	C5D-O5D-PN-O3
3	C	302	NAD	C5D-O5D-PN-O3
3	O	302	NAD	C5D-O5D-PN-O3
3	P	302	NAD	C5D-O5D-PN-O3
3	D	302	NAD	PA-O3-PN-O2N
3	A	302	NAD	PA-O3-PN-O1N
3	K	302	NAD	C5B-O5B-PA-O2A
3	N	302	NAD	C5D-O5D-PN-O1N
3	C	302	NAD	C5D-O5D-PN-O1N
3	P	302	NAD	C5D-O5D-PN-O2N
3	P	302	NAD	O4D-C4D-C5D-O5D
3	A	302	NAD	PA-O3-PN-O2N
3	I	302	NAD	PA-O3-PN-O2N
3	C	302	NAD	PA-O3-PN-O2N
3	H	302	NAD	C3D-C4D-C5D-O5D
2	M	301	TCL	C6-C5-O7-C8
3	I	302	NAD	O4B-C4B-C5B-O5B
3	K	302	NAD	PA-O3-PN-O1N
3	P	302	NAD	O4B-C4B-C5B-O5B
3	M	302	NAD	O4B-C4B-C5B-O5B
3	E	302	NAD	O4B-C4B-C5B-O5B
3	L	302	NAD	O4B-C4B-C5B-O5B
3	P	302	NAD	C3D-C4D-C5D-O5D
3	D	302	NAD	C2D-C1D-N1N-C6N
3	L	302	NAD	C5D-O5D-PN-O3
3	A	302	NAD	C5D-O5D-PN-O3
3	A	302	NAD	C2D-C1D-N1N-C6N
3	I	302	NAD	C5D-O5D-PN-O3
3	K	302	NAD	C5D-O5D-PN-O3
3	K	302	NAD	C2D-C1D-N1N-C6N
3	B	302	NAD	C5D-O5D-PN-O3
3	G	302	NAD	C5D-O5D-PN-O3
3	G	302	NAD	C2D-C1D-N1N-C6N
3	F	302	NAD	C5D-O5D-PN-O3
3	P	302	NAD	C5B-O5B-PA-O3
3	B	302	NAD	O4B-C4B-C5B-O5B
3	G	302	NAD	O4B-C4B-C5B-O5B
3	O	302	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	D	302	NAD	PA-O3-PN-O1N
3	K	302	NAD	PA-O3-PN-O2N
3	N	302	NAD	PA-O3-PN-O1N
3	C	302	NAD	PA-O3-PN-O1N
3	P	302	NAD	PN-O3-PA-O1A
3	P	302	NAD	PA-O3-PN-O1N
3	E	302	NAD	C5B-O5B-PA-O1A
3	J	302	NAD	C5D-O5D-PN-O1N
3	P	302	NAD	C5D-O5D-PN-O1N
3	D	302	NAD	O4B-C4B-C5B-O5B
3	H	302	NAD	O4B-C4B-C5B-O5B
3	A	302	NAD	O4B-C4B-C5B-O5B
3	C	302	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

28 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	NAD	2	0
3	D	302	NAD	3	0
3	H	302	NAD	4	0
3	J	302	NAD	4	0
2	P	301	TCL	4	0
3	L	302	NAD	3	0
3	A	302	NAD	2	0
2	A	301	TCL	2	0
3	I	302	NAD	4	0
2	F	301	TCL	1	0
2	N	301	TCL	2	0
3	K	302	NAD	2	0
3	M	302	NAD	8	0
3	N	302	NAD	4	0
2	J	301	TCL	2	0
3	C	302	NAD	1	0
3	B	302	NAD	1	0
3	G	302	NAD	1	0
3	F	302	NAD	1	0
3	O	302	NAD	3	0
2	O	301	TCL	2	0
2	B	301	TCL	3	0
2	G	301	TCL	1	0
3	P	302	NAD	6	0

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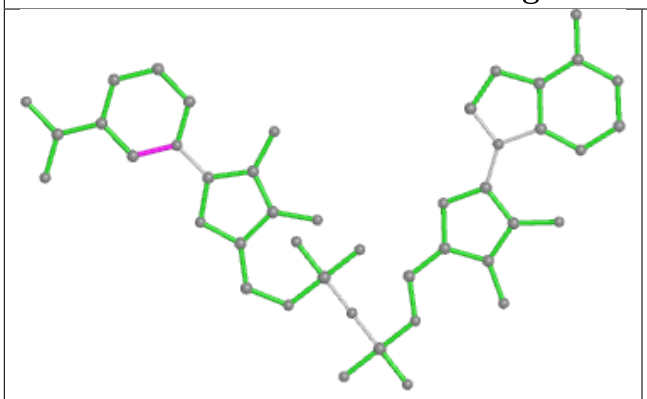
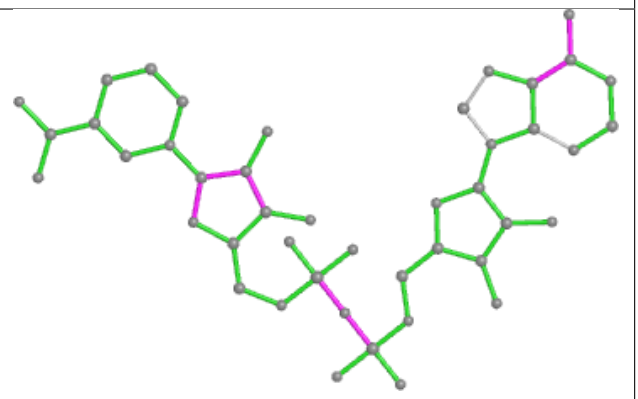
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	301	TCL	3	0
2	K	301	TCL	1	0
2	D	301	TCL	2	0
2	L	301	TCL	1	0

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.

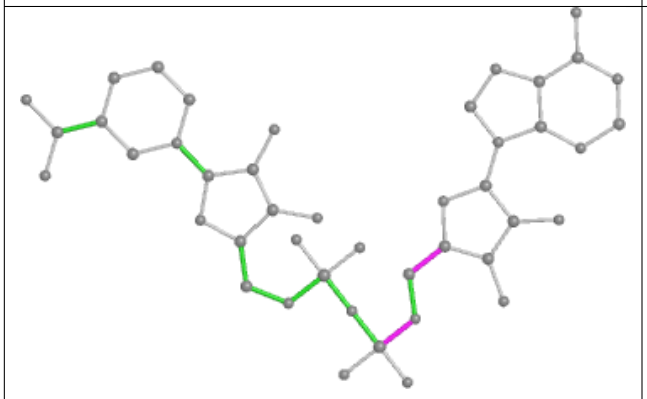
Ligand NAD E 302



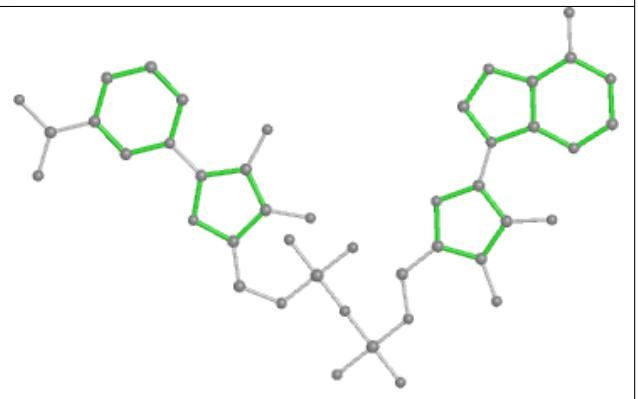
Bond lengths



Bond angles

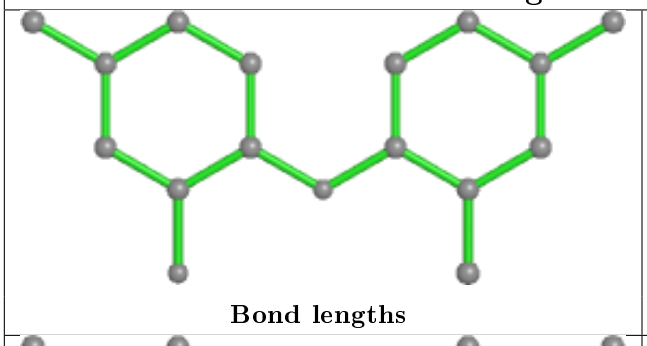


Torsions



Rings

Ligand TCL H 301



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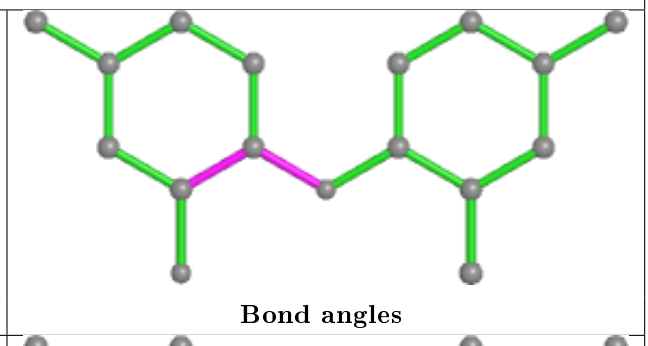

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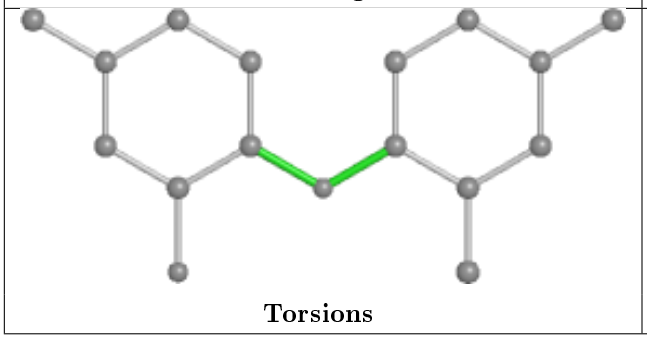
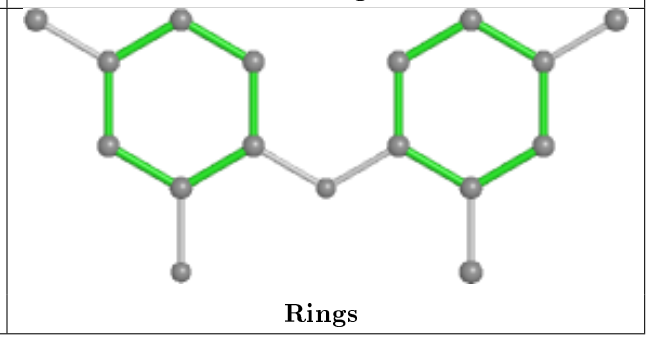
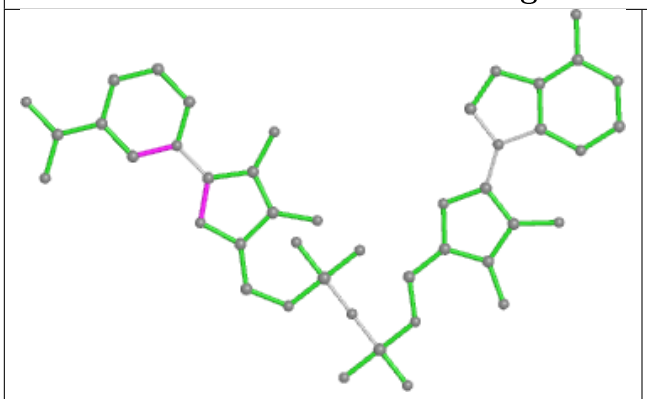


Torsions



Rings

Ligand NAD D 302



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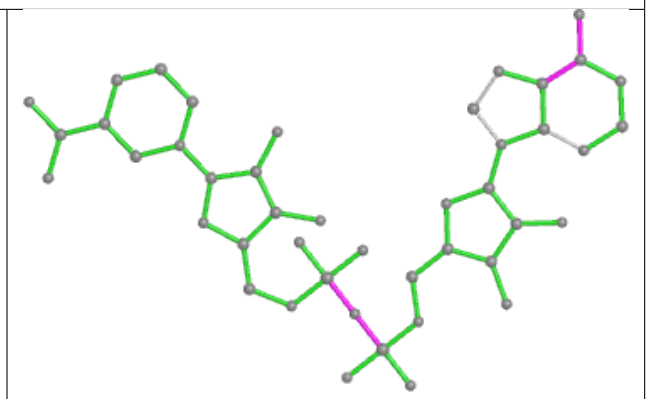

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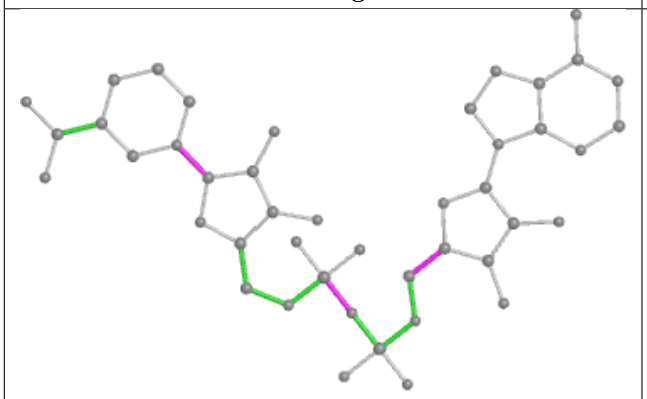

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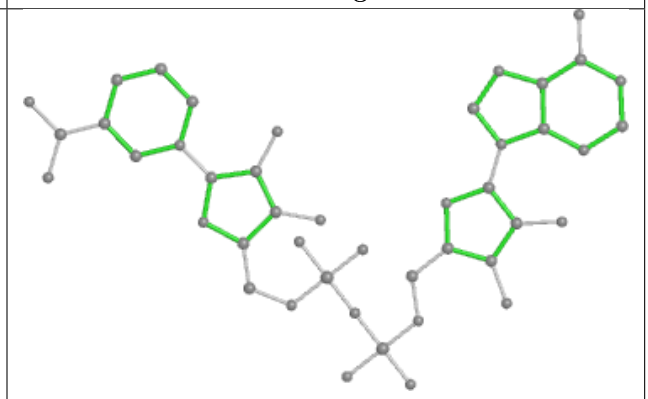
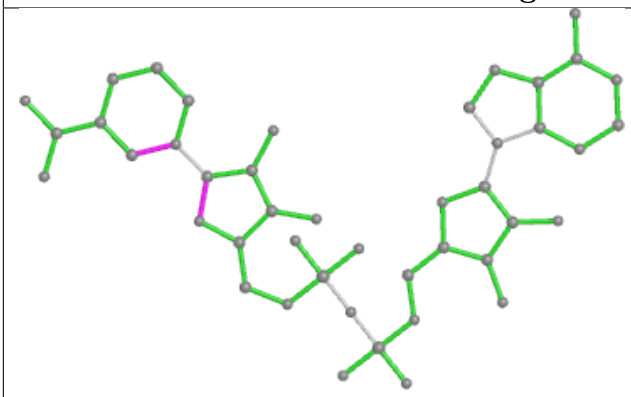


Rings

Ligand NAD H 302



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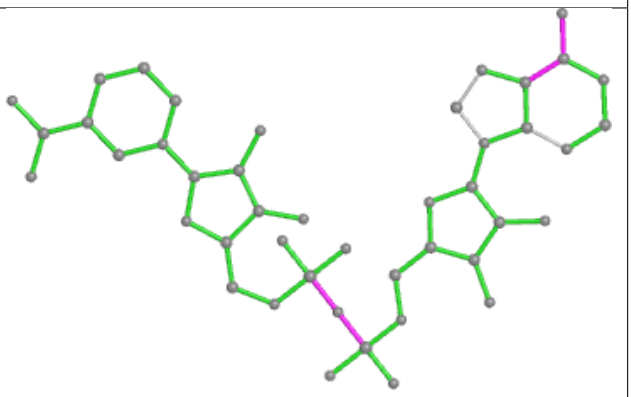

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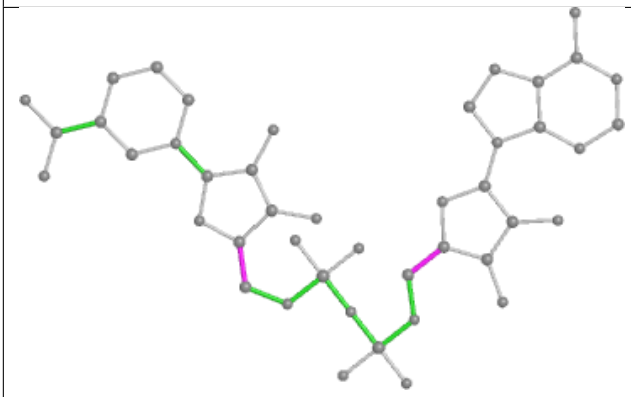

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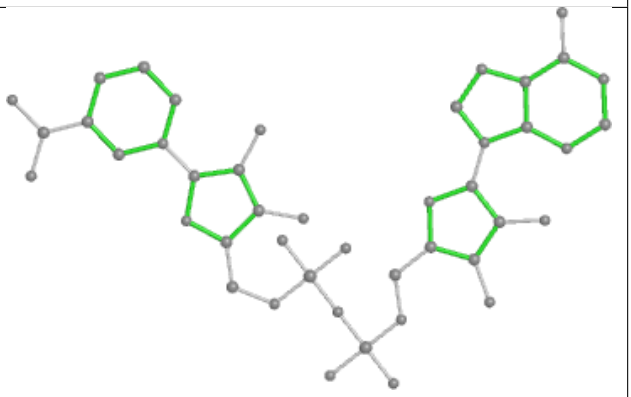
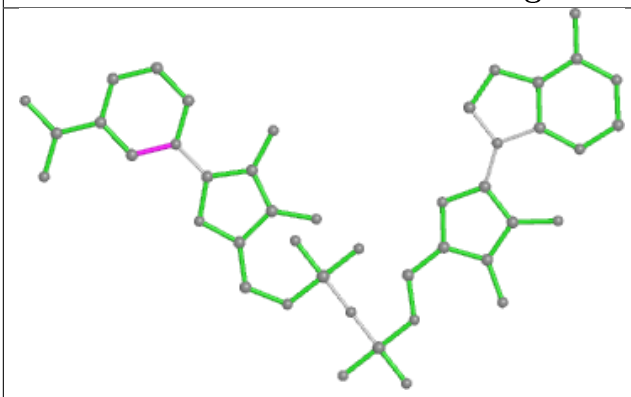


Rings

Ligand NAD J 302



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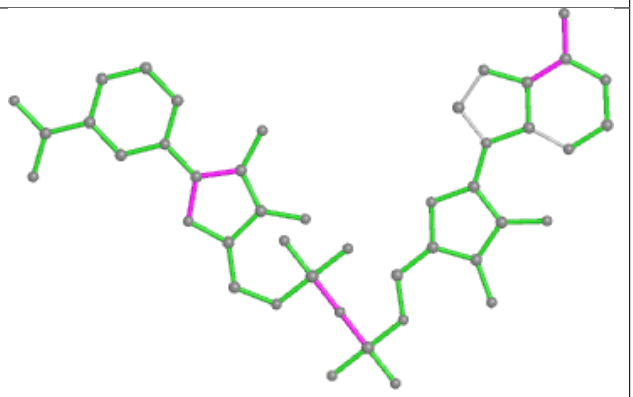
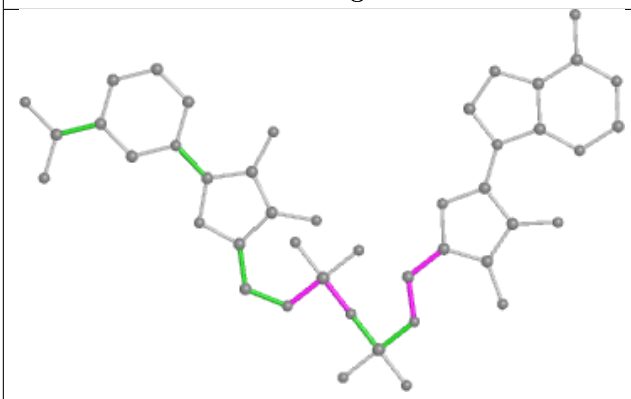


Bond angles



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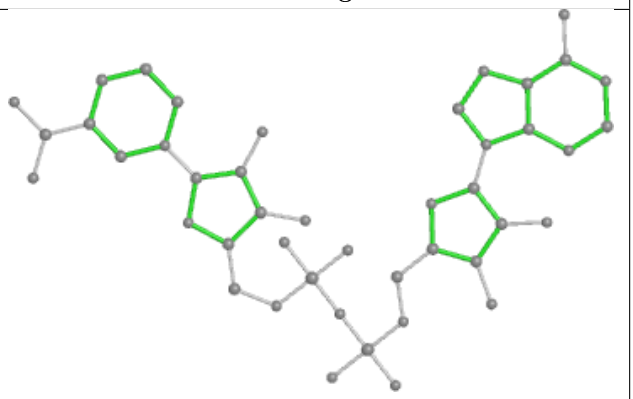
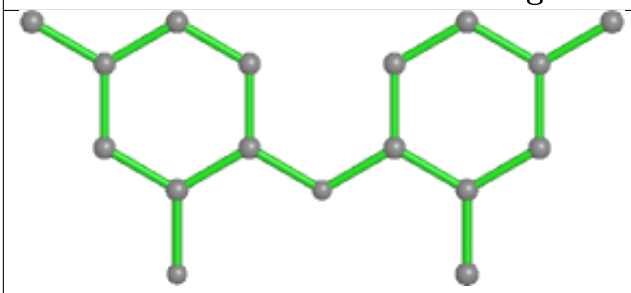


Rings

Ligand TCL P 301



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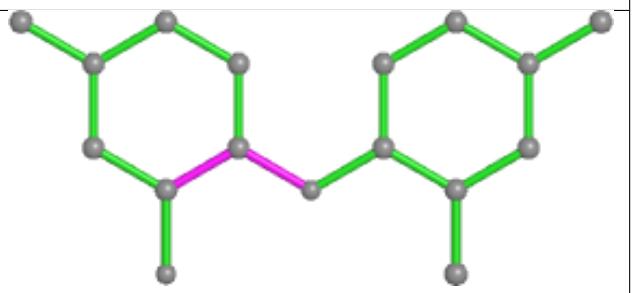

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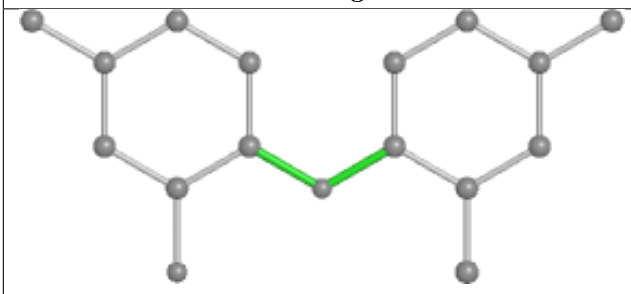

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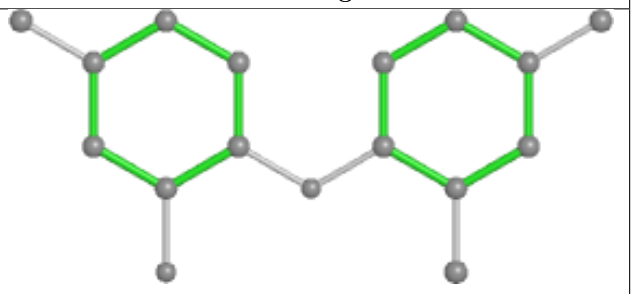
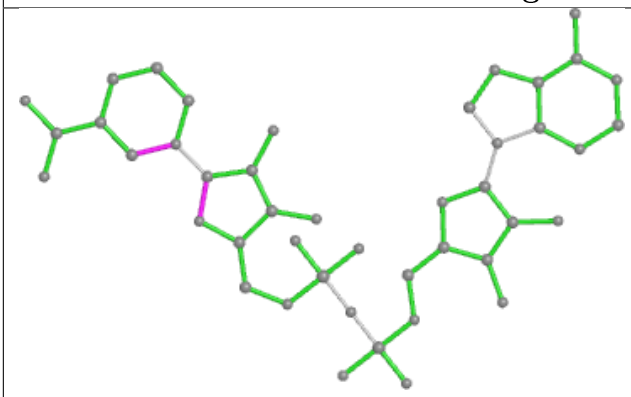


Rings

Ligand NAD L 302



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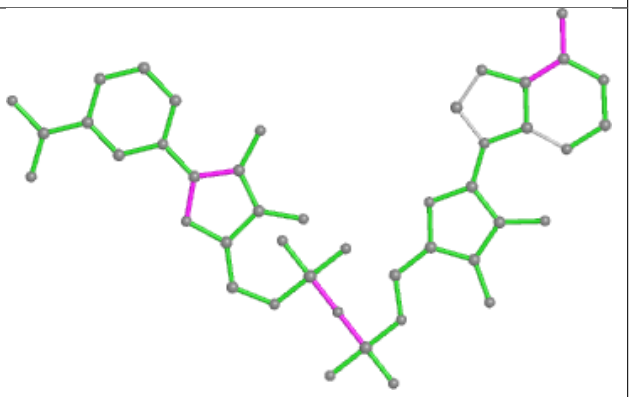

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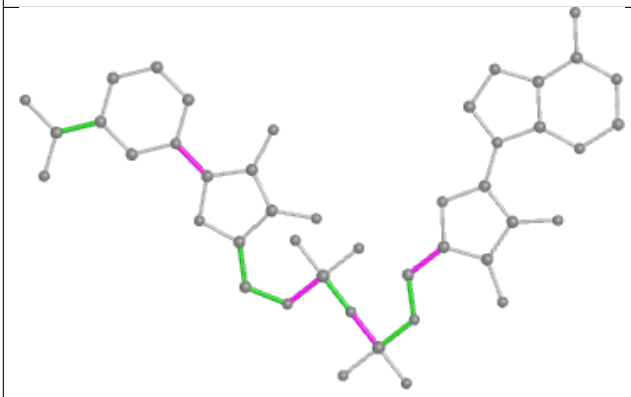

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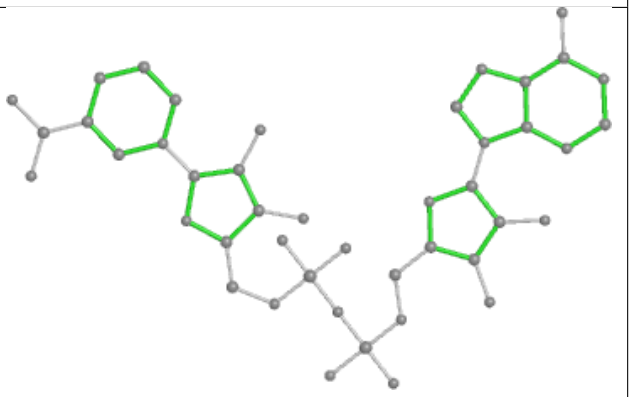
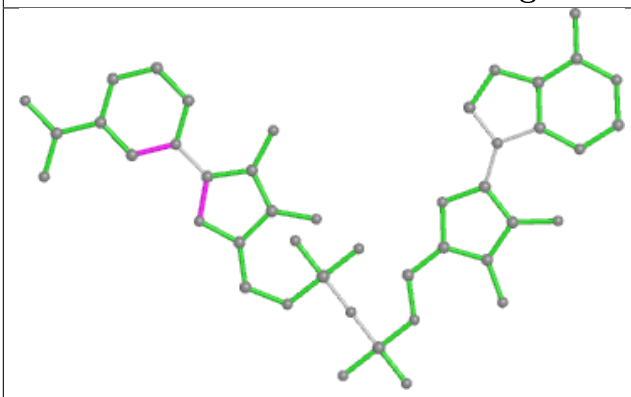


Rings

Ligand NAD A 302



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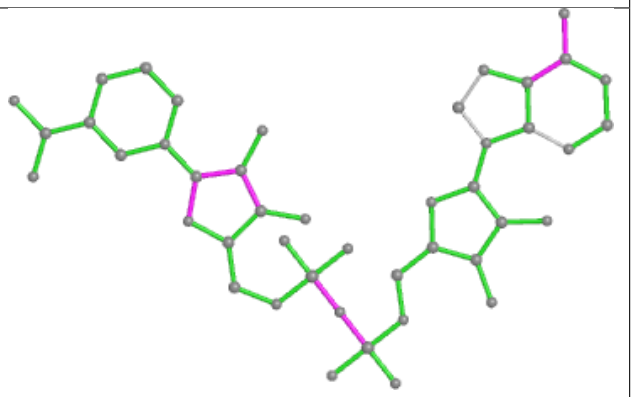

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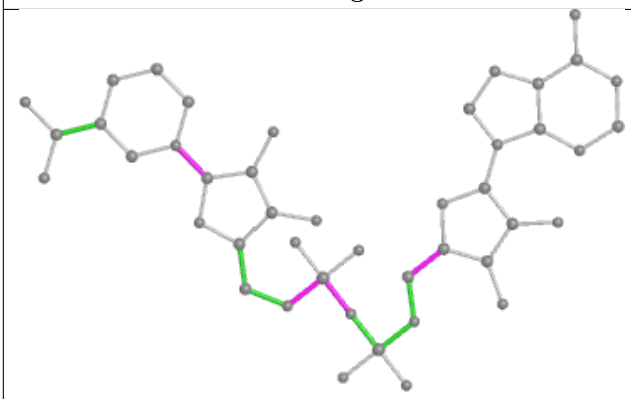

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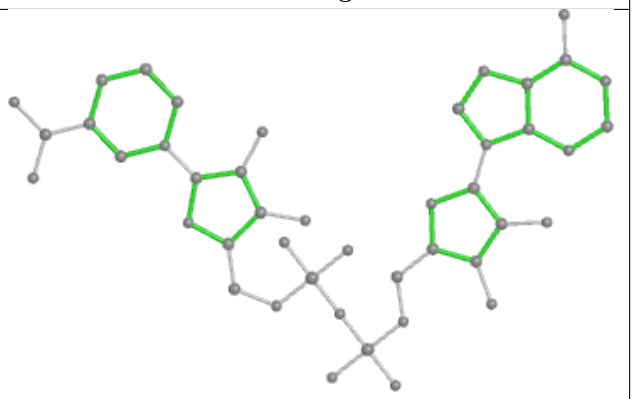
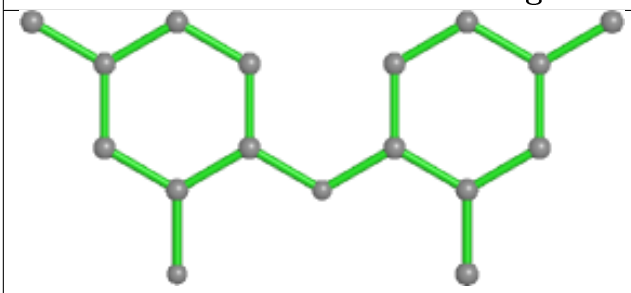


Rings

Ligand TCL A 301



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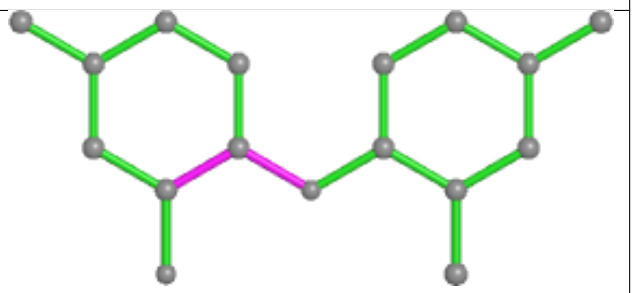

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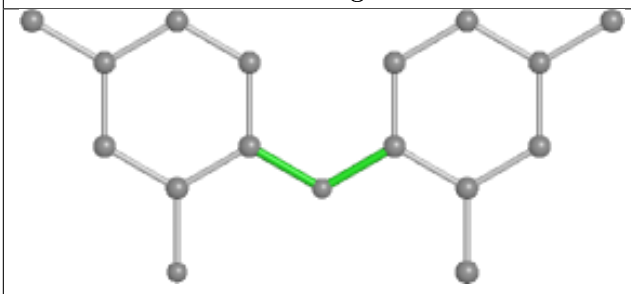

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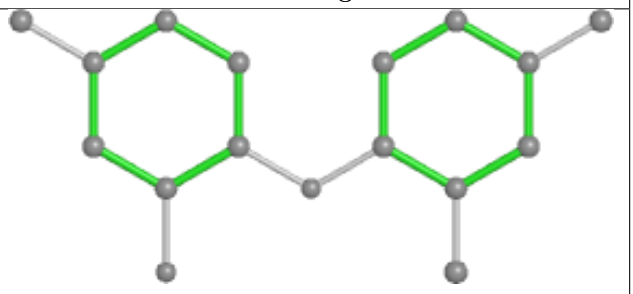
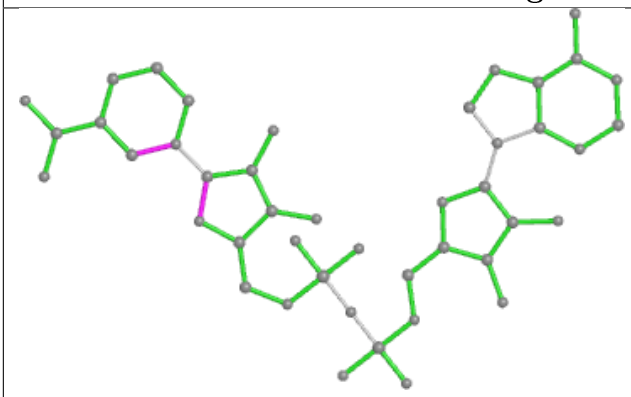


Rings

Ligand NAD I 302



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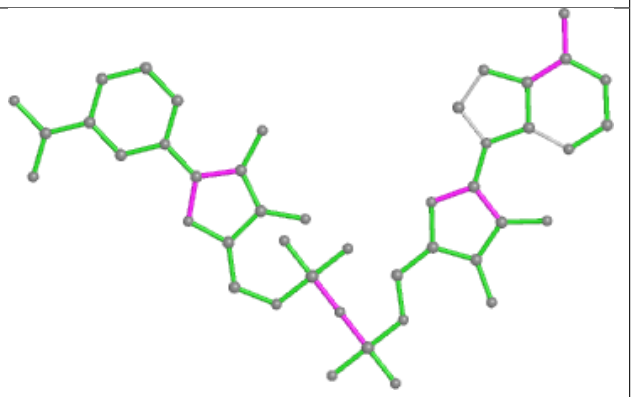

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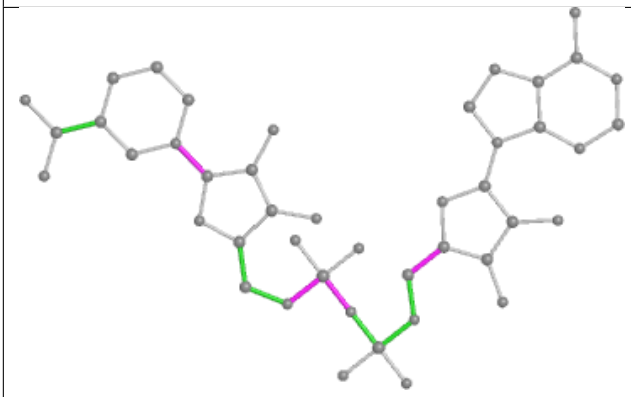

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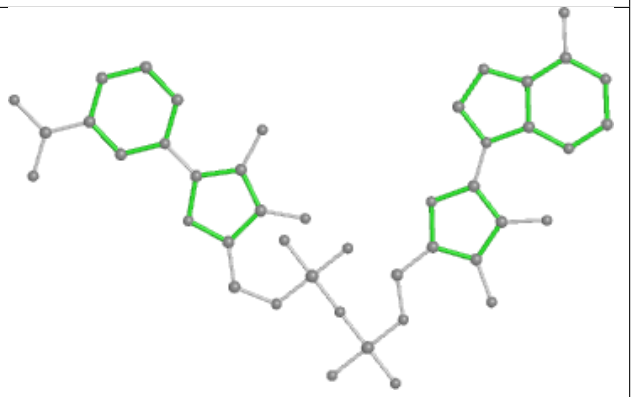
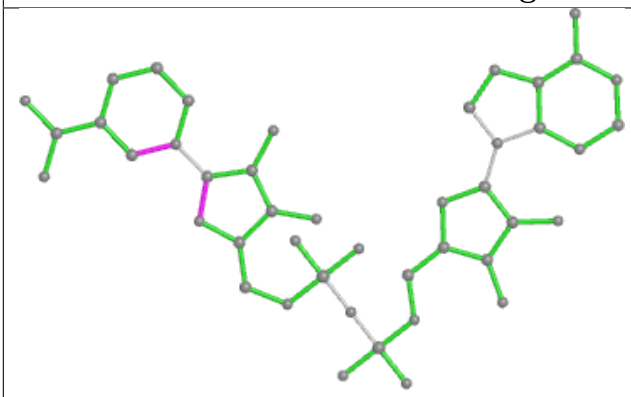


Rings

Ligand NAD K 302



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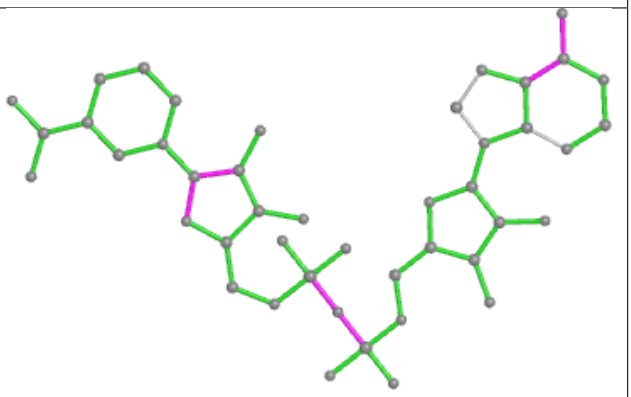

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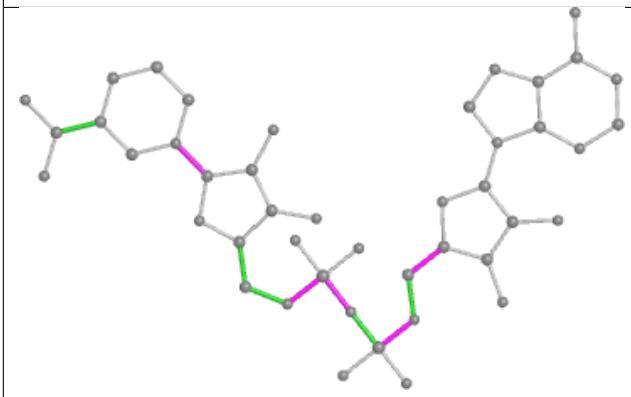

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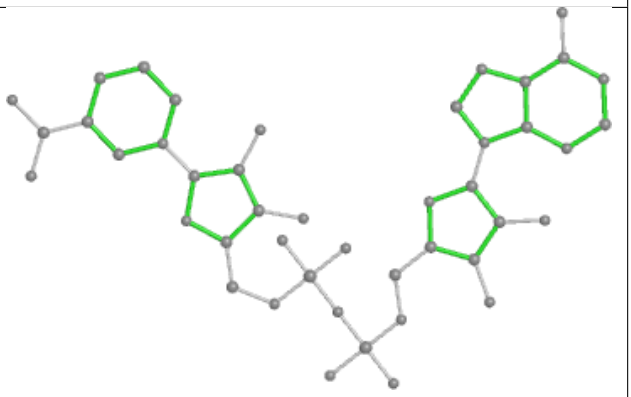
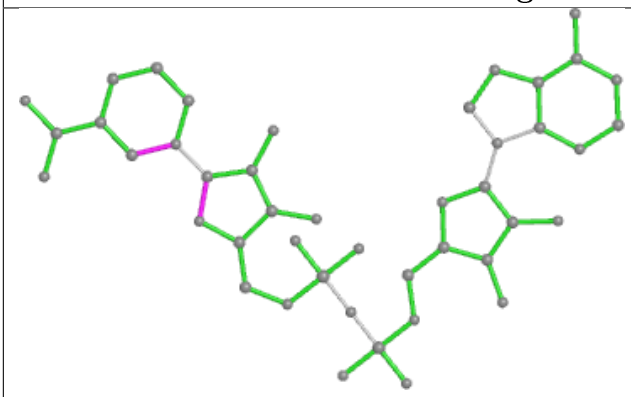


Rings

Ligand NAD M 302



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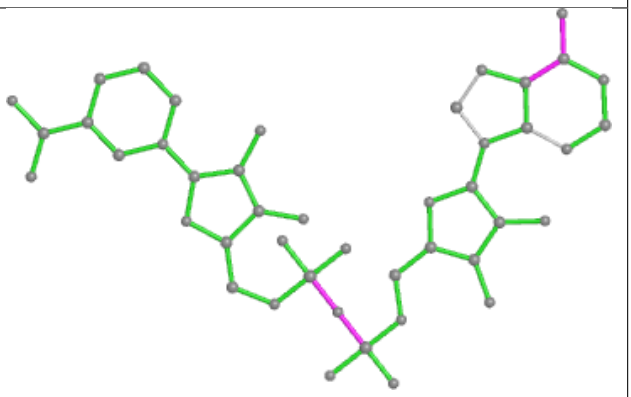

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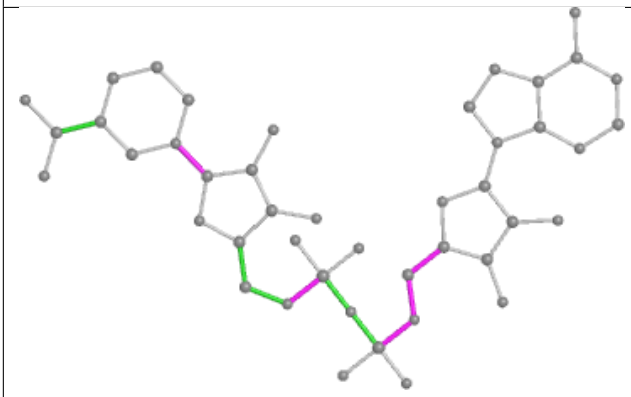

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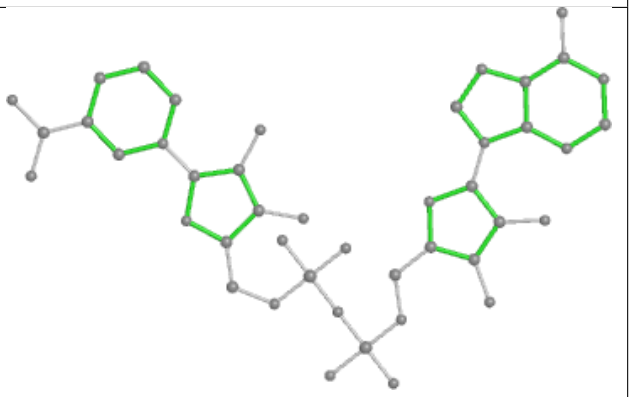
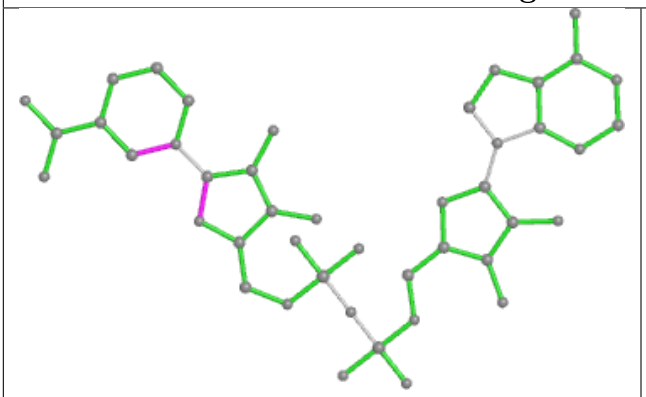


Rings

Ligand NAD N 302



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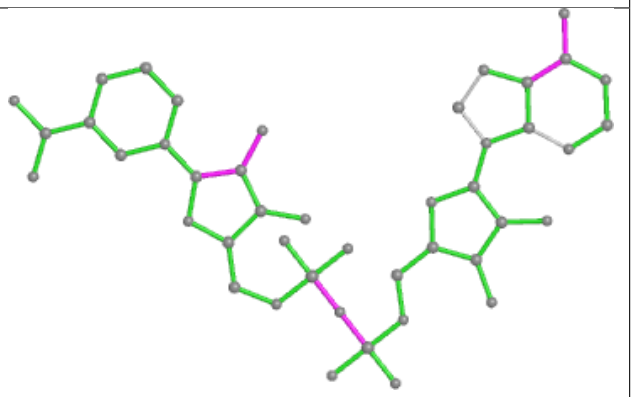

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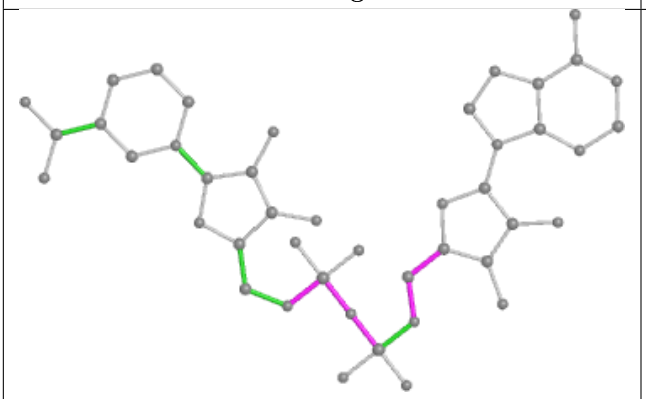

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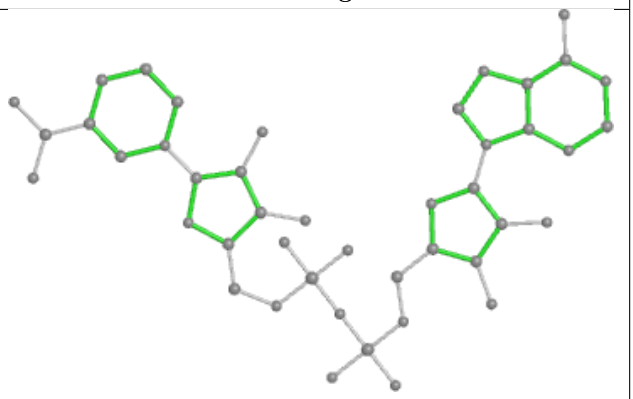
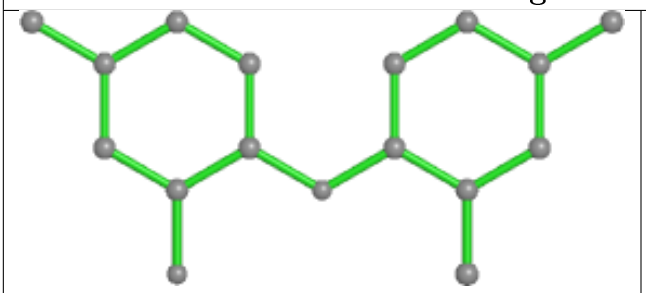


Rings

Ligand TCL J 301



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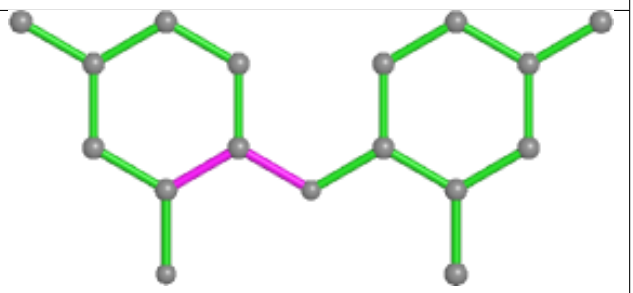
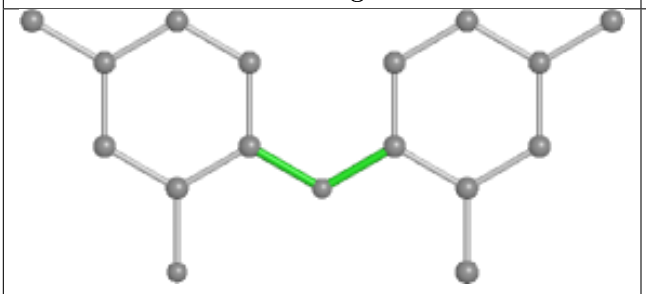


Bond angles



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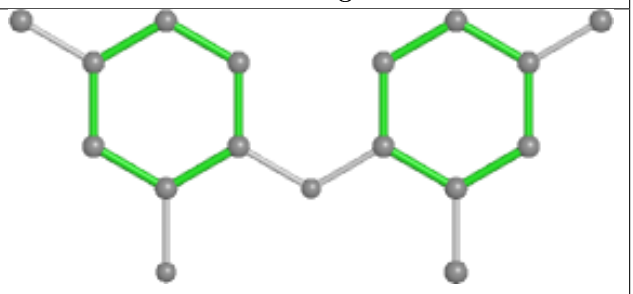
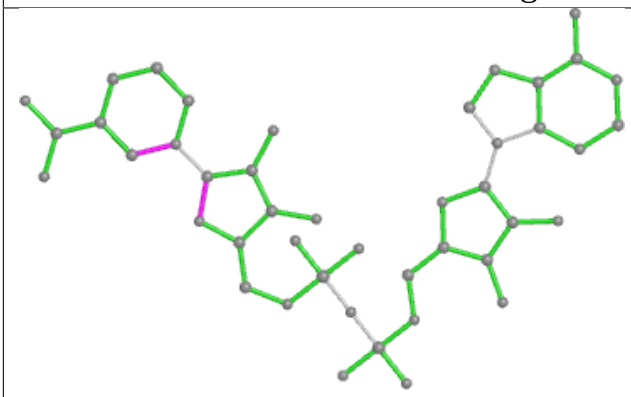
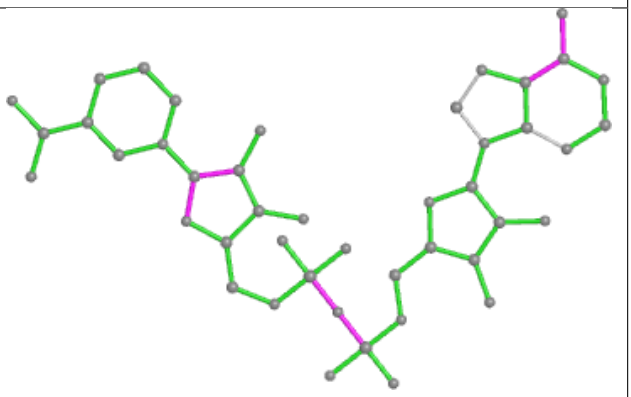


Rings

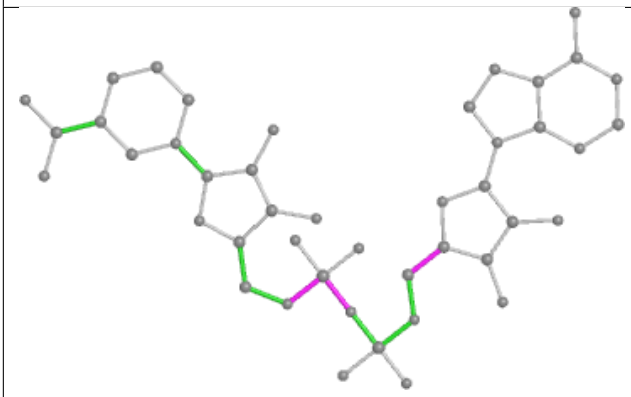
Ligand NAD C 302



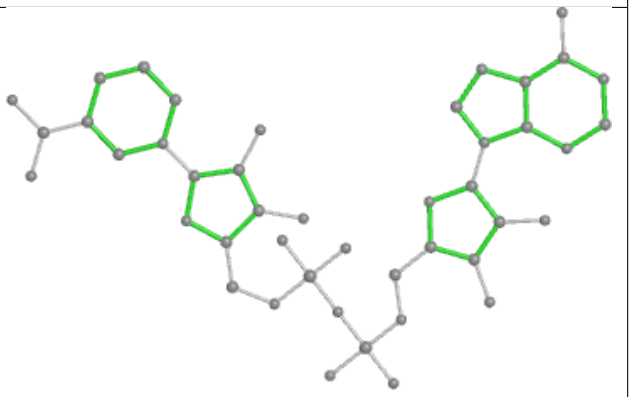
Bond lengths



Bond angles

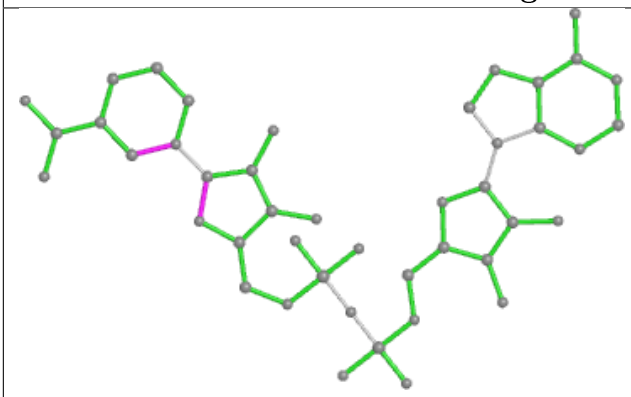


Torsions

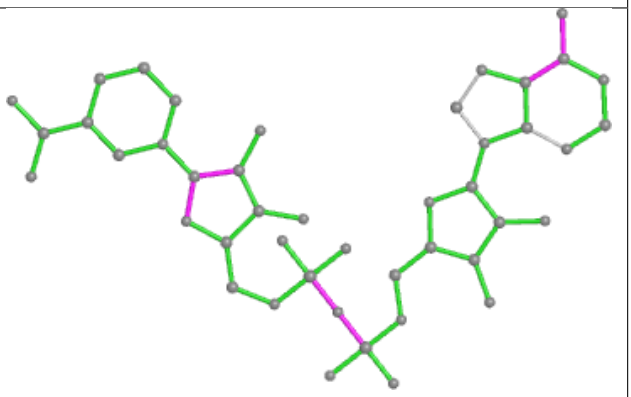


Rings

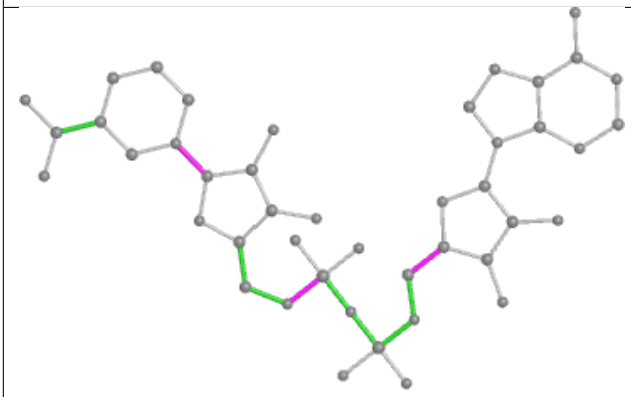
Ligand NAD B 302



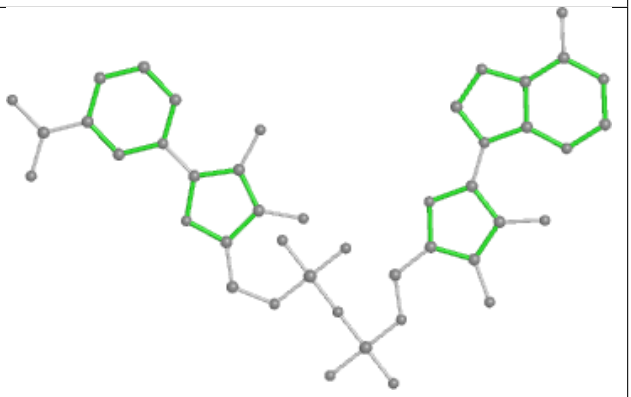
Bond lengths



Bond angles

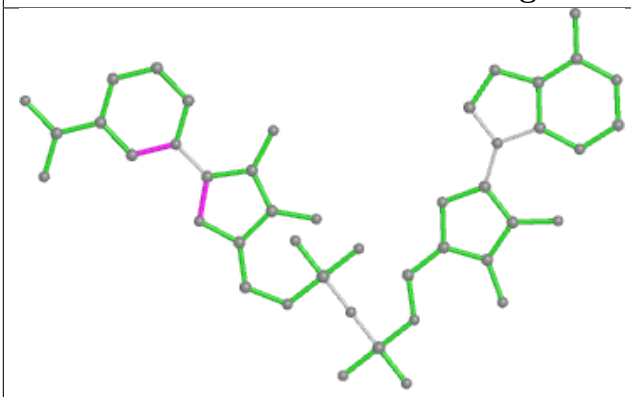


Torsions

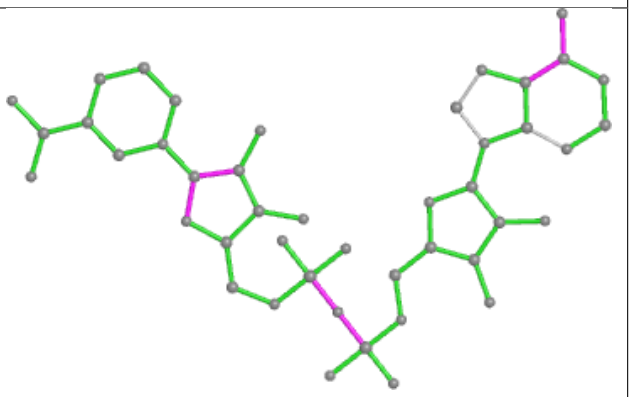


Rings

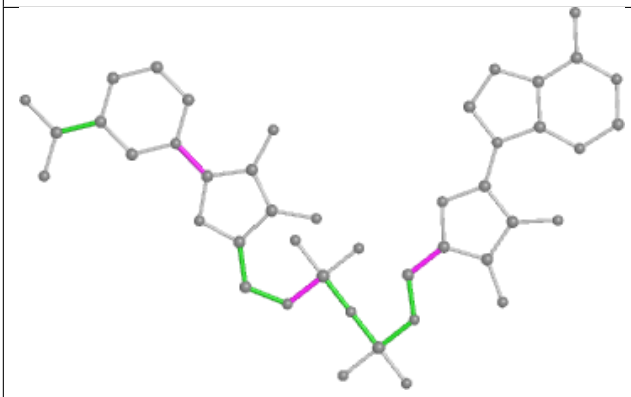
Ligand NAD G 302



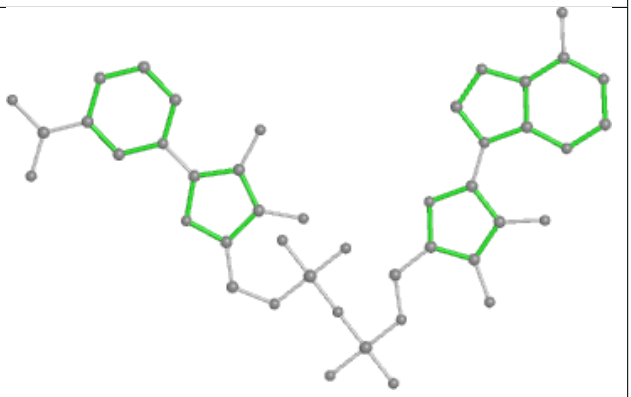
Bond lengths



Bond angles

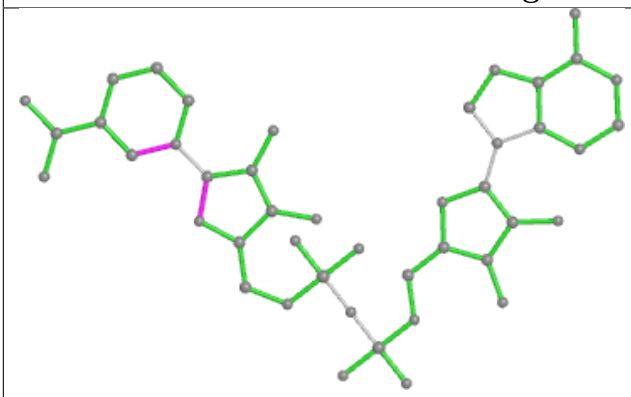


Torsions

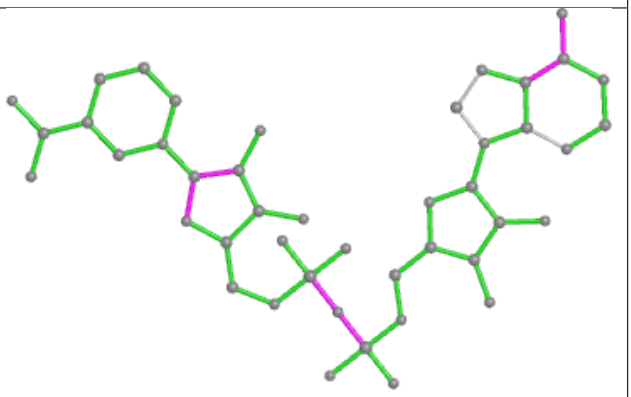


Rings

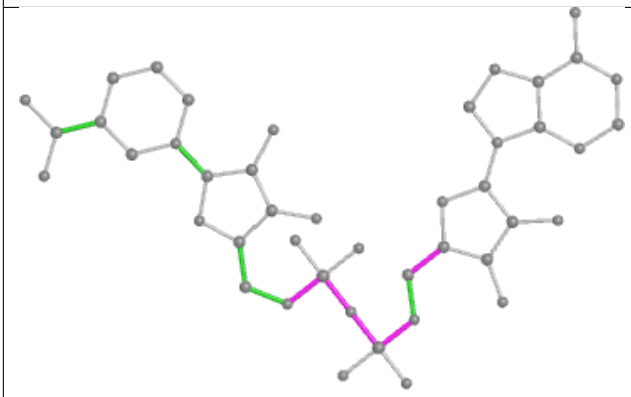
Ligand NAD F 302



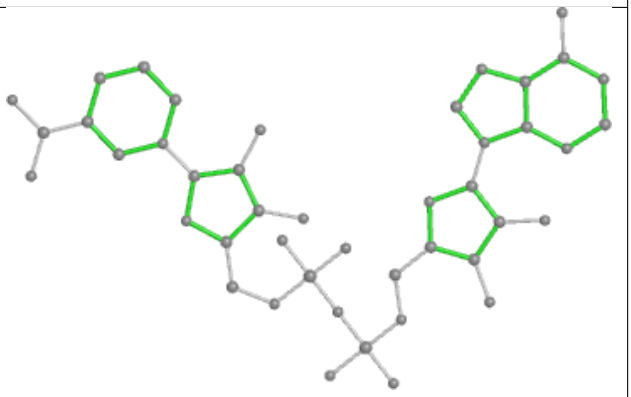
Bond lengths



Bond angles

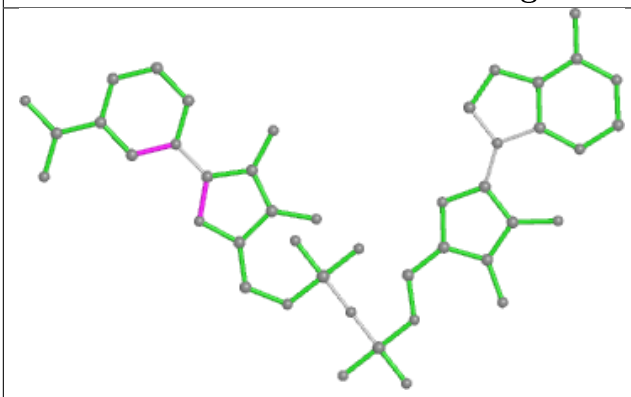


Torsions

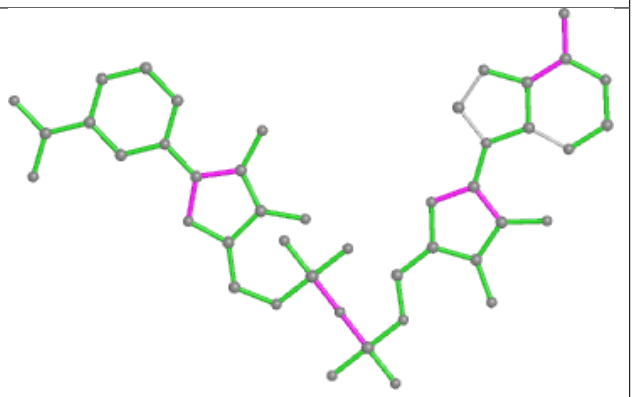


Rings

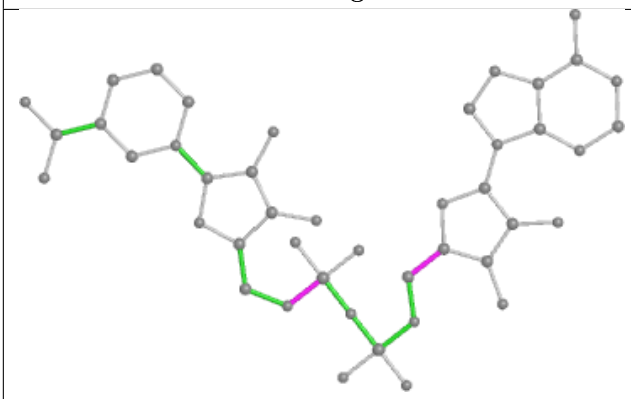
Ligand NAD O 302



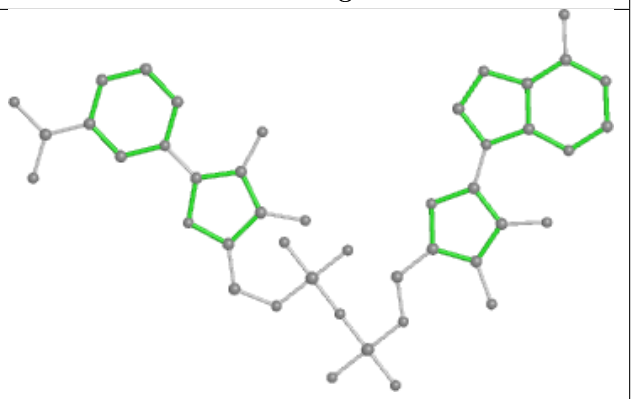
Bond lengths



Bond angles

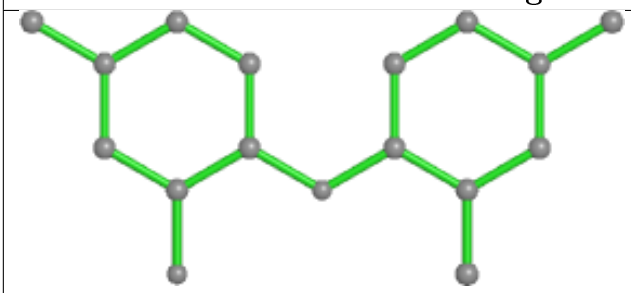


Torsions

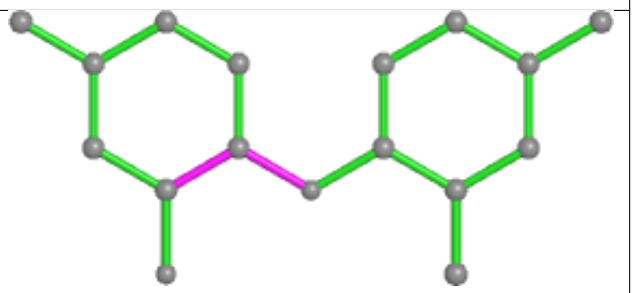


Rings

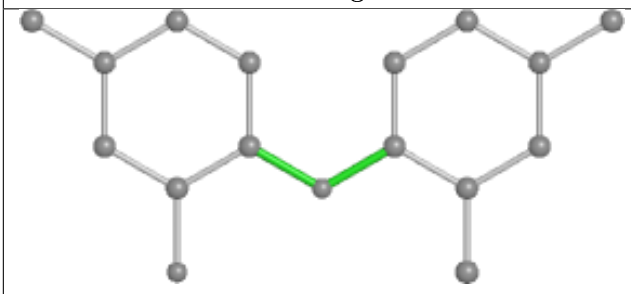
Ligand TCL O 301



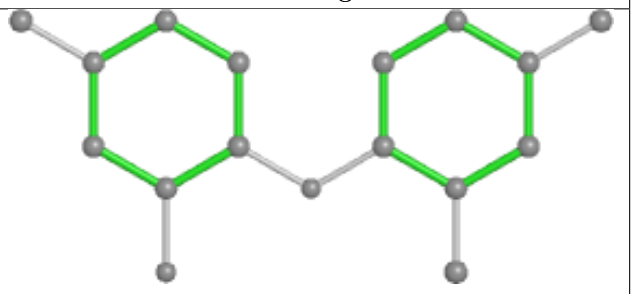
Bond lengths



Bond angles

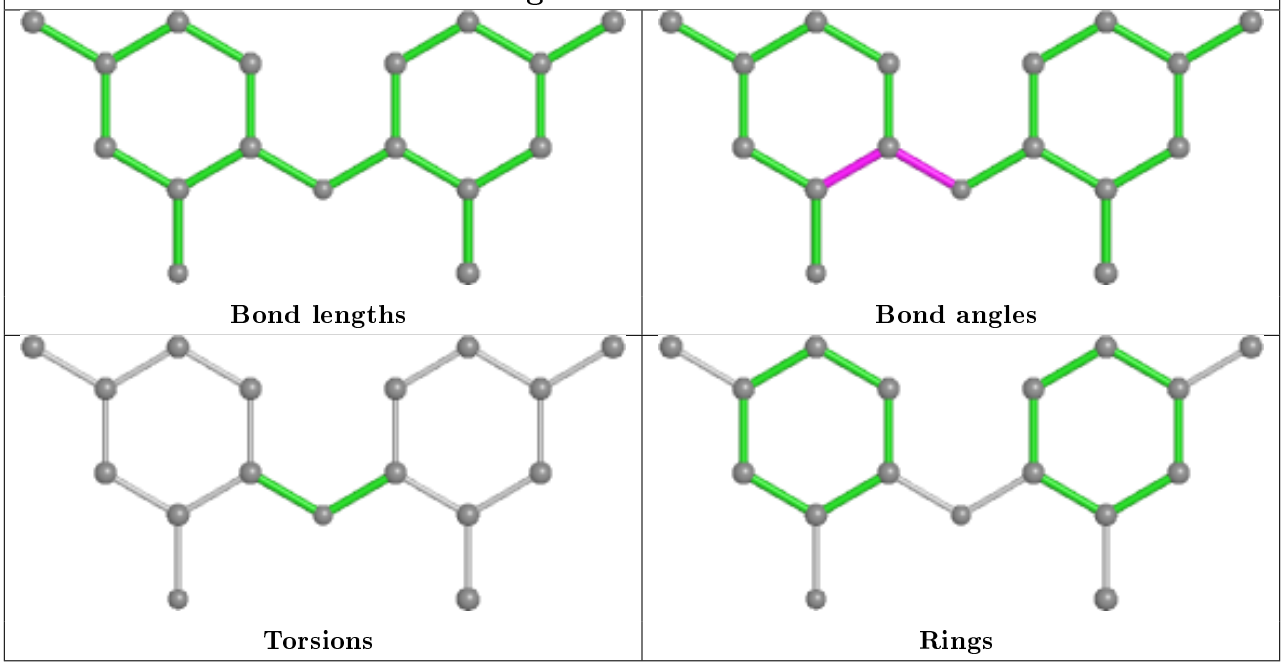


Torsions

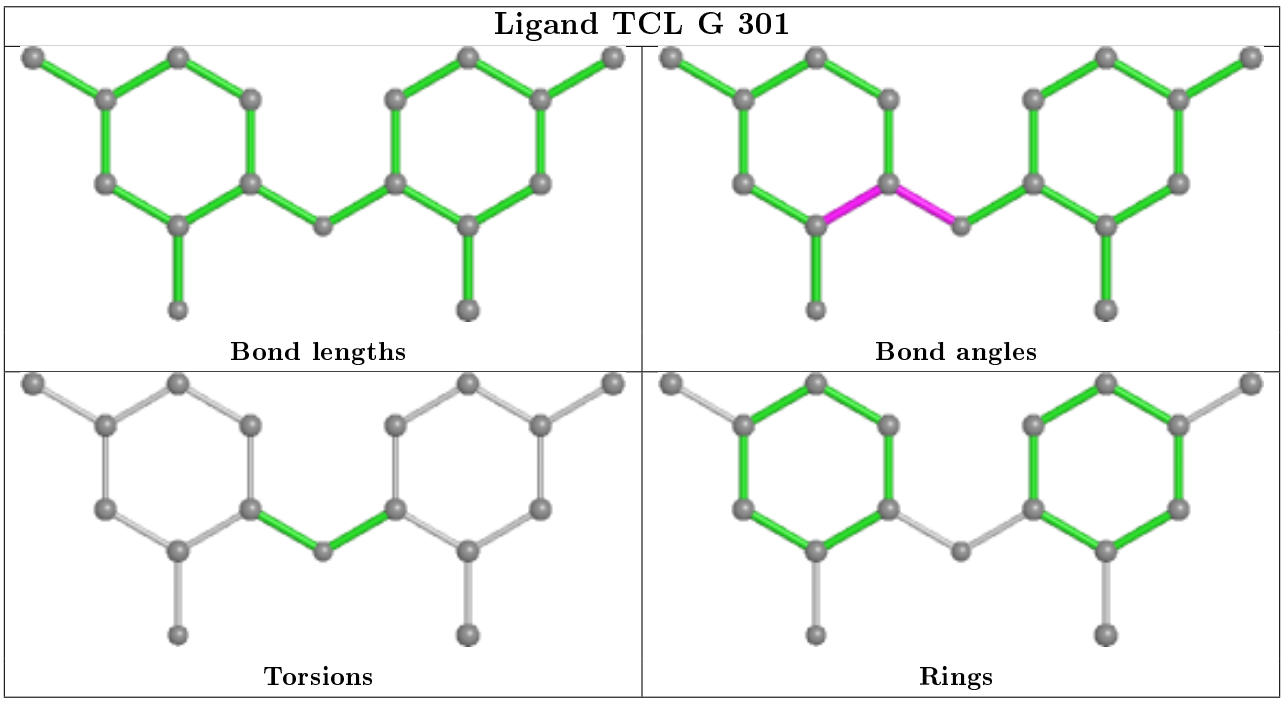


Rings

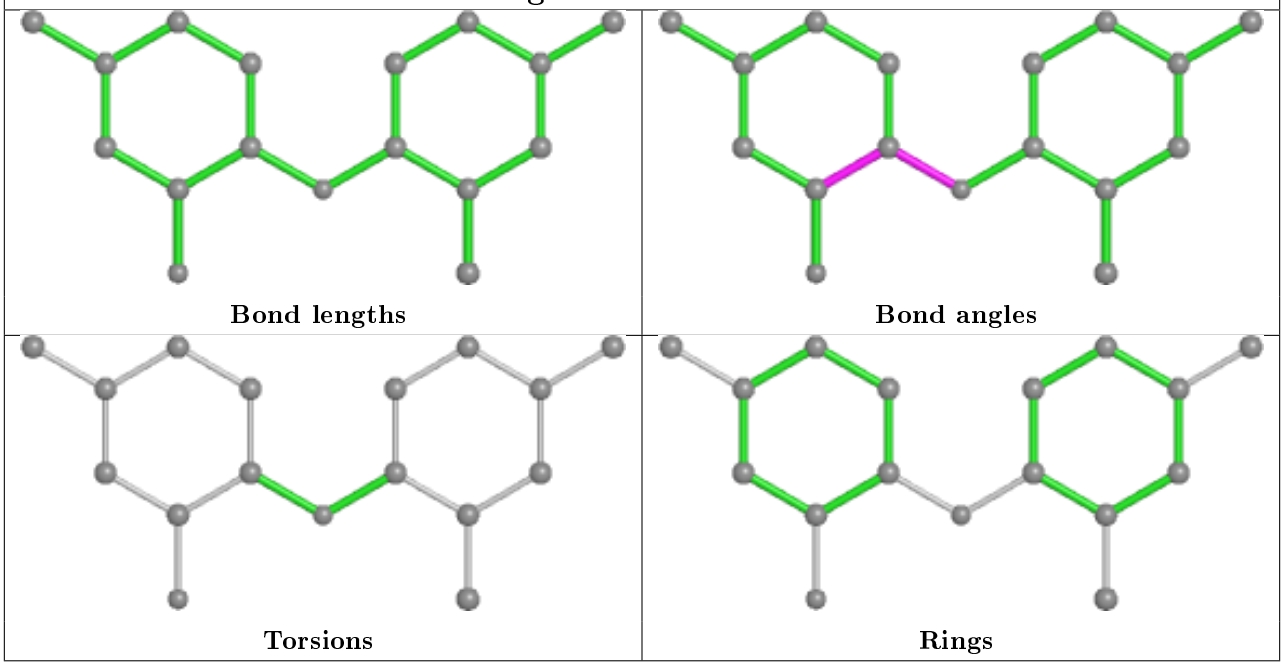
Ligand TCL B 301



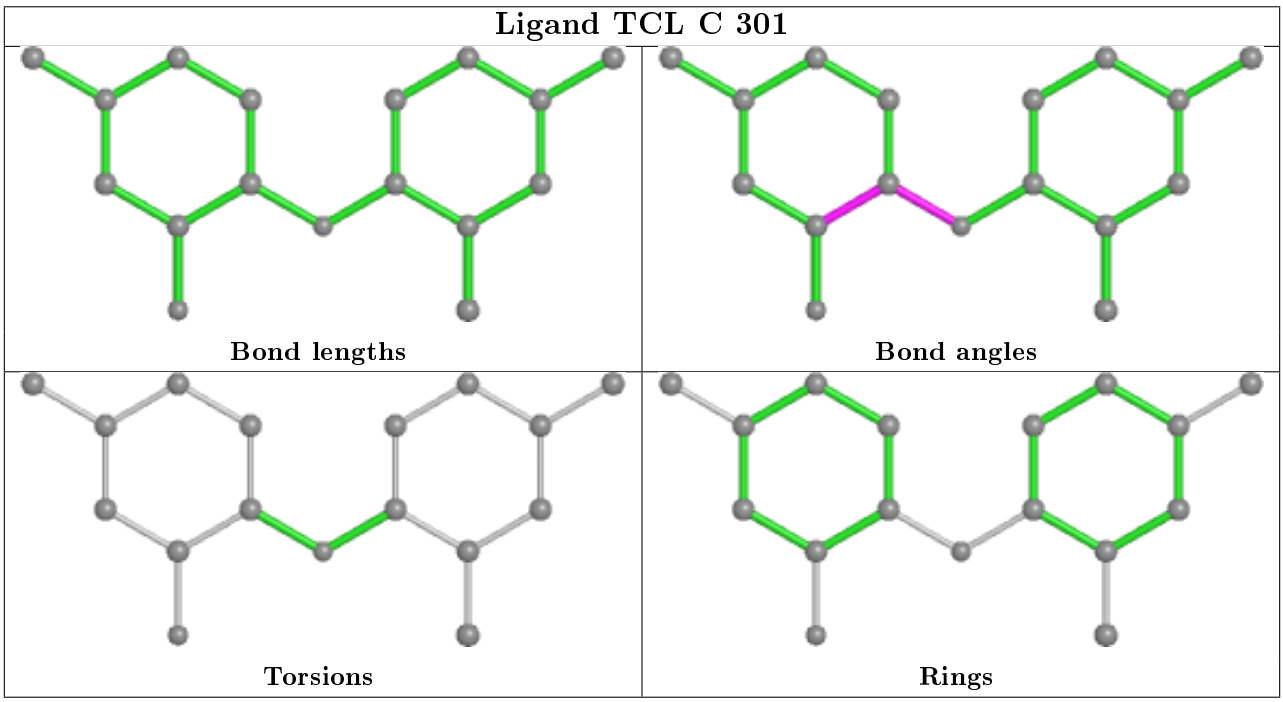
Ligand TCL G 301



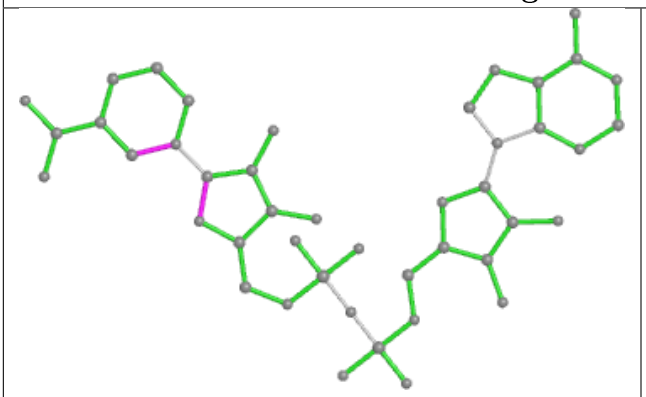
Ligand TCL E 301



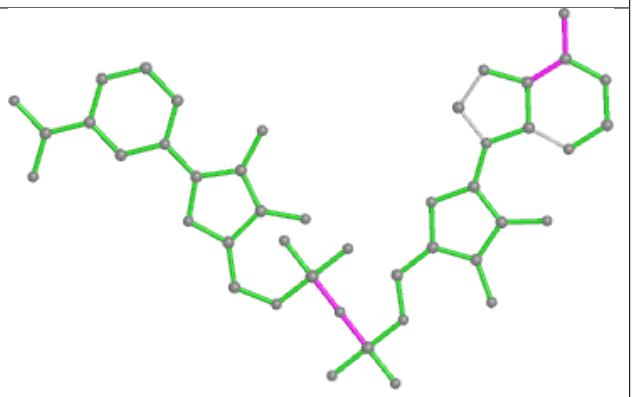
Ligand TCL C 301



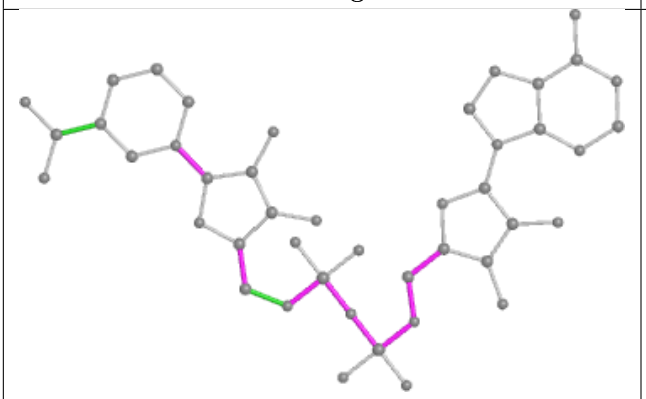
Ligand NAD P 302



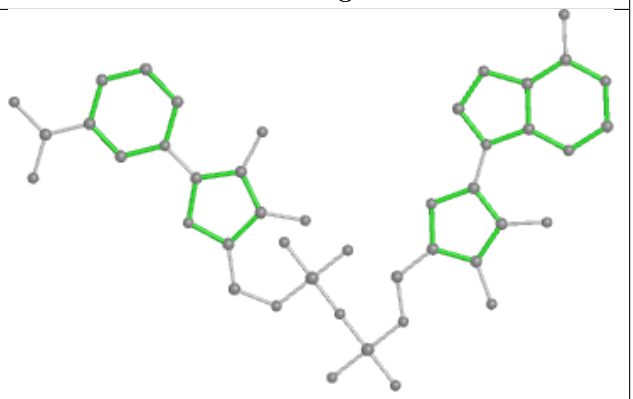
Bond lengths



Bond angles

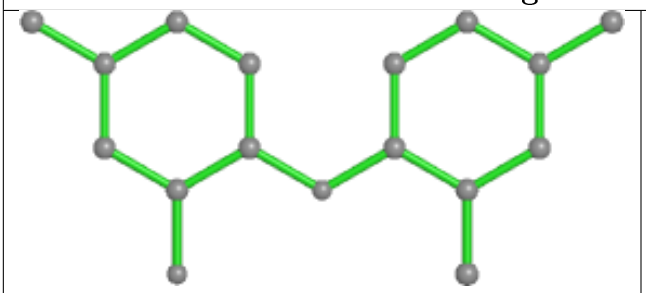


Torsions

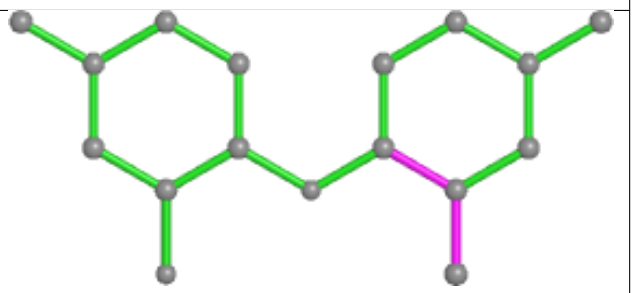


Rings

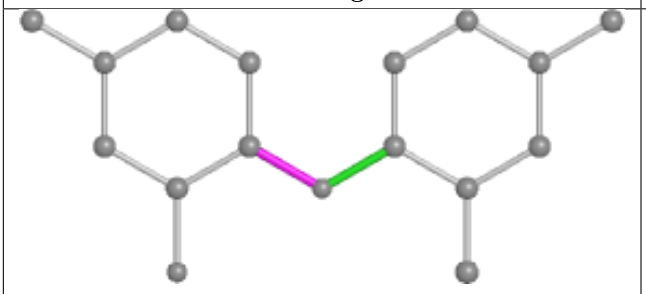
Ligand TCL M 301



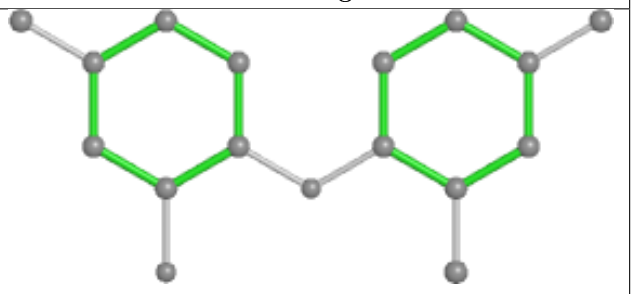
Bond lengths



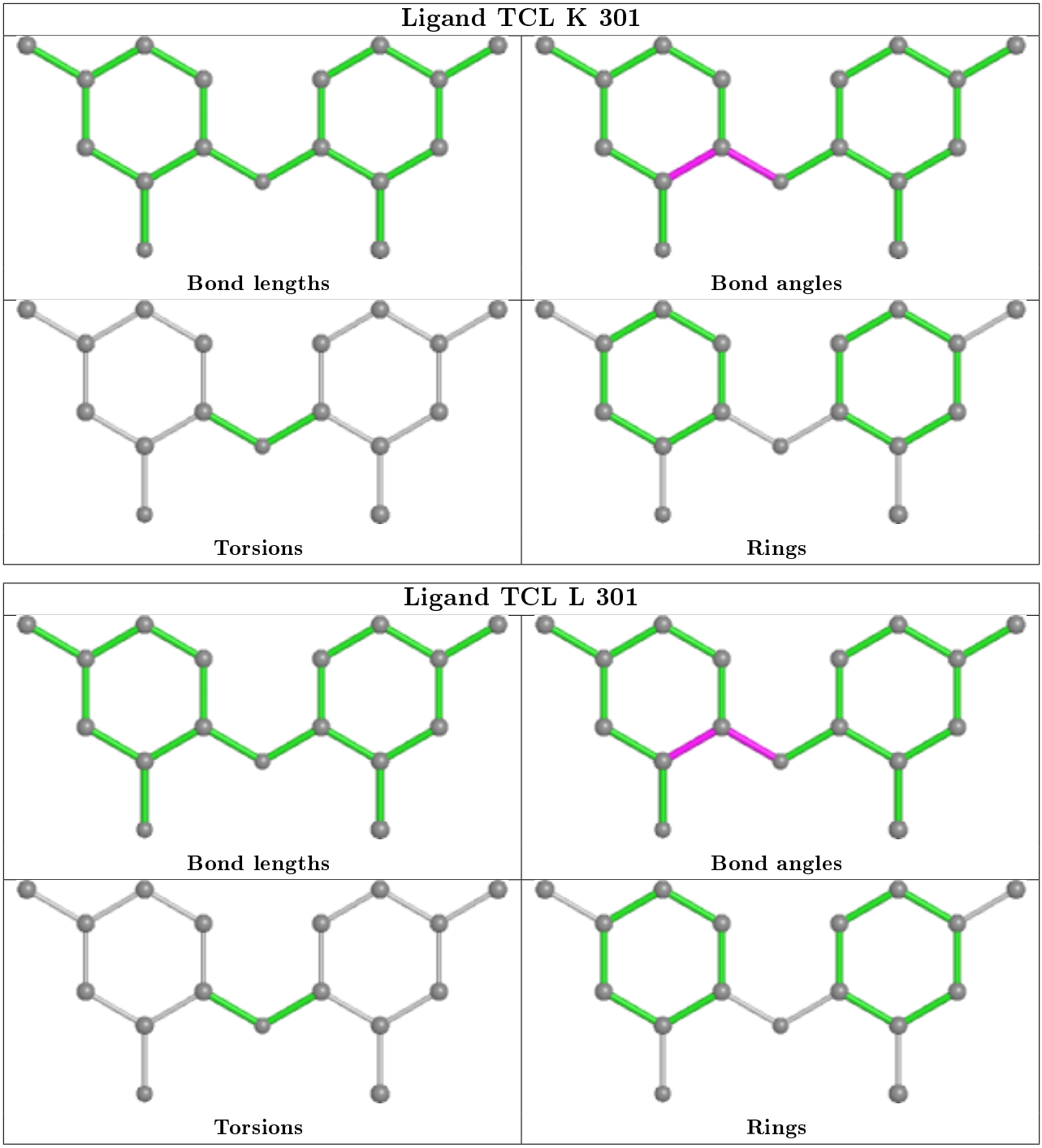
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	255/276 (92%)	-0.18	1 (0%) 92 91	28, 43, 76, 111	0
1	B	255/276 (92%)	-0.19	2 (0%) 86 84	30, 40, 59, 93	0
1	C	255/276 (92%)	0.08	6 (2%) 59 53	32, 49, 90, 132	0
1	D	255/276 (92%)	-0.16	1 (0%) 92 91	29, 47, 88, 128	0
1	E	255/276 (92%)	-0.12	0 100 100	37, 48, 74, 122	0
1	F	255/276 (92%)	0.08	7 (2%) 54 48	36, 52, 96, 123	0
1	G	255/276 (92%)	-0.14	2 (0%) 86 84	36, 49, 75, 133	0
1	H	255/276 (92%)	0.08	7 (2%) 54 48	39, 54, 94, 139	0
1	I	255/276 (92%)	0.24	9 (3%) 44 36	29, 55, 103, 148	0
1	J	255/276 (92%)	0.32	15 (5%) 22 17	31, 55, 103, 154	0
1	K	255/276 (92%)	-0.11	2 (0%) 86 84	29, 44, 73, 134	0
1	L	255/276 (92%)	-0.03	3 (1%) 79 76	31, 50, 87, 111	0
1	M	255/276 (92%)	1.32	66 (25%) 0 0	47, 82, 135, 165	0
1	N	255/276 (92%)	1.06	50 (19%) 1 0	48, 70, 114, 152	0
1	O	255/276 (92%)	0.33	12 (4%) 31 25	39, 57, 90, 121	0
1	P	255/276 (92%)	1.15	46 (18%) 1 0	46, 80, 128, 193	0
All	All	4080/4416 (92%)	0.23	229 (5%) 24 19	28, 53, 103, 193	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	5	ASP	9.0
1	M	88	LEU	7.2
1	P	200	ILE	6.9
1	M	181	GLY	6.9
1	J	97	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
1	M	45	LYS	6.7
1	M	42	ASP	6.7
1	N	102	GLY	6.3
1	J	41	GLY	5.5
1	J	200	ILE	5.5
1	M	6	GLY	5.4
1	O	240	VAL	5.4
1	M	2	GLY	5.4
1	M	139	ALA	5.4
1	N	40	VAL	5.4
1	P	145	SER	5.3
1	M	4	LEU	5.3
1	M	199	GLY	5.1
1	P	198	SER	5.0
1	M	44	PHE	4.9
1	M	37	PHE	4.8
1	P	43	ARG	4.7
1	I	59	LEU	4.7
1	P	195	LEU	4.5
1	P	203	PHE	4.5
1	M	182	VAL	4.4
1	P	15	LEU	4.4
1	M	80	THR	4.3
1	P	206	ILE	4.3
1	M	62	PRO	4.2
1	N	95	ALA	4.2
1	N	36	ALA	4.1
1	M	40	VAL	4.1
1	N	105	LEU	4.1
1	N	73	ALA	4.0
1	P	156	TYR	4.0
1	N	20	ILE	4.0
1	N	201	LYS	4.0
1	N	117	HIS	4.0
1	H	193	LYS	3.9
1	M	33	ALA	3.9
1	M	141	LEU	3.8
1	N	24	ILE	3.8
1	C	46	ASP	3.8
1	P	219	ASN	3.8
1	M	82	TRP	3.8
1	P	153	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	N	104	PHE	3.8
1	N	43	ARG	3.7
1	N	223	GLU	3.7
1	N	10	LEU	3.7
1	P	41	GLY	3.6
1	J	199	GLY	3.6
1	J	78	LEU	3.6
1	M	78	LEU	3.5
1	P	207	LEU	3.5
1	J	42	ASP	3.5
1	M	172	TYR	3.5
1	N	214	SER	3.5
1	M	127	LEU	3.5
1	N	220	VAL	3.5
1	I	15	LEU	3.4
1	M	134	MET	3.4
1	M	126	ALA	3.4
1	H	201	LYS	3.4
1	N	41	GLY	3.4
1	N	198	SER	3.4
1	F	108	LEU	3.4
1	M	118	ASP	3.3
1	N	42	ASP	3.3
1	N	200	ILE	3.3
1	M	230	ALA	3.3
1	J	47	ARG	3.3
1	C	42	ASP	3.3
1	M	232	LEU	3.3
1	P	202	SER	3.3
1	P	146	TYR	3.3
1	J	201	LYS	3.3
1	L	200	ILE	3.2
1	P	249	SER	3.2
1	K	43	ARG	3.2
1	P	59	LEU	3.2
1	P	147	LEU	3.2
1	M	11	LEU	3.2
1	P	217	LYS	3.2
1	I	39	TYR	3.1
1	M	73	ALA	3.1
1	N	12	THR	3.1
1	M	56	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	40	VAL	3.1
1	M	86	ASP	3.1
1	N	210	VAL	3.1
1	O	172	TYR	3.0
1	C	41	GLY	3.0
1	N	251	PHE	3.0
1	N	88	LEU	3.0
1	H	199	GLY	3.0
1	F	193	LYS	3.0
1	O	43	ARG	3.0
1	M	101	ALA	3.0
1	M	92	ILE	3.0
1	L	97	ARG	3.0
1	N	22	TYR	3.0
1	M	122	TYR	2.9
1	M	133	PRO	2.9
1	O	61	PHE	2.9
1	M	242	ALA	2.9
1	M	74	LEU	2.9
1	M	189	ALA	2.9
1	B	43	ARG	2.9
1	P	225	VAL	2.8
1	N	65	VAL	2.8
1	P	191	PRO	2.8
1	N	159	MET	2.8
1	P	190	GLY	2.8
1	M	179	ALA	2.7
1	N	68	ASP	2.7
1	M	238	SER	2.7
1	N	132	LEU	2.7
1	N	141	LEU	2.7
1	N	152	ALA	2.7
1	O	242	ALA	2.7
1	M	184	VAL	2.7
1	M	85	LEU	2.7
1	N	254	VAL	2.7
1	M	22	TYR	2.7
1	N	97	ARG	2.7
1	H	200	ILE	2.6
1	J	94	PHE	2.6
1	O	42	ASP	2.6
1	I	48	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	51	PHE	2.6
1	N	9	ILE	2.6
1	M	138	ASP	2.6
1	K	97	ARG	2.6
1	P	40	VAL	2.5
1	F	18	ARG	2.5
1	I	60	VAL	2.5
1	O	236	LEU	2.5
1	P	78	LEU	2.5
1	A	83	ASP	2.5
1	G	43	ARG	2.5
1	P	63	CYS	2.5
1	J	46	ASP	2.5
1	M	180	LYS	2.5
1	H	18	ARG	2.5
1	N	215	PRO	2.5
1	O	20	ILE	2.5
1	N	150	GLU	2.5
1	P	221	THR	2.5
1	P	187	ILE	2.5
1	N	28	CYS	2.5
1	N	205	LYS	2.4
1	C	83	ASP	2.4
1	F	97	ARG	2.4
1	O	237	ALA	2.4
1	N	145	SER	2.4
1	P	70	GLN	2.4
1	M	236	LEU	2.4
1	F	200	ILE	2.4
1	P	24	ILE	2.4
1	J	44	PHE	2.4
1	M	97	ARG	2.4
1	M	35	LEU	2.4
1	M	142	LEU	2.4
1	N	195	LEU	2.4
1	P	205	LYS	2.4
1	P	55	PHE	2.4
1	M	119	ILE	2.3
1	N	119	ILE	2.3
1	N	146	TYR	2.3
1	P	87	GLY	2.3
1	M	137	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	141	LEU	2.3
1	M	58	GLU	2.3
1	P	210	VAL	2.3
1	D	97	ARG	2.3
1	P	22	TYR	2.3
1	H	40	VAL	2.3
1	M	145	SER	2.3
1	J	92	ILE	2.3
1	M	136	SER	2.2
1	B	97	ARG	2.2
1	M	237	ALA	2.2
1	I	43	ARG	2.2
1	P	218	ARG	2.2
1	F	206	ILE	2.2
1	L	100	ILE	2.2
1	P	220	VAL	2.2
1	N	196	ALA	2.2
1	N	38	THR	2.2
1	N	113	PHE	2.2
1	P	213	ASN	2.2
1	I	51	PHE	2.2
1	N	55	PHE	2.2
1	M	240	VAL	2.2
1	P	212	SER	2.2
1	P	211	GLU	2.2
1	C	137	ASP	2.2
1	M	135	LEU	2.1
1	O	127	LEU	2.1
1	N	207	LEU	2.1
1	P	144	LEU	2.1
1	P	201	LYS	2.1
1	M	84	SER	2.1
1	N	115	ILE	2.1
1	J	128	ALA	2.1
1	G	3	PHE	2.1
1	O	77	SER	2.1
1	M	129	LYS	2.1
1	M	3	PHE	2.1
1	I	42	ASP	2.1
1	O	128	ALA	2.1
1	M	8	ARG	2.1
1	M	65	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	11	LEU	2.1
1	N	90	HIS	2.0
1	M	43	ARG	2.0
1	F	58	GLU	2.0
1	M	63	CYS	2.0
1	N	92	ILE	2.0
1	H	202	SER	2.0
1	M	140	SER	2.0
1	P	20	ILE	2.0
1	P	112	ASN	2.0
1	I	49	THR	2.0
1	C	44	PHE	2.0
1	J	43	ARG	2.0
1	M	34	GLU	2.0

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 carbohydrates 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, 95^{th} 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
2	TCL	M	301	17/17	0.65	0.26	77,134,158,181	0
2	TCL	J	301	17/17	0.85	0.25	80,86,104,133	0
3	NAD	M	302	44/44	0.85	0.24	83,110,137,144	0
2	TCL	P	301	17/17	0.86	0.22	64,85,116,170	0
2	TCL	F	301	17/17	0.90	0.18	67,73,87,88	0
3	NAD	P	302	44/44	0.91	0.16	47,69,94,112	0
3	NAD	N	302	44/44	0.91	0.19	55,78,102,120	0
2	TCL	K	301	17/17	0.91	0.24	36,52,94,107	0
2	TCL	D	301	17/17	0.92	0.17	30,60,91,106	0

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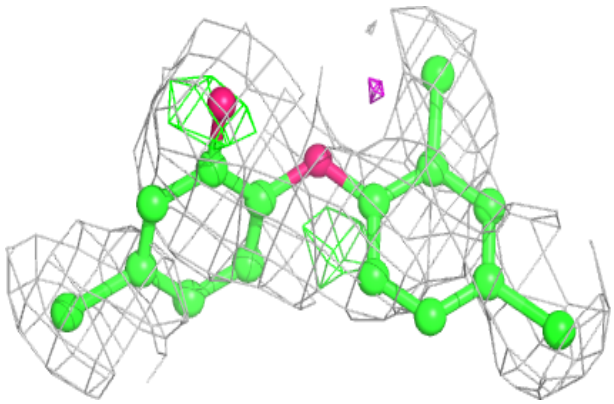
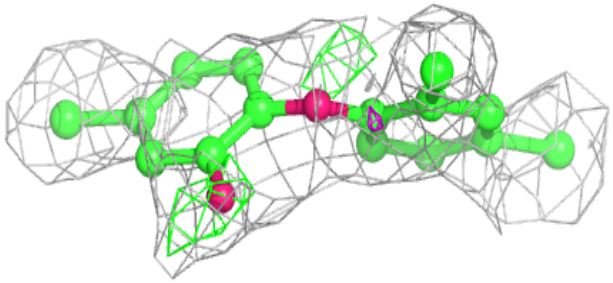
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TCL	L	301	17/17	0.92	0.18	41,55,72,84	0
3	NAD	F	302	44/44	0.93	0.14	31,59,76,92	0
2	TCL	N	301	17/17	0.94	0.19	56,68,74,127	0
2	TCL	H	301	17/17	0.94	0.17	44,57,67,221	0
3	NAD	H	302	44/44	0.94	0.16	42,66,90,103	0
2	TCL	I	301	17/17	0.94	0.23	42,53,80,90	0
3	NAD	J	302	44/44	0.94	0.19	33,53,70,97	0
2	TCL	G	301	17/17	0.94	0.16	38,48,67,78	0
3	NAD	O	302	44/44	0.95	0.17	39,51,72,80	0
2	TCL	O	301	17/17	0.95	0.15	39,46,88,98	0
2	TCL	B	301	17/17	0.95	0.17	31,46,68,117	0
3	NAD	L	302	44/44	0.95	0.16	34,48,64,77	0
3	NAD	I	302	44/44	0.95	0.17	38,51,66,79	0
3	NAD	A	302	44/44	0.96	0.15	29,40,62,74	0
2	TCL	A	301	17/17	0.96	0.15	30,38,82,122	0
3	NAD	C	302	44/44	0.96	0.13	33,47,70,90	0
3	NAD	D	302	44/44	0.96	0.13	27,39,66,90	0
2	TCL	E	301	17/17	0.96	0.17	38,49,79,82	0
2	TCL	C	301	17/17	0.96	0.15	33,55,74,95	0
3	NAD	E	302	44/44	0.97	0.16	38,46,62,74	0
3	NAD	B	302	44/44	0.97	0.14	31,38,51,61	0
3	NAD	G	302	44/44	0.97	0.14	37,48,60,68	0
3	NAD	K	302	44/44	0.97	0.14	30,38,60,67	0

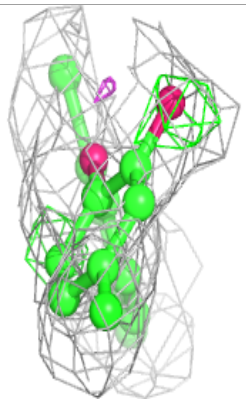
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TCL M 301:

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

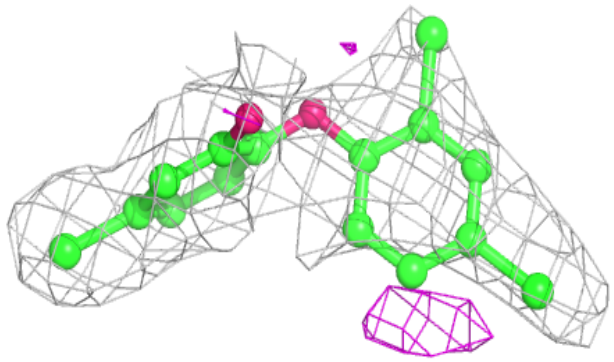


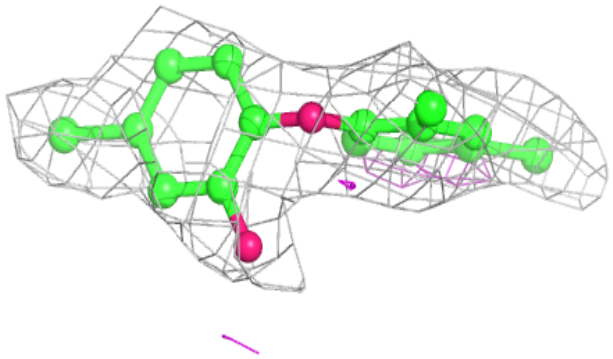


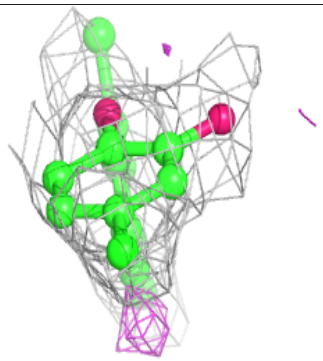


Electron density around TCL J 301:

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

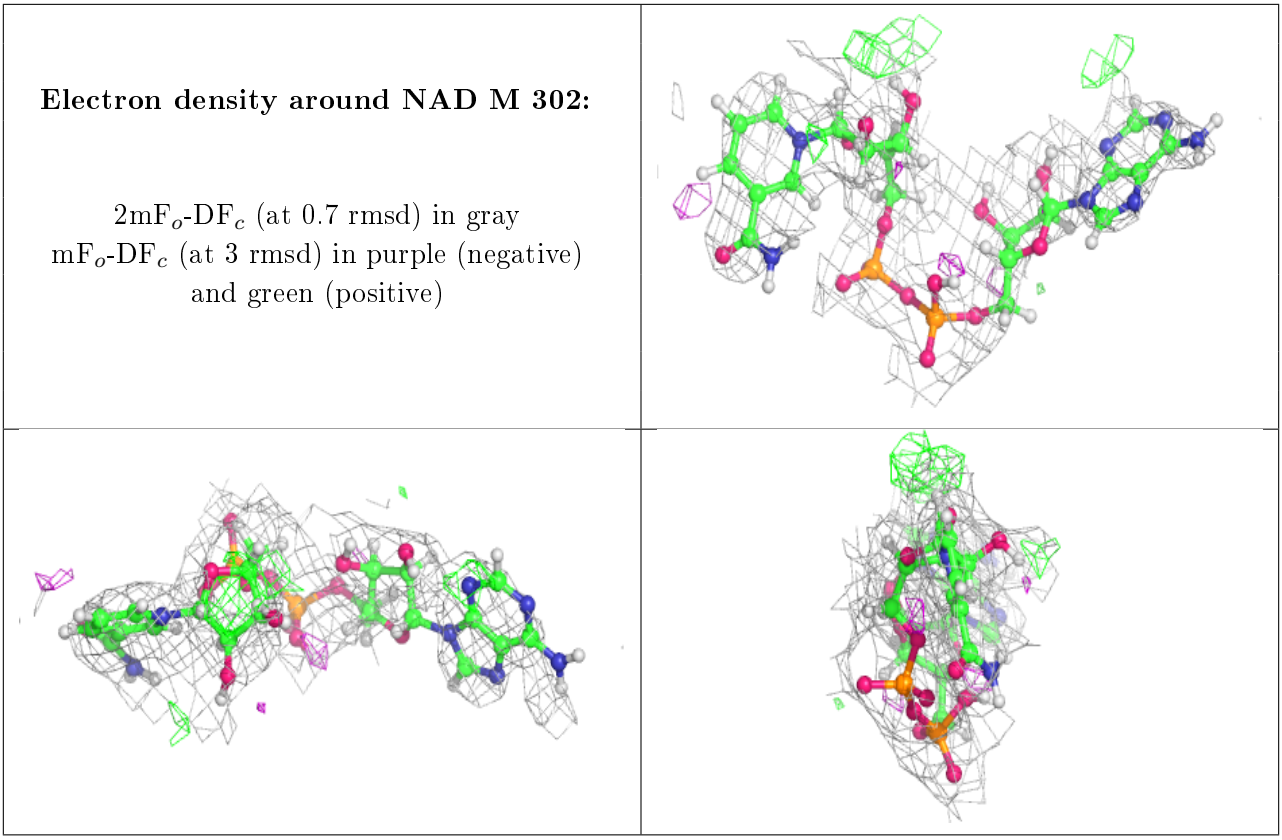






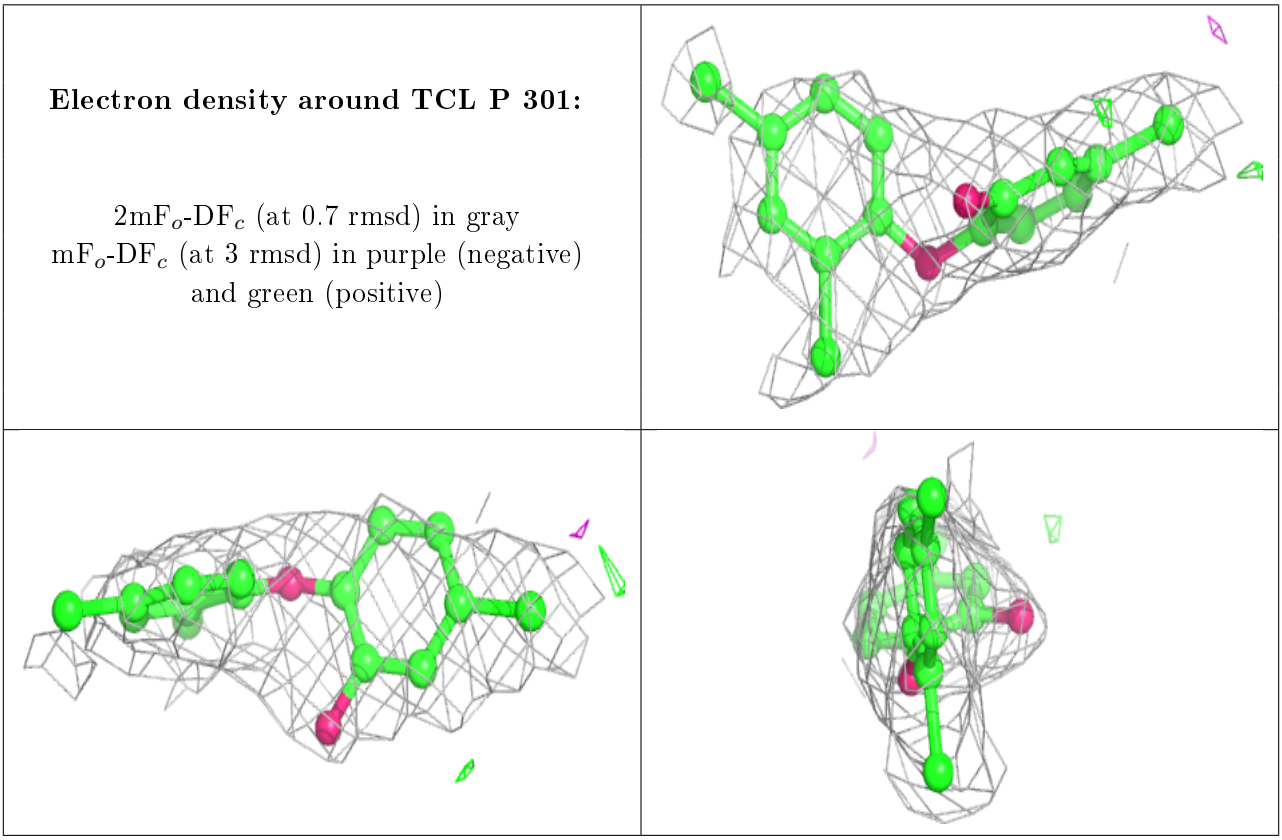
Electron density around NAD M 302:

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



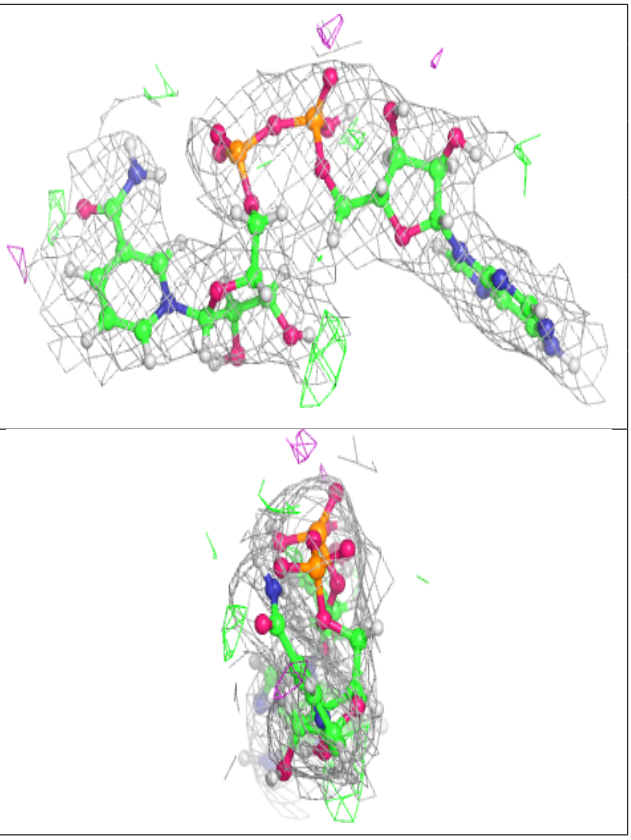
Electron density around TCL P 301:

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



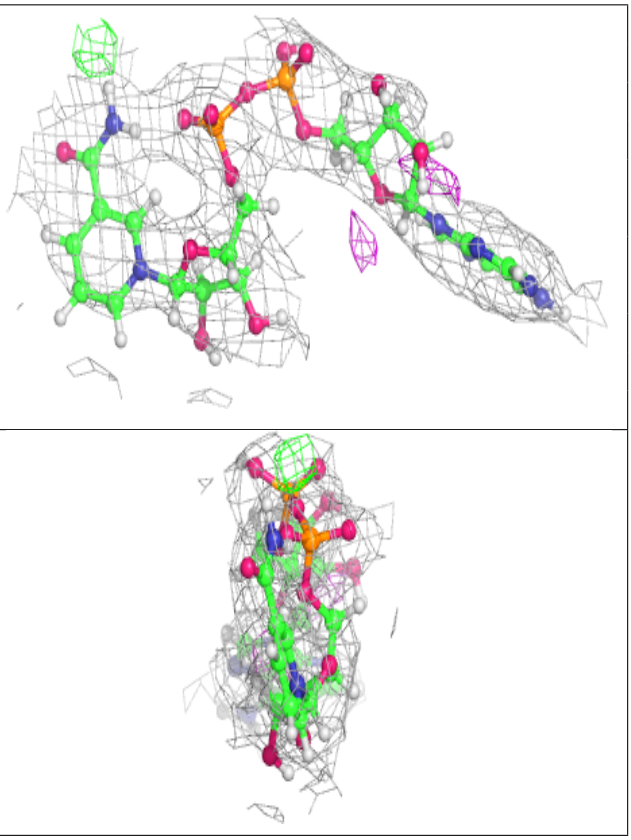
Electron density around NAD P 302:

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



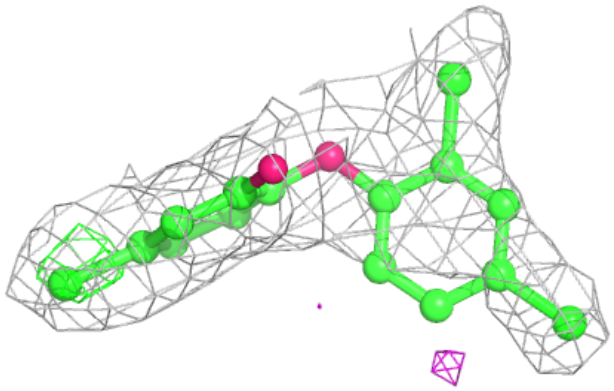
Electron density around NAD N 302:

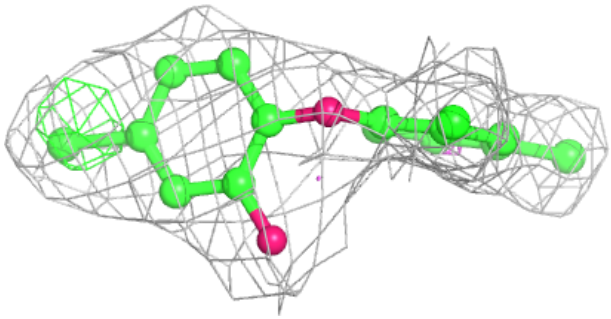
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

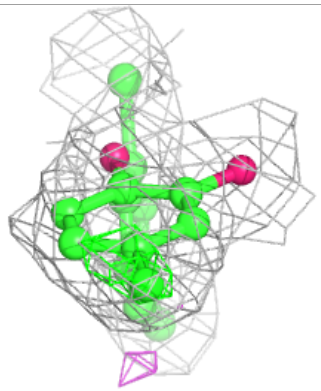


Electron density around TCL K 301:

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

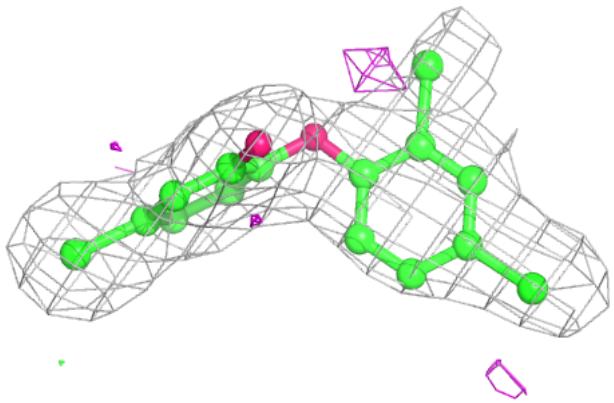


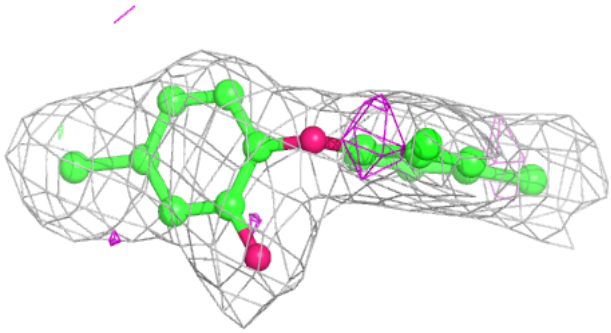


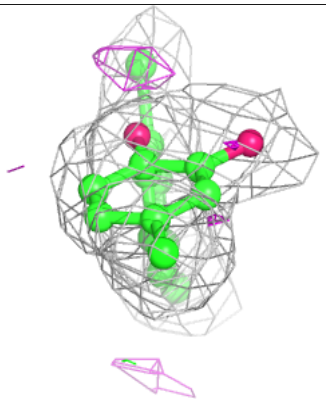


Electron density around TCL L 301:

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

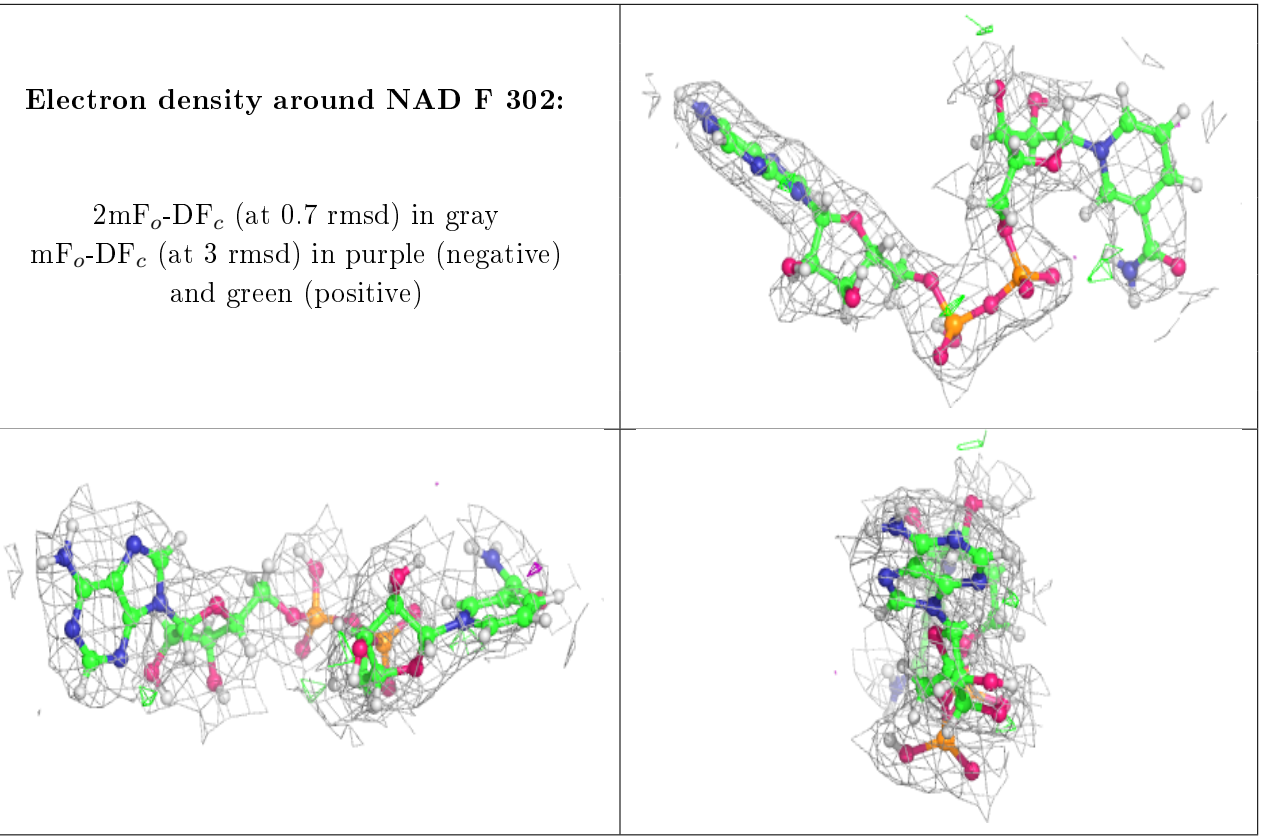






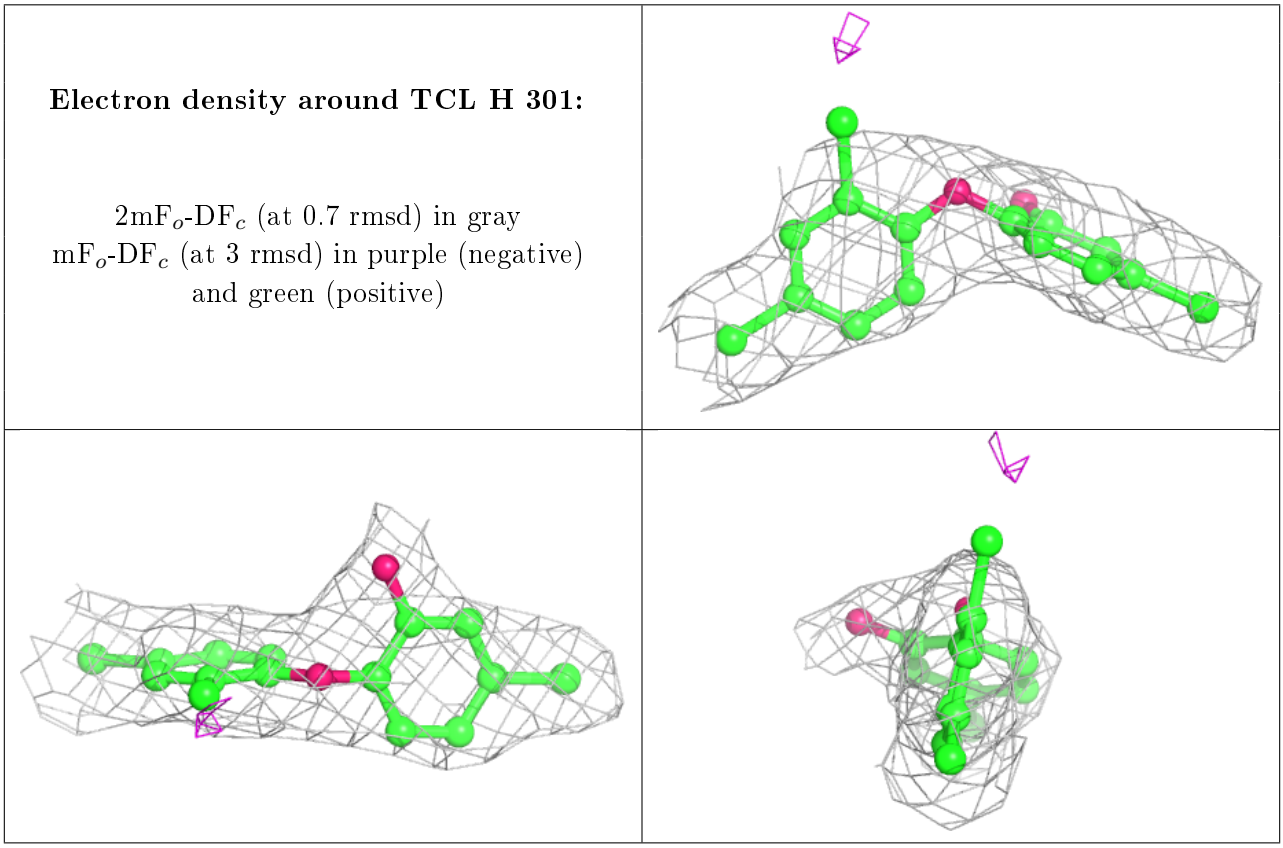
Electron density around NAD F 302:

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



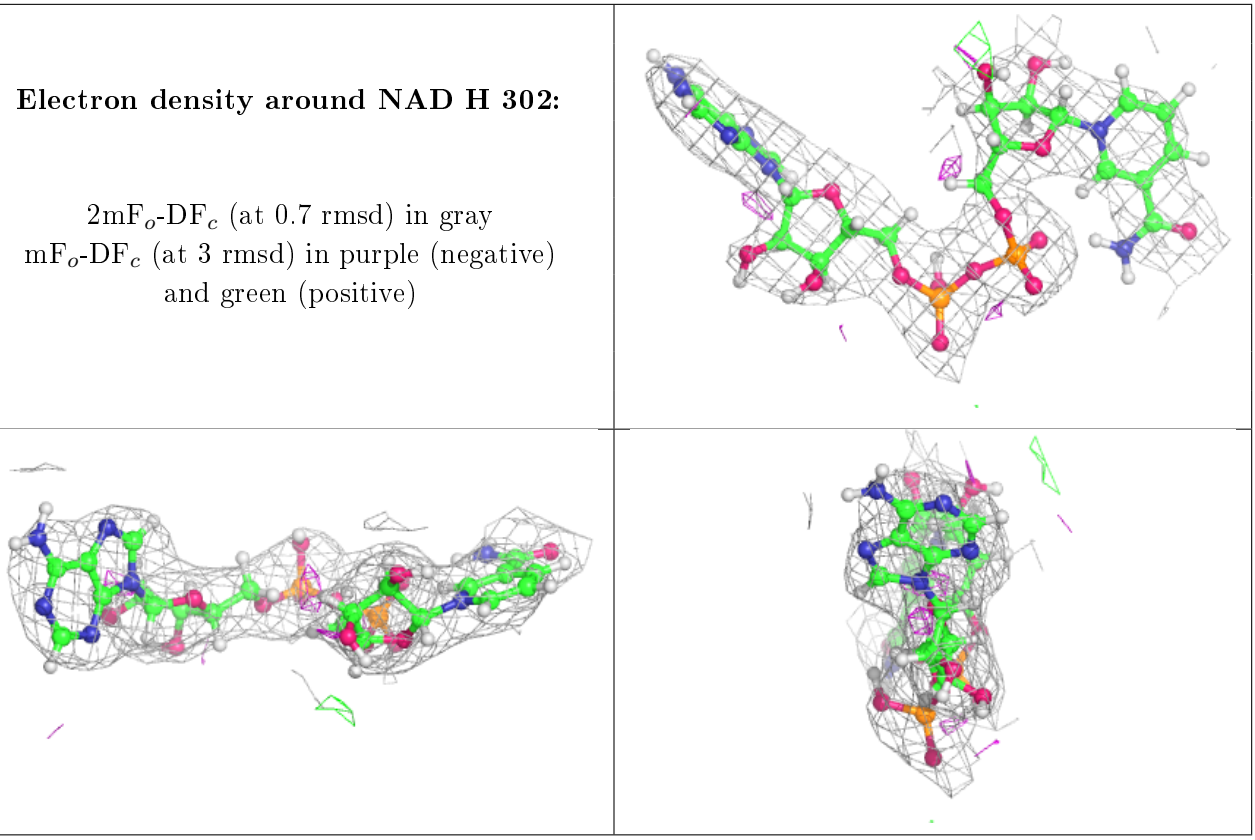
Electron density around TCL H 301:

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



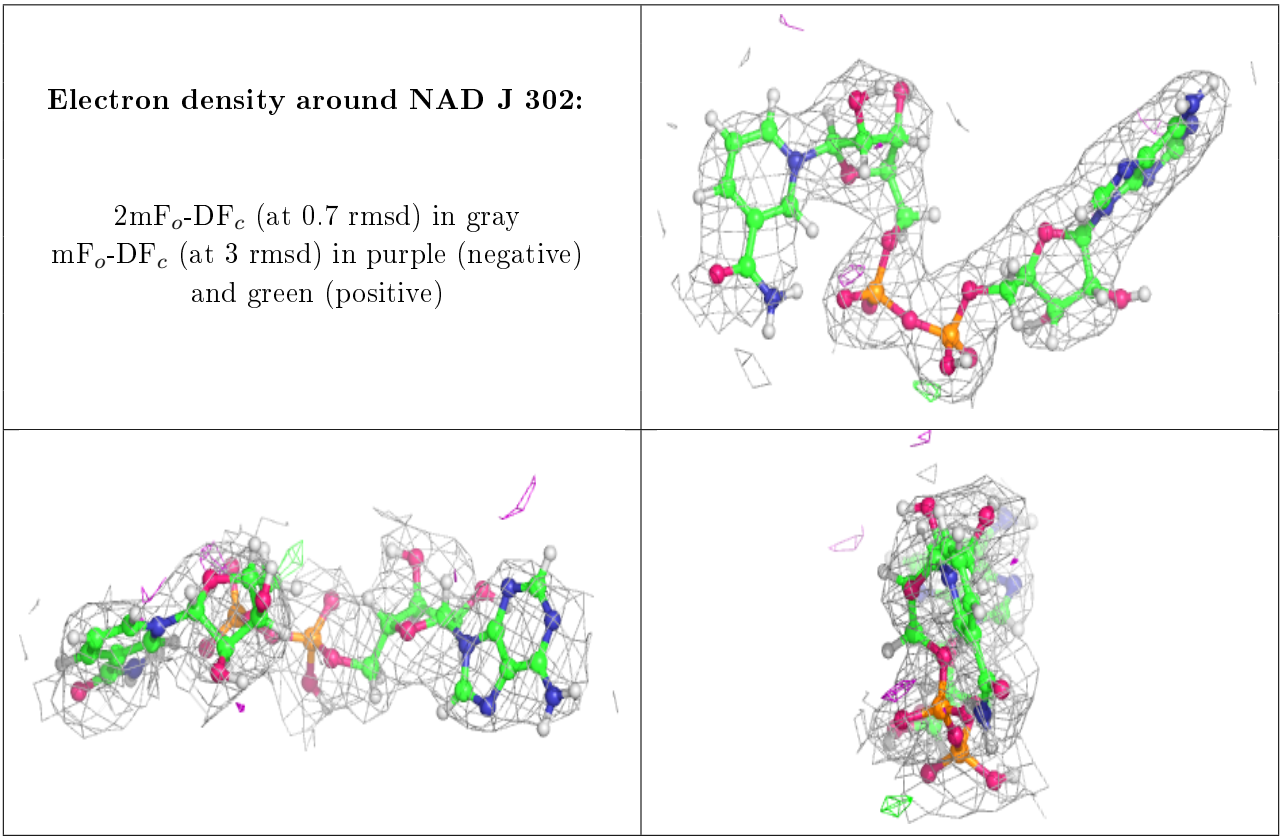
Electron density around NAD H 302:

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



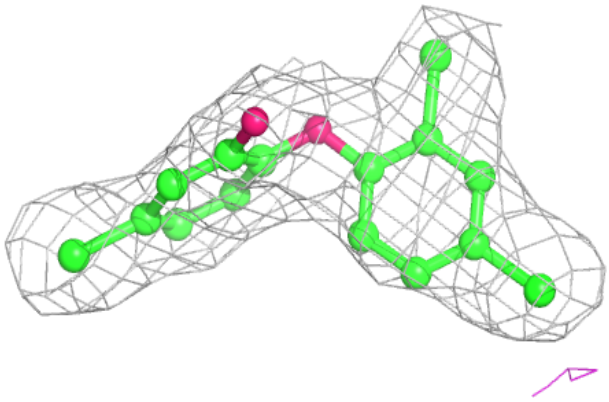
Electron density around NAD J 302:

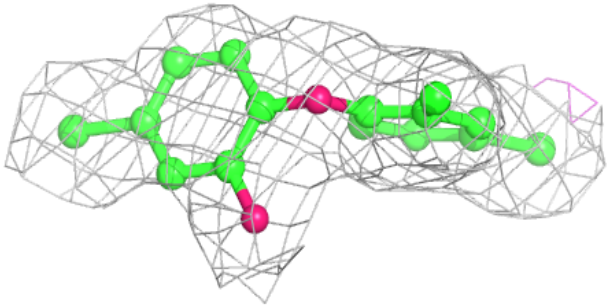
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

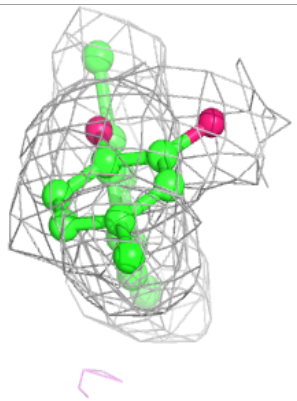


Electron density around TCL G 301:

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

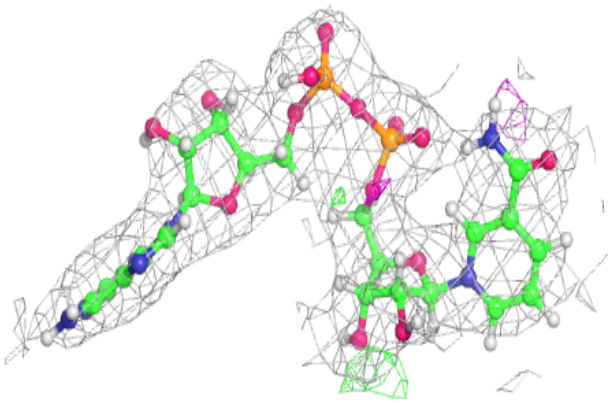


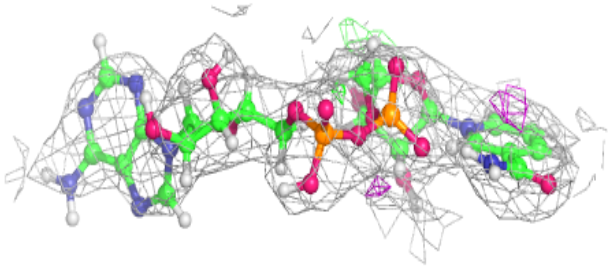


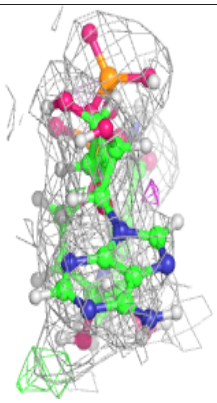


Electron density around NAD O 302:

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

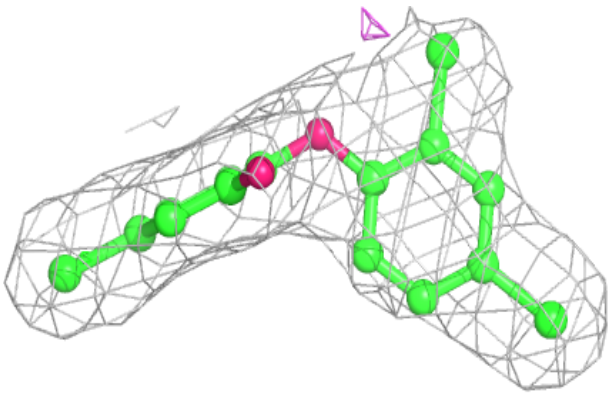


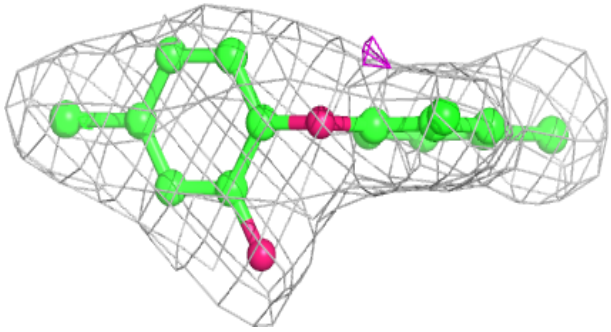


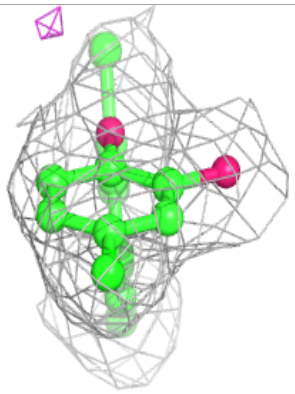


Electron density around TCL O 301:

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

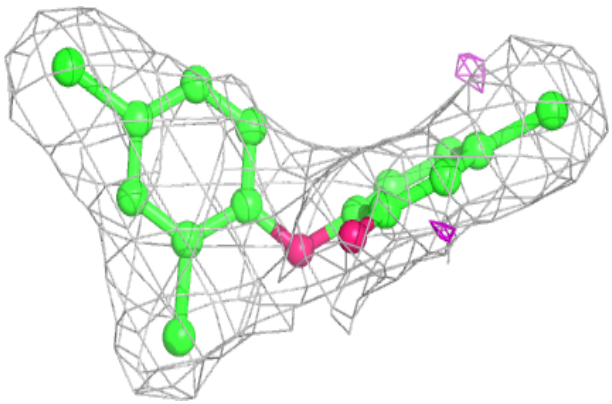


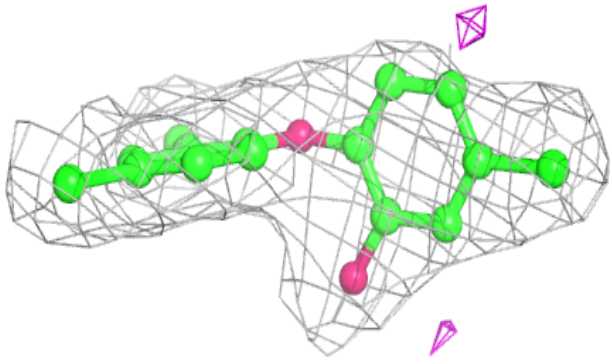


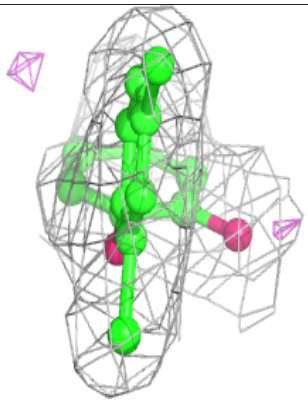


Electron density around TCL B 301:

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

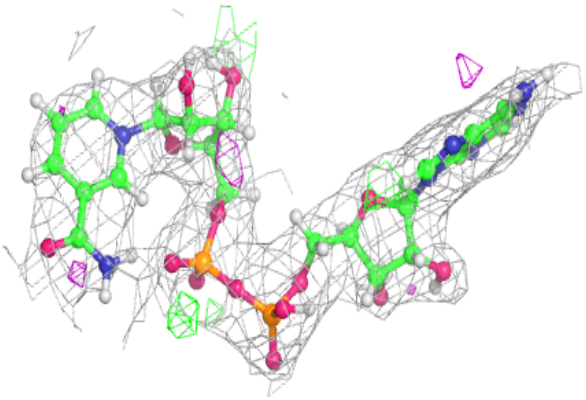


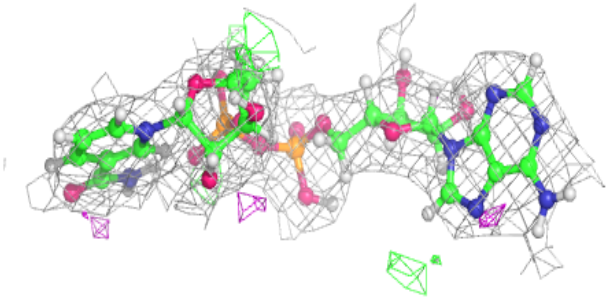


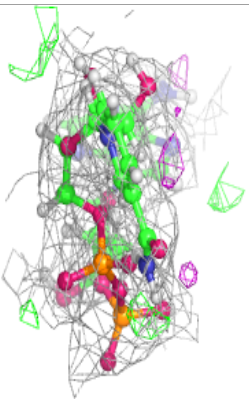


Electron density around NAD L 302:

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

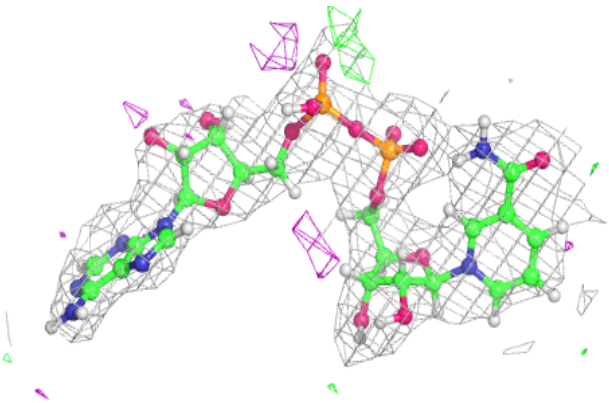


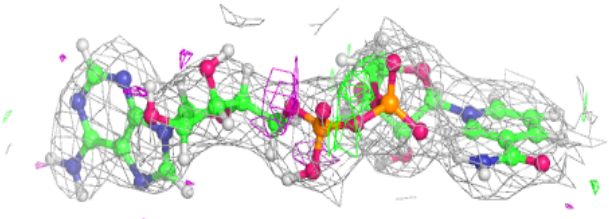


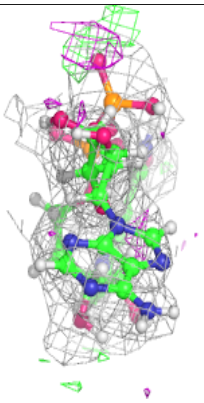


Electron density around NAD I 302:

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

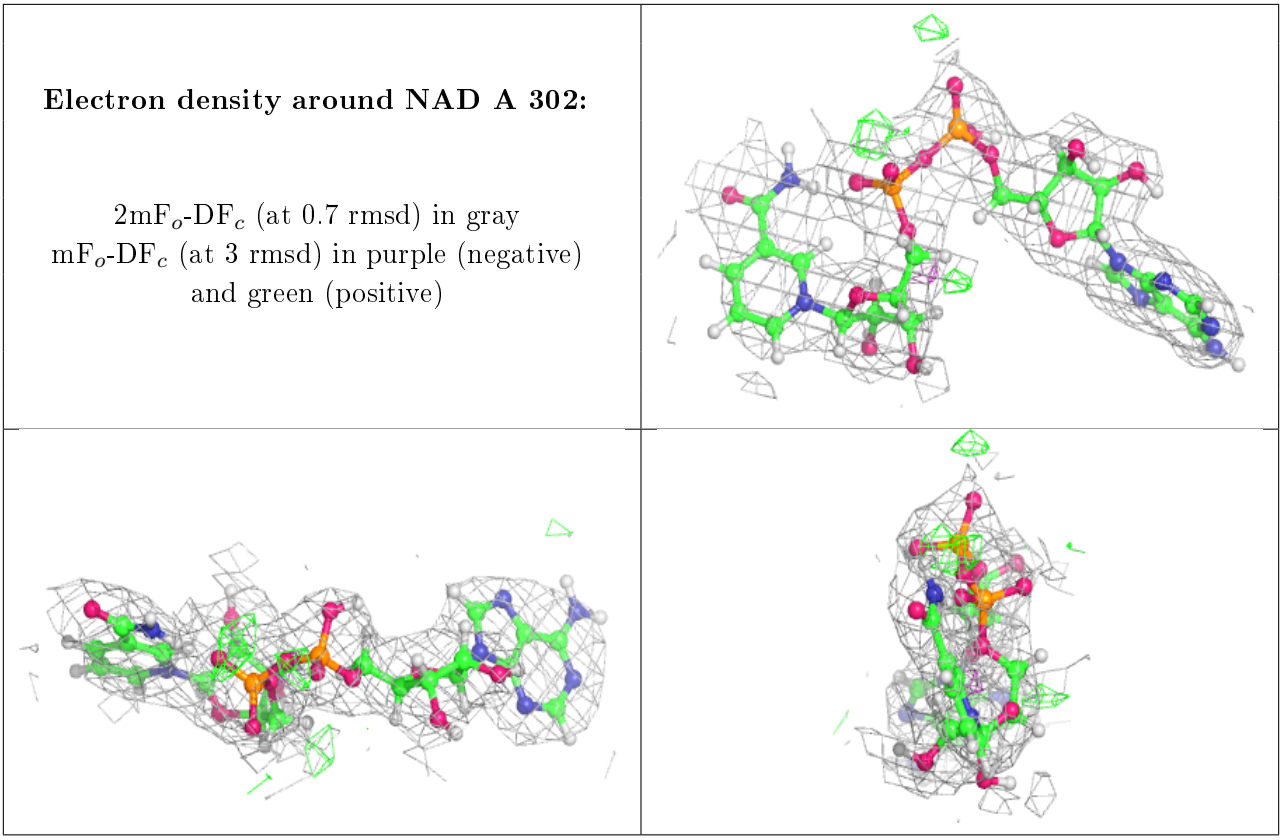






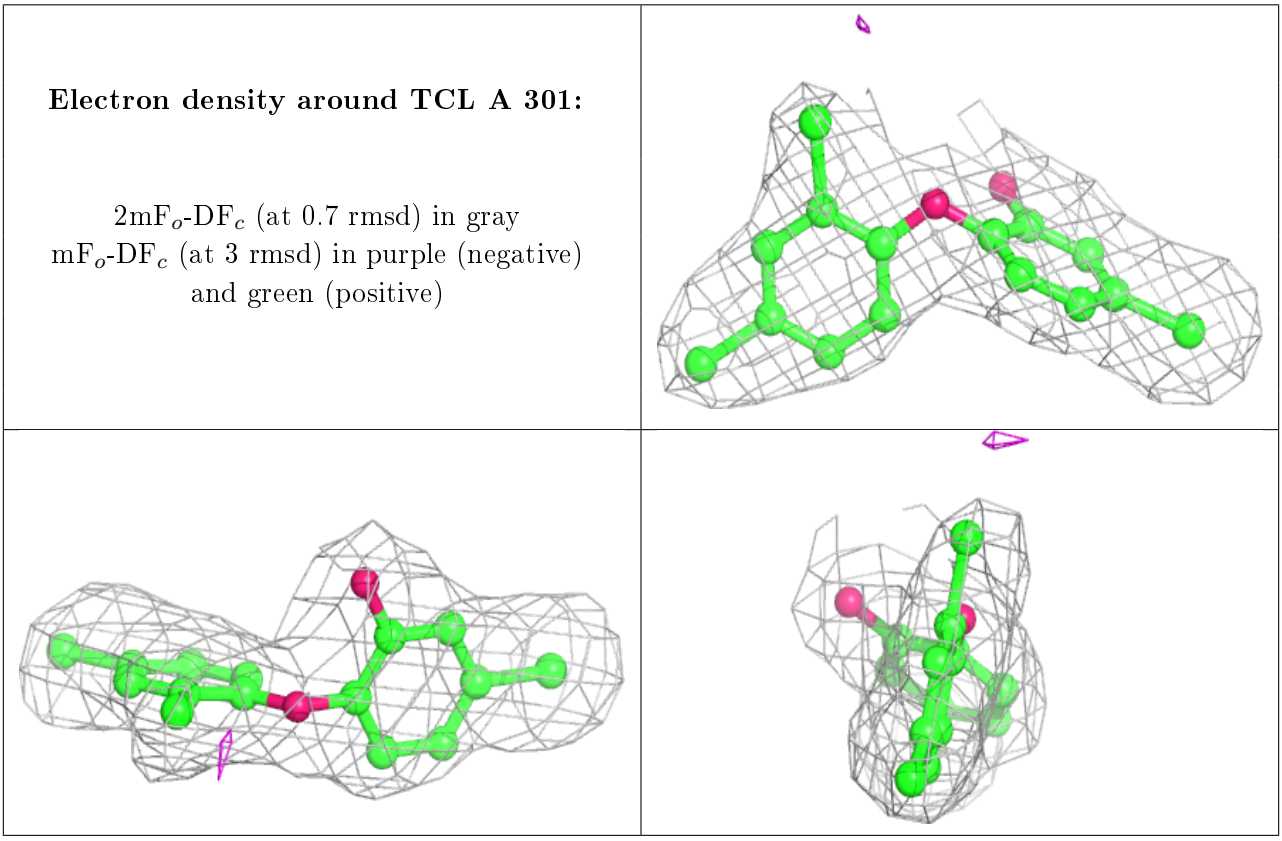
Electron density around NAD A 302:

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



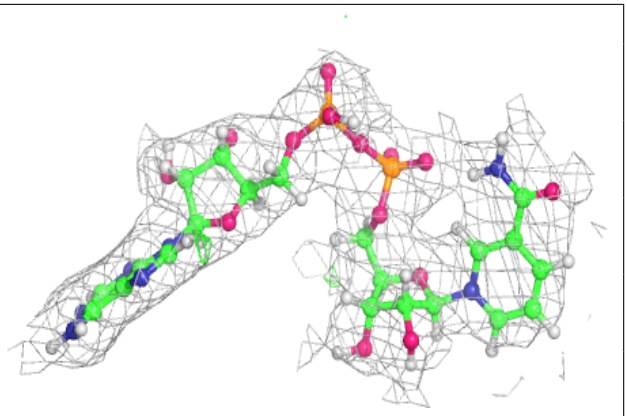
Electron density around TCL A 301:

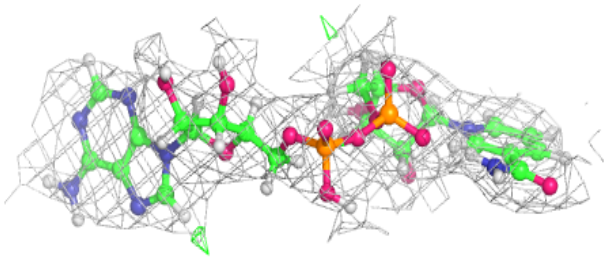
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

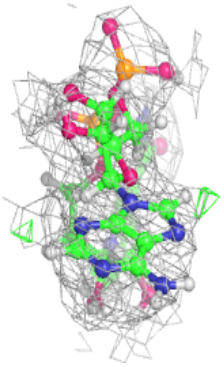


Electron density around NAD C 302:

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

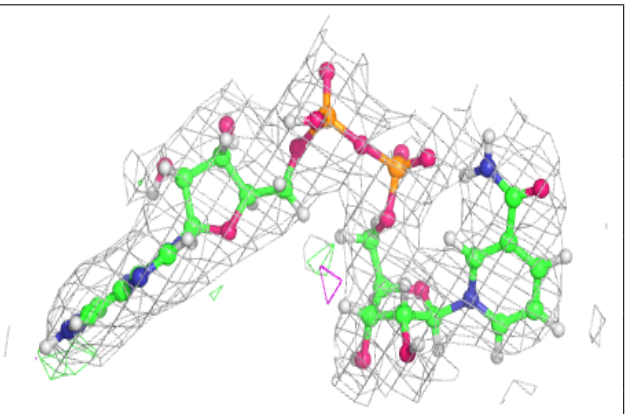


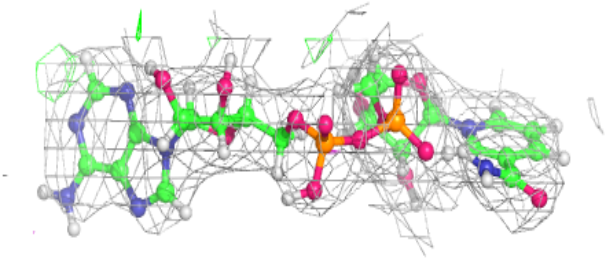


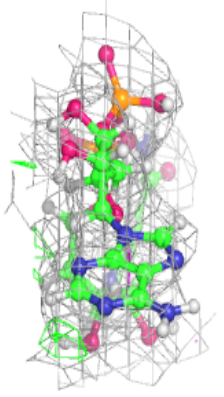


Electron density around NAD D 302:

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

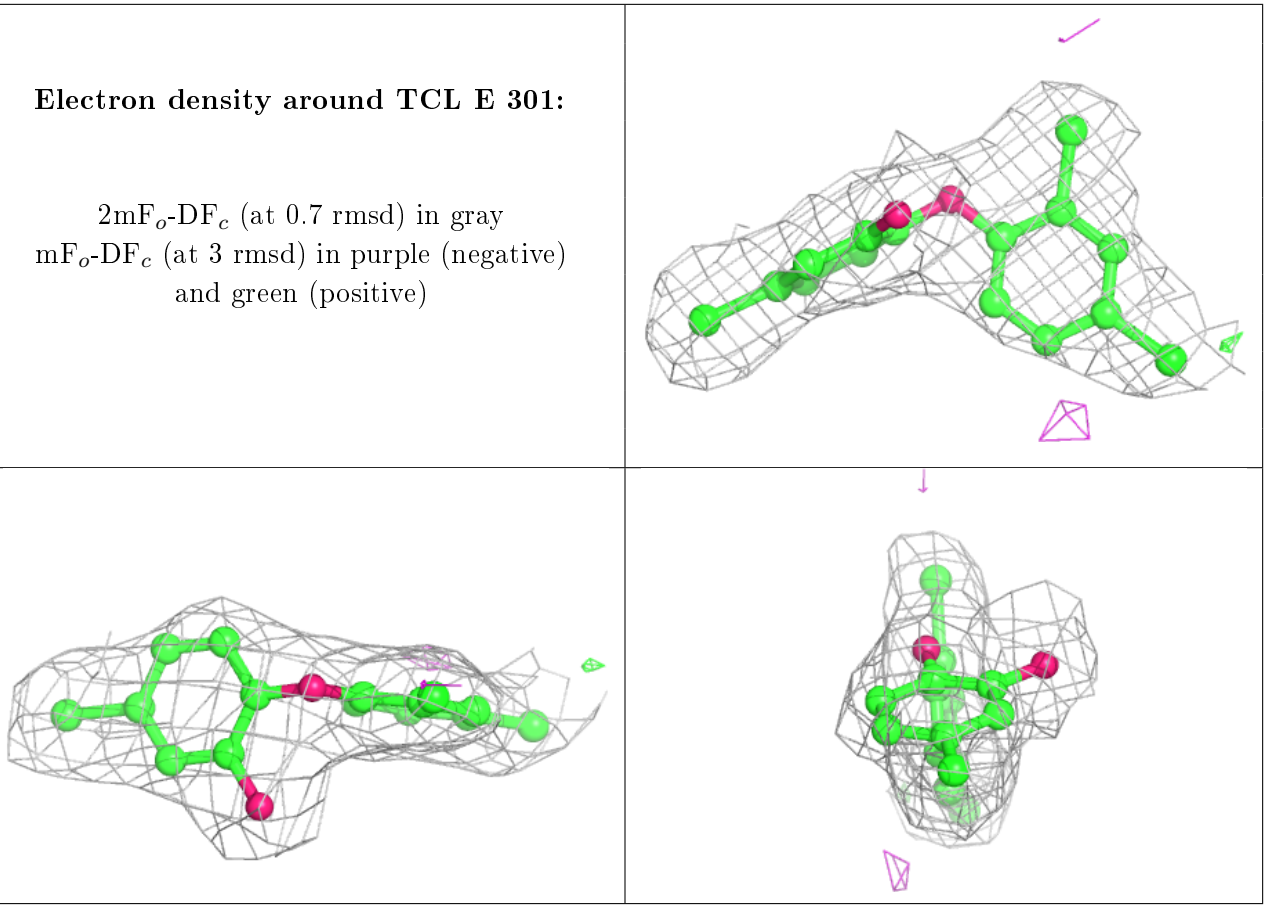






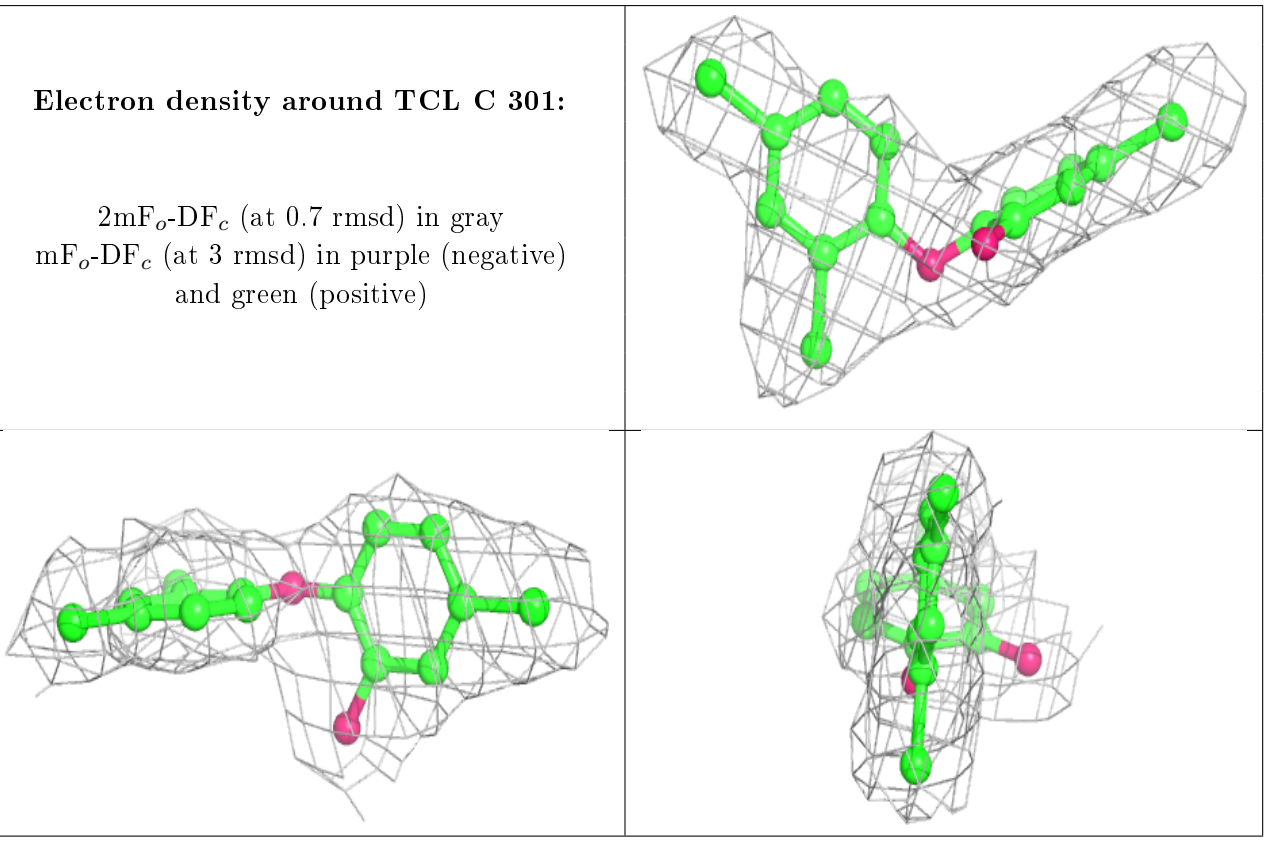
Electron density around TCL E 301:

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



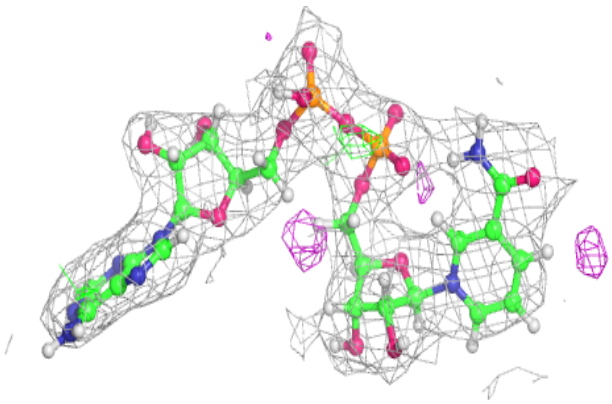
Electron density around TCL C 301:

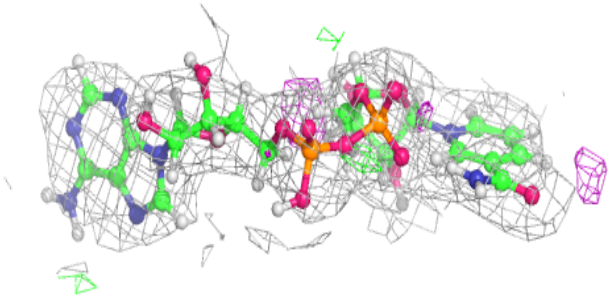
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

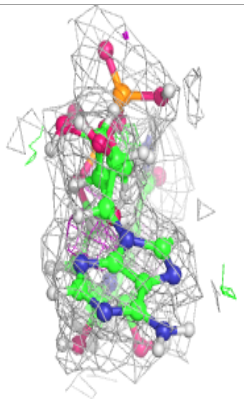


Electron density around NAD E 302:

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

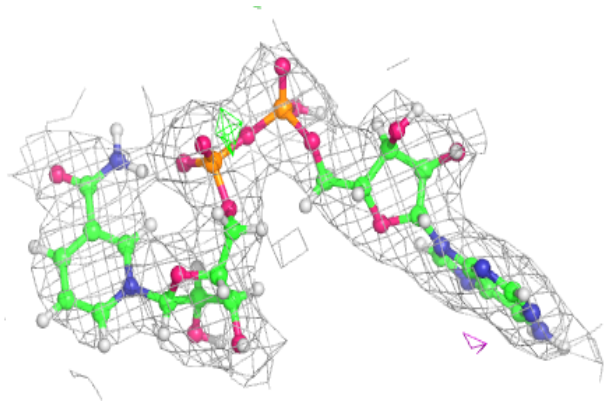


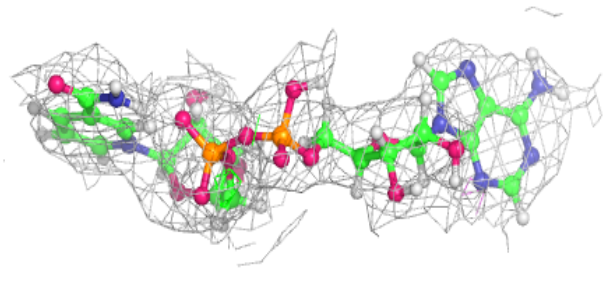


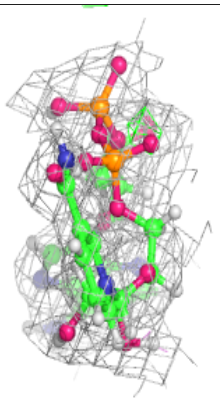


Electron density around NAD B 302:

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

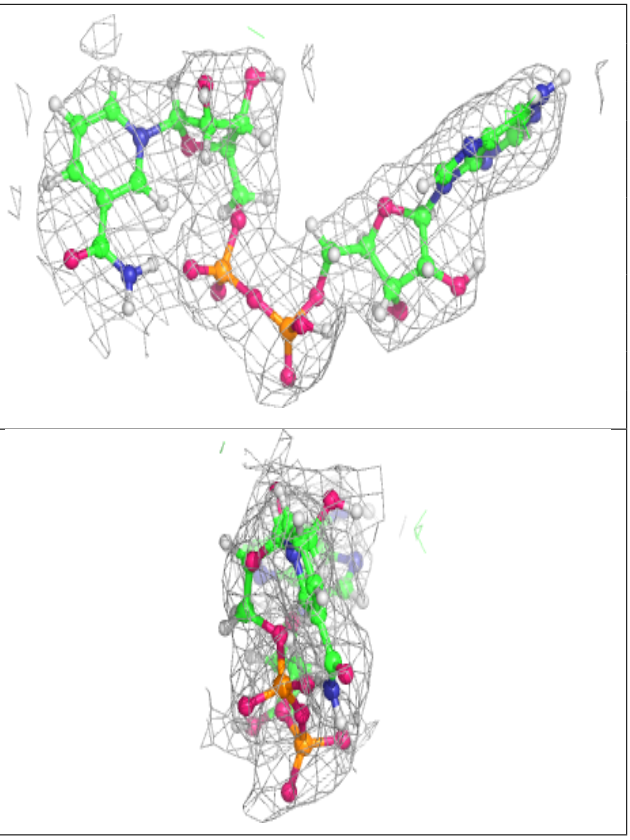






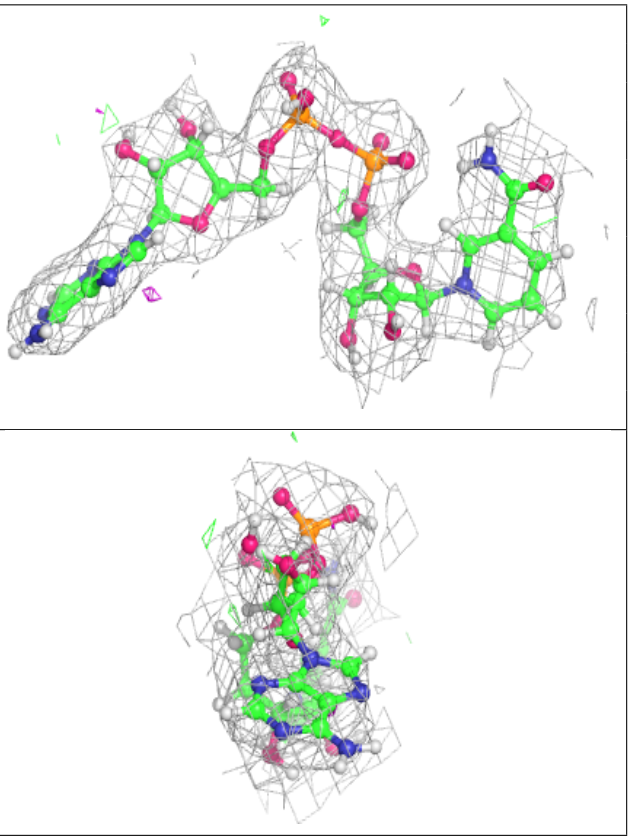
Electron density around NAD G 302:

$2mF_o$-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 K 302:

$2mF_o$-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.