wwPDB X-ray Structure Validation Summary Report (i)

Aug 2, 2023 – 07:50 AM EDT

PDB ID	:	1BVR
Title	:	M.TB. ENOYL-ACP REDUCTASE (INHA) IN COMPLEX WITH NAD+ AND C16-FATTY-ACYL-SUBSTRATE
Authors	:	Rozwarski, D.A.; Vilcheze, C.; Sugantino, M.; Bittman, R.; Jacobs, W.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	1998-09-17
Resolution	:	2.80 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

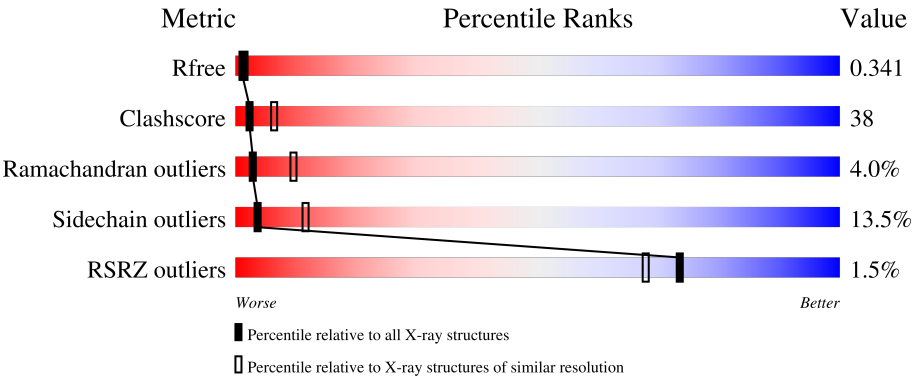
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	268	50% 45% 5%
1	B	268	51% 43% 5%
1	C	268	49% 46% 5%
1	D	268	47% 44% 8%

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Mol	Chain	Length	Quality of chain
1	E	268	21% 53% 23%
1	F	268	3% 47% 47% 6%

2 Entry composition (i)

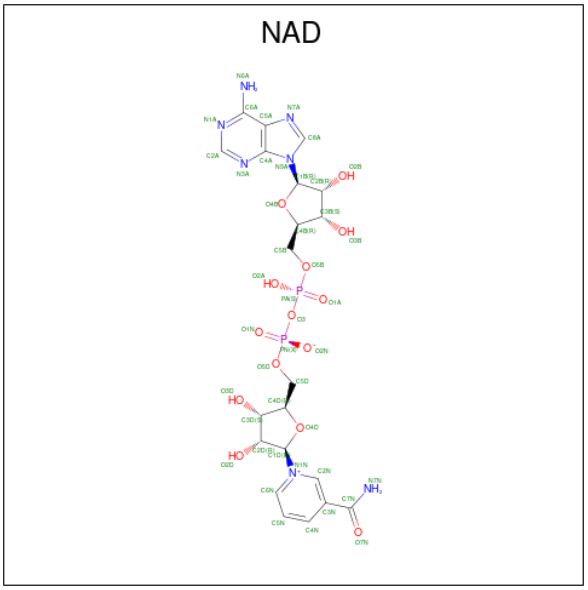
There are 4 unique types of molecules in this entry. The entry contains 12987 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (ENOYL-ACYL CARRIER PROTEIN (ACP) REDUCTASE).

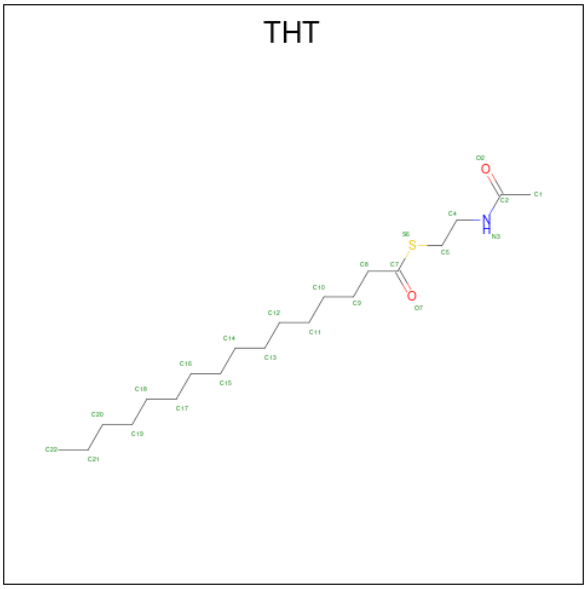
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	B	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	C	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	D	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	E	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			
1	F	268	Total	C	N	O	S	0	0	0
			1994	1263	348	373	10			

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



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

- Molecule 3 is TRANS-2-HEXADECENOYL-(N-ACETYL-CYSTEAMINE)-THIOESTER (three-letter code: THT) (formula: $C_{20}H_{39}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	20	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			24	20	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			24	20	1	2	1		
3	F	1	Total	C	N	O	S	0	0
			24	20	1	2	1		

- Molecule 4 is water.

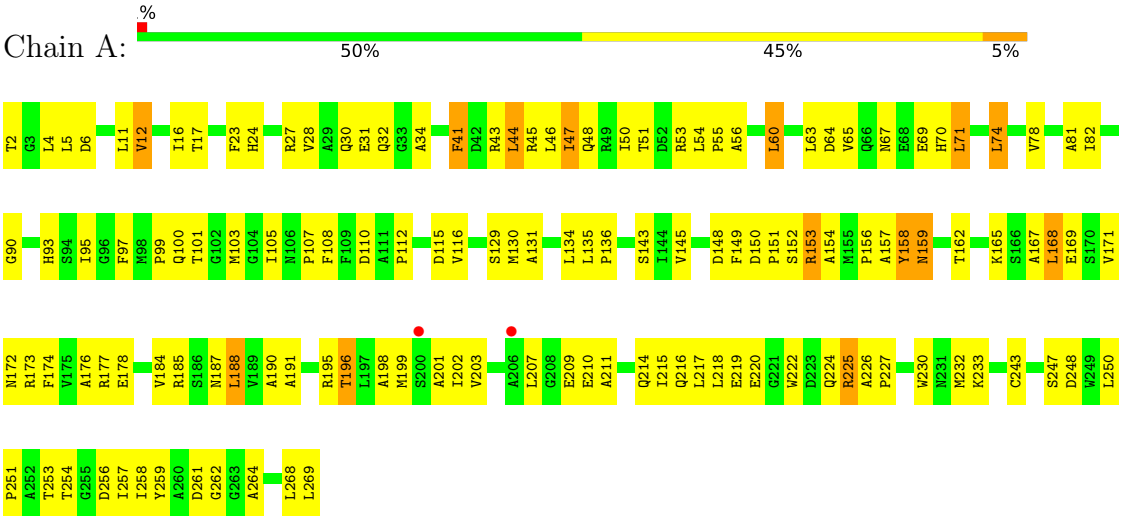
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	110	Total O 110 110	0	0
4	B	114	Total O 114 114	0	0
4	C	106	Total O 106 106	0	0
4	D	104	Total O 104 104	0	0
4	E	119	Total O 119 119	0	0
4	F	110	Total O 110 110	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

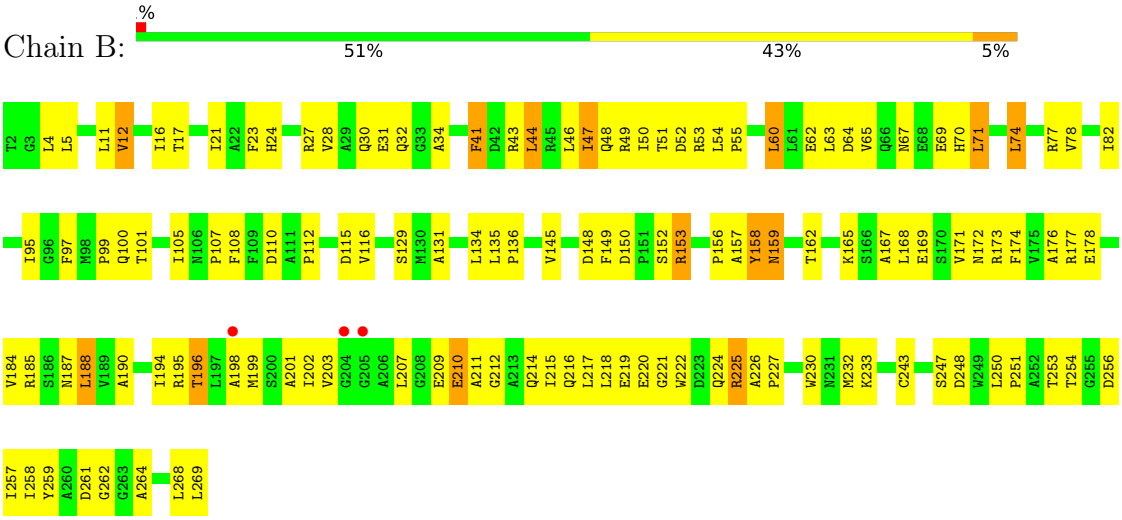
• Molecule 1: PROTEIN (ENOYL-ACYL CARRIER PROTEIN (ACP) REDUCTASE)

Chain A:



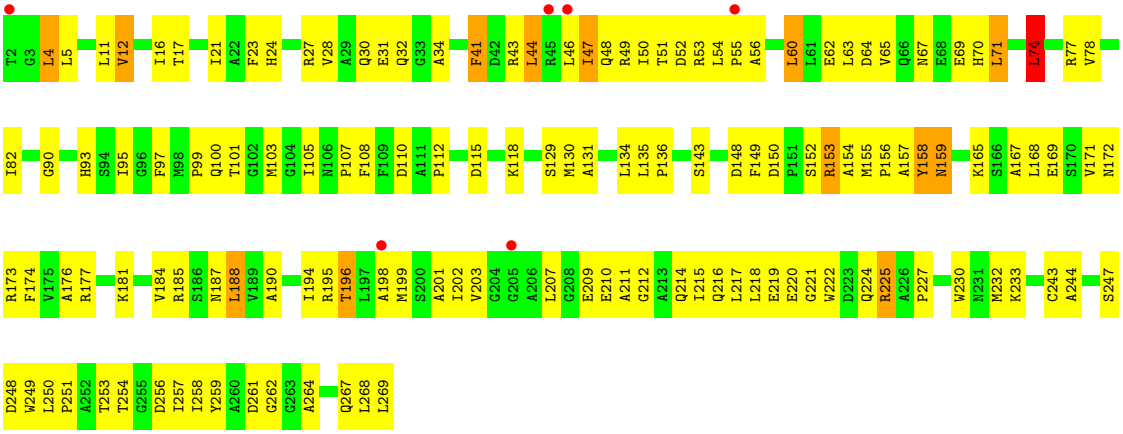
• Molecule 1: PROTEIN (ENOYL-ACYL CARRIER PROTEIN (ACP) REDUCTASE)

Chain B:



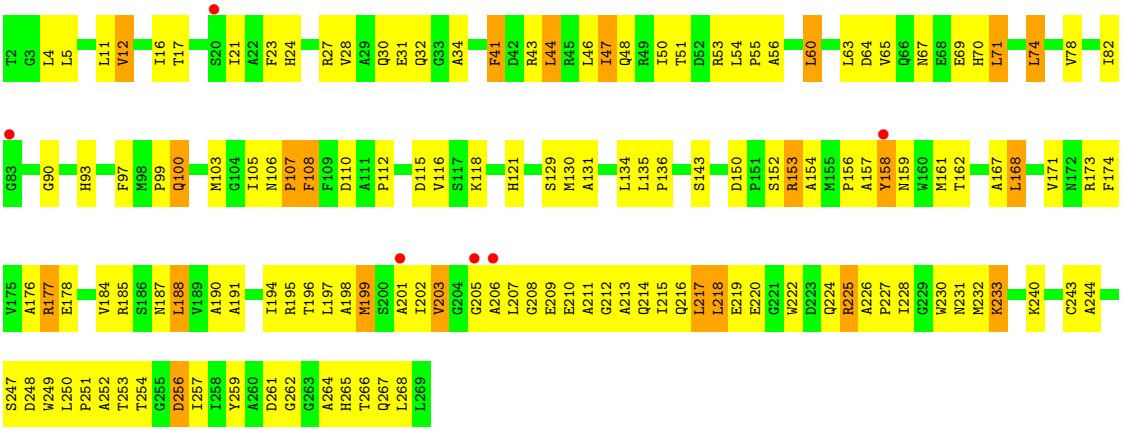
• Molecule 1: PROTEIN (ENOYL-ACYL CARRIER PROTEIN (ACP) REDUCTASE)

Chain C:



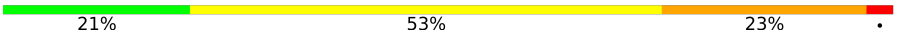
• Molecule 1: PROTEIN (ENOYL-ACYL CARRIER PROTEIN (ACP) REDUCTASE)

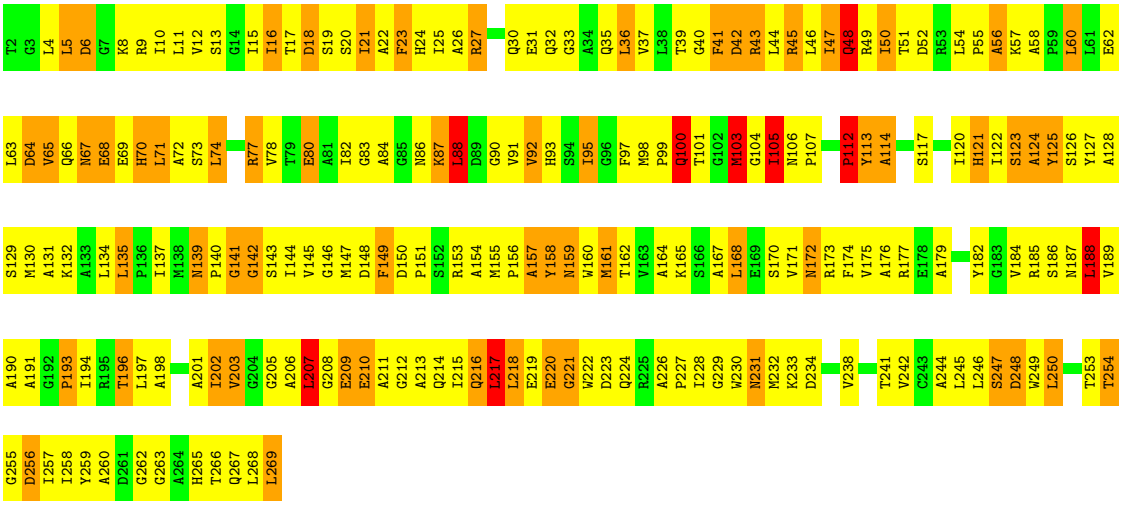
Chain D:



• Molecule 1: PROTEIN (ENOYL-ACYL CARRIER PROTEIN (ACP) REDUCTASE)

Chain E:





• Molecule 1: PROTEIN (ENOYL-ACYL CARRIER PROTEIN (ACP) REDUCTASE)

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.08Å 83.45Å 192.81Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.2 (10.00-2.80) 90.1 (10.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.80Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.217 , 0.344 0.217 , 0.341	Depositor DCC
R_{free} test set	3460 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.11 , 104.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: THT, 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	0.59	0/2032	0.76	0/2758
1	B	0.60	0/2032	0.78	0/2758
1	C	0.60	0/2032	0.76	0/2758
1	D	0.65	0/2032	0.81	0/2758
1	E	0.86	0/2032	1.13	14/2758 (0.5%)
1	F	0.59	0/2032	0.77	0/2758
All	All	0.66	0/12192	0.85	14/16548 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	217	LEU	CA-CB-CG	6.70	130.71	115.30
1	E	27	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	E	255	GLY	N-CA-C	-5.84	98.50	113.10
1	E	188	LEU	CA-CB-CG	5.67	128.34	115.30
1	E	41	PHE	N-CA-C	5.60	126.11	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	113	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1994	0	2008	127	0
1	B	1994	0	2008	121	0
1	C	1994	0	2008	150	0
1	D	1994	0	2008	136	0
1	E	1994	0	2008	338	0
1	F	1994	0	2008	141	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
2	E	44	0	25	9	0
2	F	44	0	26	1	0
3	A	24	0	39	17	0
3	B	24	0	39	15	0
3	C	24	0	39	17	0
3	F	24	0	39	17	0
4	A	110	0	0	13	0
4	B	114	0	0	15	0
4	C	106	0	0	11	0
4	D	104	0	0	11	0
4	E	119	0	0	46	0
4	F	110	0	0	13	0
All	All	12987	0	12359	948	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 948 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:198:ALA:HB2	3:F:1310:THT:HC12	1.22	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ALA:HB2	3:A:1302:THT:HC12	1.18	1.08
1:B:198:ALA:HB2	3:B:1304:THT:HC12	1.25	1.08
1:C:198:ALA:HB2	3:C:1306:THT:HC12	1.19	1.08
1:E:135:LEU:HD11	1:E:144:ILE:HD11	1.38	1.02

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	266/268 (99%)	238 (90%)	22 (8%)	6 (2%)	6 21
1	B	266/268 (99%)	238 (90%)	21 (8%)	7 (3%)	5 18
1	C	266/268 (99%)	241 (91%)	18 (7%)	7 (3%)	5 18
1	D	266/268 (99%)	231 (87%)	27 (10%)	8 (3%)	4 15
1	E	266/268 (99%)	190 (71%)	46 (17%)	30 (11%)	0 1
1	F	266/268 (99%)	239 (90%)	21 (8%)	6 (2%)	6 21
All	All	1596/1608 (99%)	1377 (86%)	155 (10%)	64 (4%)	3 9

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	GLU
1	D	103	MET
1	D	197	LEU
1	E	21	ILE
1	E	56	ALA

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	203/204 (100%)	182 (90%)	21 (10%)	7 21
1	B	203/204 (100%)	182 (90%)	21 (10%)	7 21
1	C	203/204 (100%)	181 (89%)	22 (11%)	6 19
1	D	203/204 (100%)	179 (88%)	24 (12%)	5 16
1	E	203/204 (100%)	148 (73%)	55 (27%)	0 1
1	F	203/204 (100%)	182 (90%)	21 (10%)	7 21
All	All	1218/1224 (100%)	1054 (86%)	164 (14%)	4 11

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	105	ILE
1	F	12	VAL
1	E	139	ASN
1	E	207	LEU
1	F	129	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	100	GLN
1	F	70	HIS
1	F	214	GLN
1	E	231	ASN
1	D	100	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	THT	B	1304	-	23,23,23	1.37	4 (17%)	23,24,24	1.98	5 (21%)
3	THT	A	1302	-	23,23,23	1.15	2 (8%)	23,24,24	1.91	5 (21%)
3	THT	F	1310	-	23,23,23	1.20	3 (13%)	23,24,24	1.80	4 (17%)
2	NAD	A	1301	-	42,48,48	1.40	5 (11%)	50,73,73	1.41	4 (8%)
2	NAD	B	1303	-	42,48,48	1.45	3 (7%)	50,73,73	1.50	9 (18%)
2	NAD	D	1307	-	42,48,48	1.56	5 (11%)	50,73,73	1.56	9 (18%)
2	NAD	C	1305	-	42,48,48	1.44	4 (9%)	50,73,73	1.41	6 (12%)
3	THT	C	1306	-	23,23,23	1.50	4 (17%)	23,24,24	1.99	4 (17%)
2	NAD	F	1309	-	42,48,48	1.36	4 (9%)	50,73,73	1.43	6 (12%)
2	NAD	E	1308	-	42,48,48	1.32	5 (11%)	50,73,73	2.32	21 (42%)

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	THT	B	1304	-	-	15/22/22/22	-
3	THT	A	1302	-	-	15/22/22/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THT	F	1310	-	-	15/22/22/22	-
2	NAD	A	1301	-	-	13/26/62/62	0/5/5/5
2	NAD	B	1303	-	-	13/26/62/62	0/5/5/5
2	NAD	D	1307	-	-	14/26/62/62	0/5/5/5
2	NAD	C	1305	-	-	14/26/62/62	0/5/5/5
3	THT	C	1306	-	-	15/22/22/22	-
2	NAD	F	1309	-	-	14/26/62/62	0/5/5/5
2	NAD	E	1308	-	-	18/26/62/62	0/5/5/5

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1307	NAD	C2N-N1N	6.34	1.42	1.35
2	A	1301	NAD	C2N-N1N	5.76	1.42	1.35
2	B	1303	NAD	C2N-N1N	5.62	1.41	1.35
2	C	1305	NAD	C2N-N1N	5.47	1.41	1.35
2	F	1309	NAD	C2N-N1N	5.27	1.41	1.35

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1304	THT	C8-C7-S6	5.85	120.26	113.46
3	C	1306	THT	C8-C7-S6	5.67	120.06	113.46
2	E	1308	NAD	O4D-C1D-C2D	-5.35	99.11	106.93
3	A	1302	THT	C8-C7-S6	5.30	119.62	113.46
2	E	1308	NAD	C1B-N9A-C4A	-5.22	117.47	126.64

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	NAD	C5B-O5B-PA-O1A
2	A	1301	NAD	O4D-C1D-N1N-C2N
2	A	1301	NAD	O4D-C1D-N1N-C6N
2	A	1301	NAD	C2D-C1D-N1N-C2N
2	A	1301	NAD	C2D-C1D-N1N-C6N

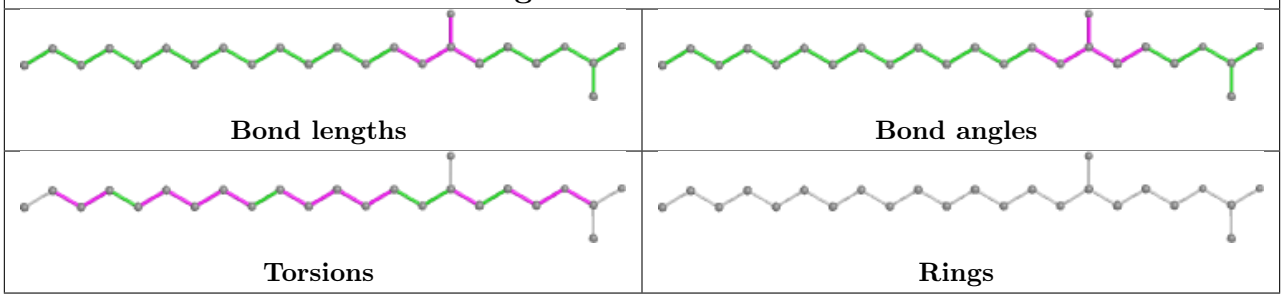
There are no ring outliers.

10 monomers are involved in 82 short contacts:

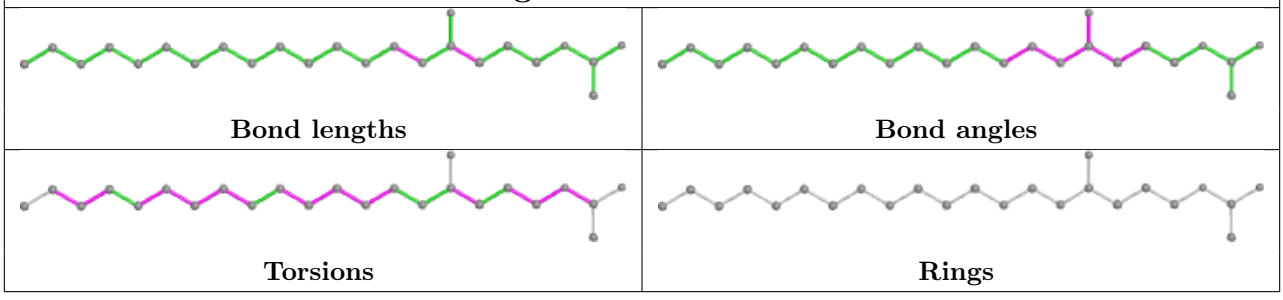
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1304	THT	15	0
3	A	1302	THT	17	0
3	F	1310	THT	17	0
2	A	1301	NAD	2	0
2	B	1303	NAD	1	0
2	D	1307	NAD	2	0
2	C	1305	NAD	1	0
3	C	1306	THT	17	0
2	F	1309	NAD	1	0
2	E	1308	NAD	9	0

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.

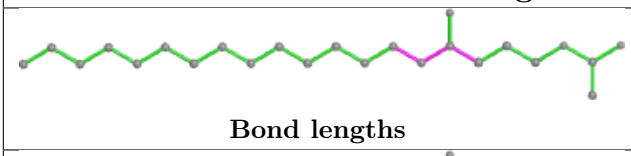
Ligand THT B 1304



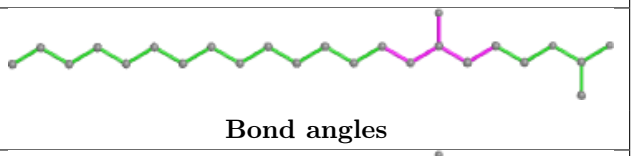
Ligand THT A 1302



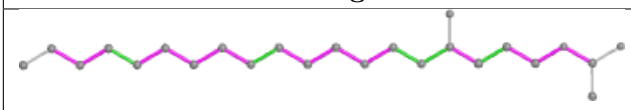
Ligand THT F 1310



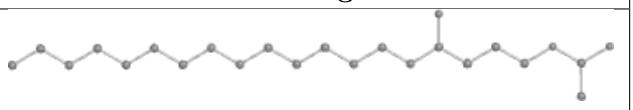
Bond lengths



Bond angles

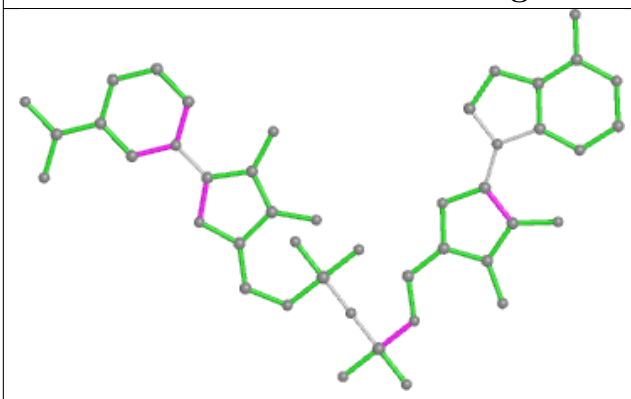


Torsions

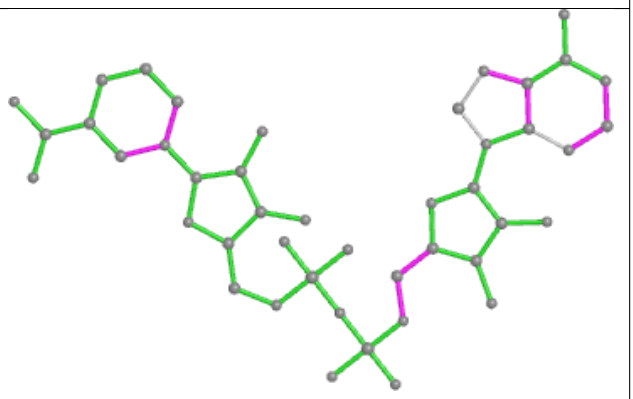


Rings

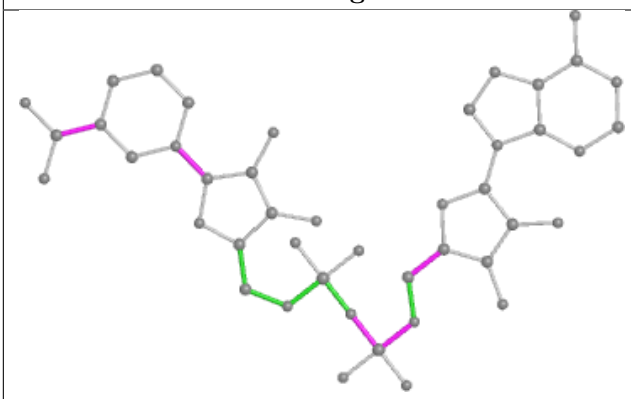
Ligand NAD A 1301



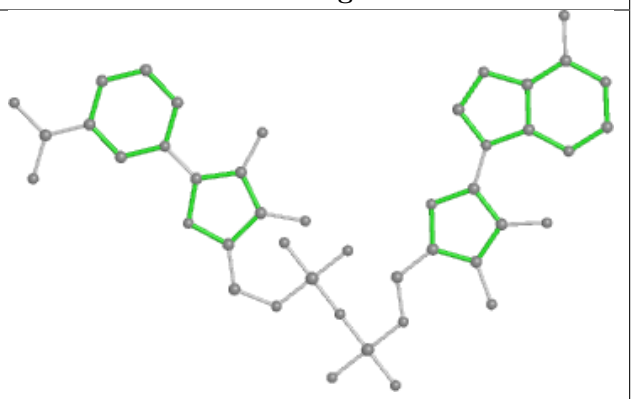
Bond lengths



Bond angles

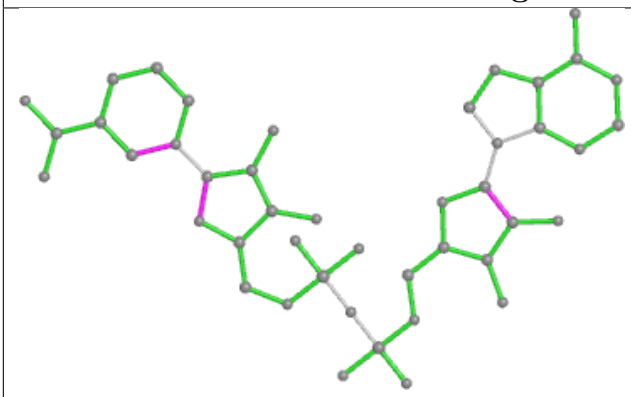


Torsions

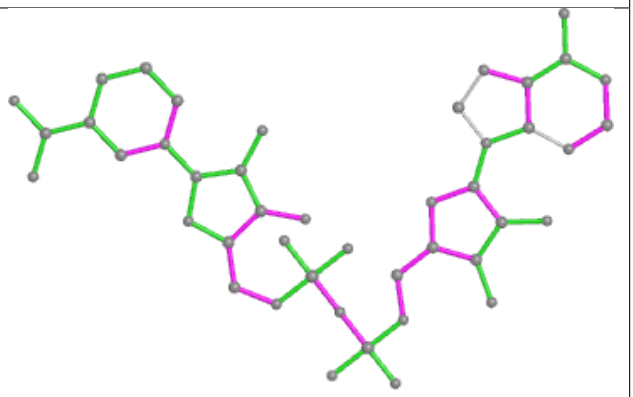


Rings

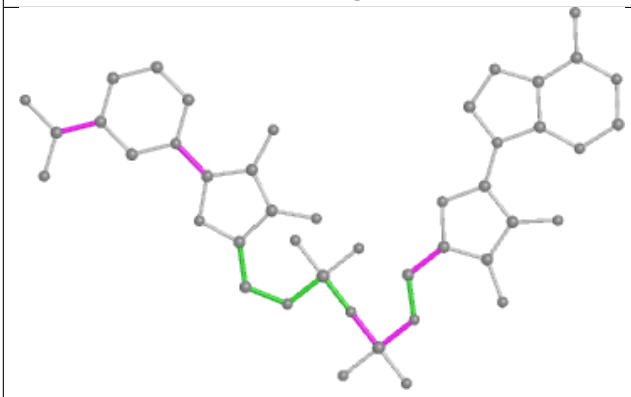
Ligand NAD B 1303



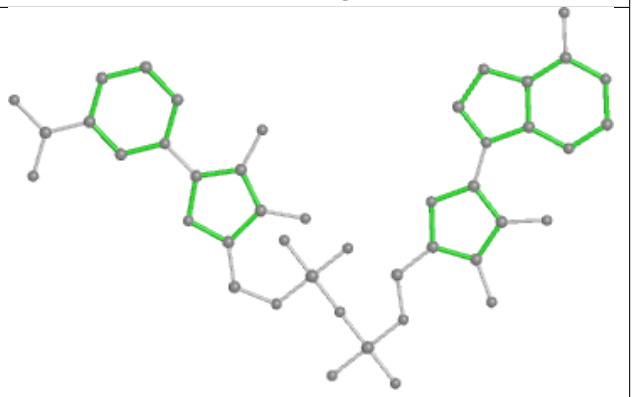
Bond lengths



Bond angles

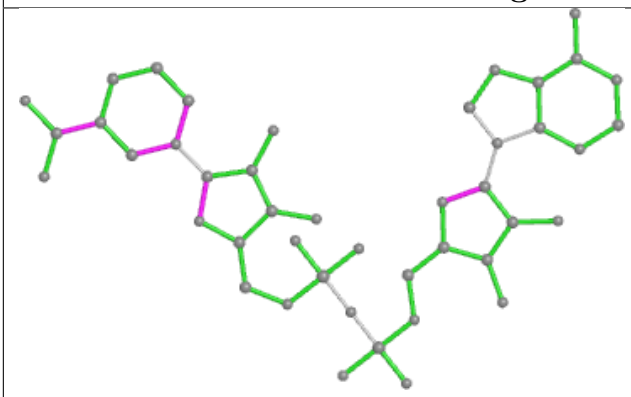


Torsions

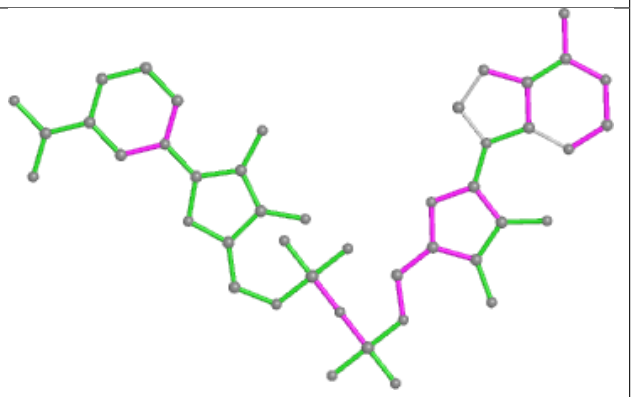


Rings

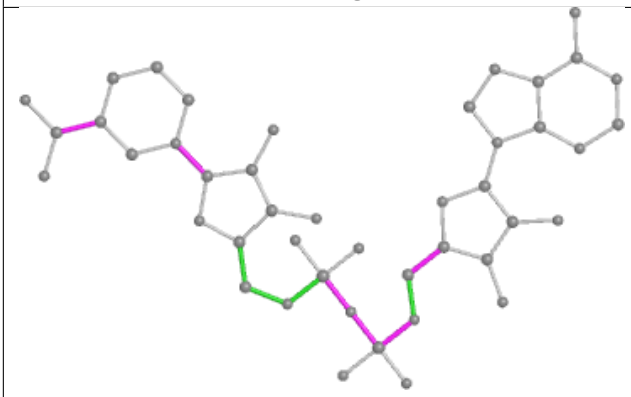
Ligand NAD D 1307



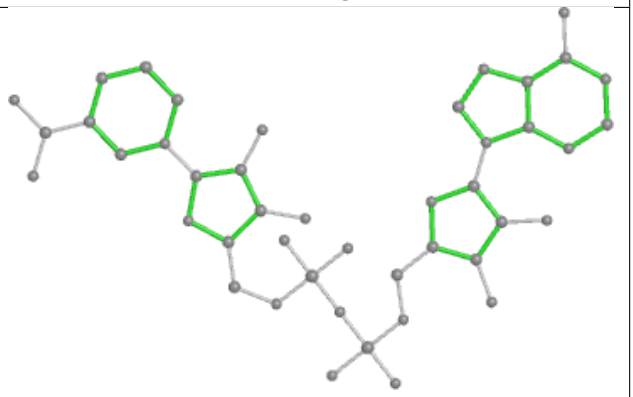
Bond lengths



Bond angles

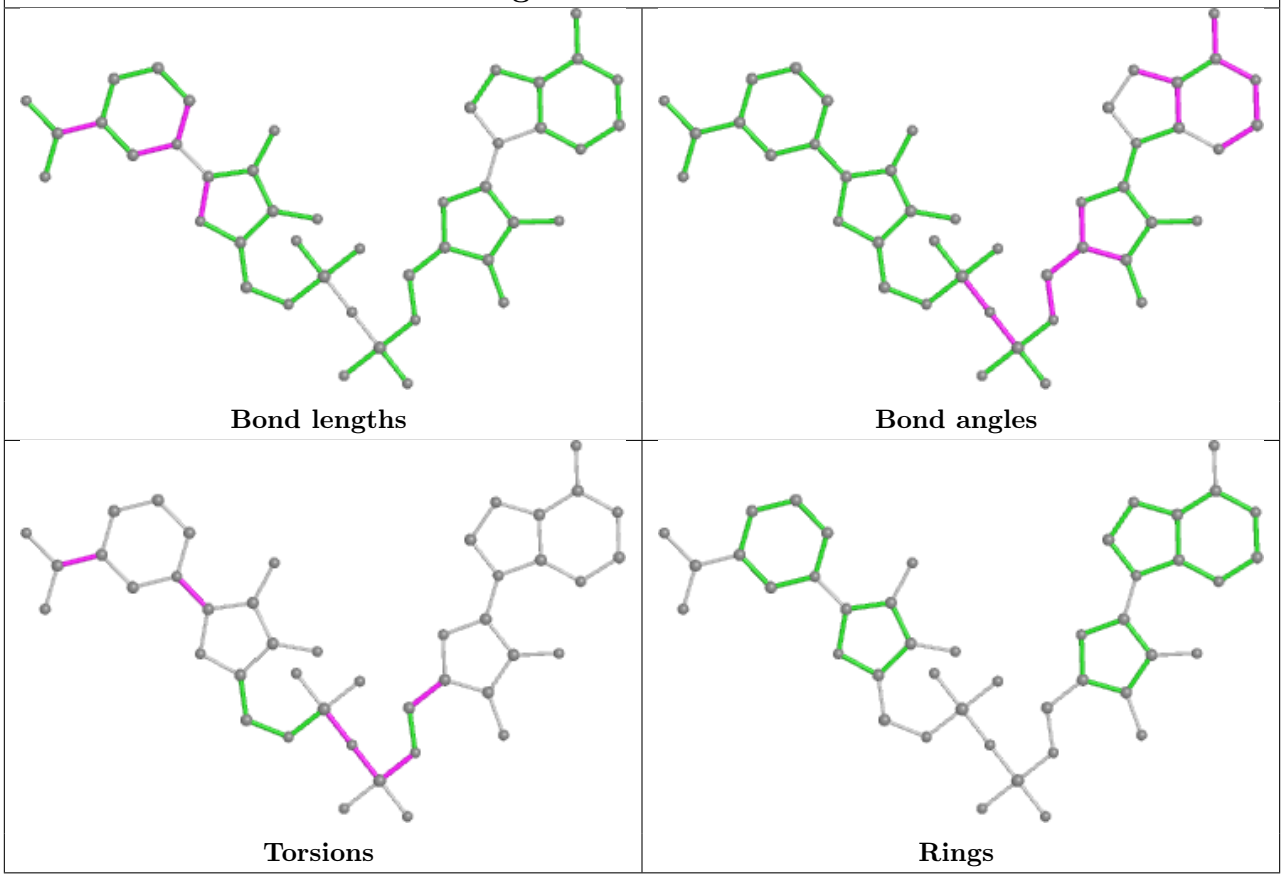


Torsions

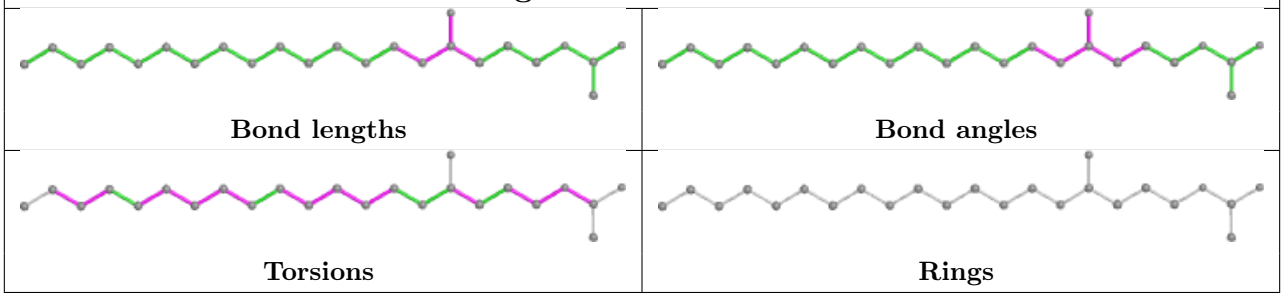


Rings

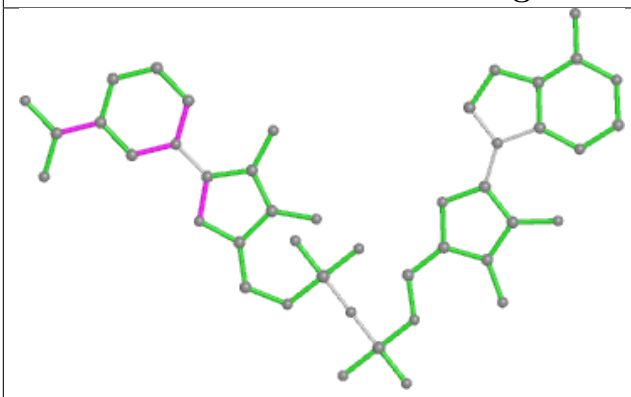
Ligand NAD C 1305



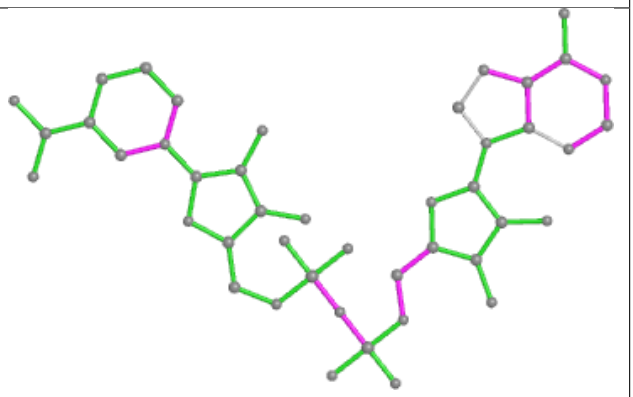
Ligand THT C 1306



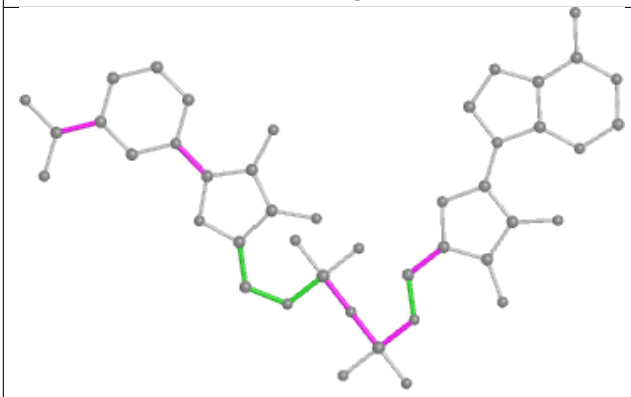
Ligand NAD F 1309



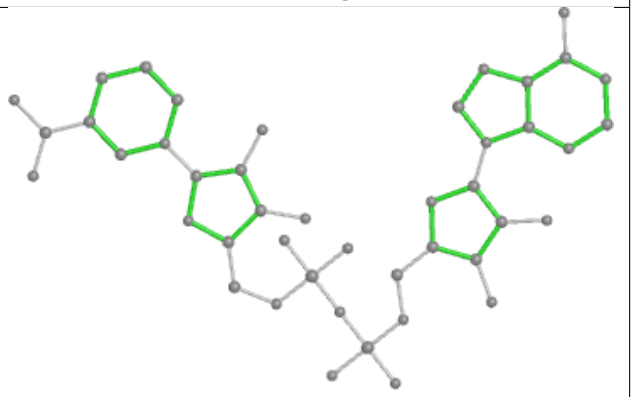
Bond lengths



Bond angles

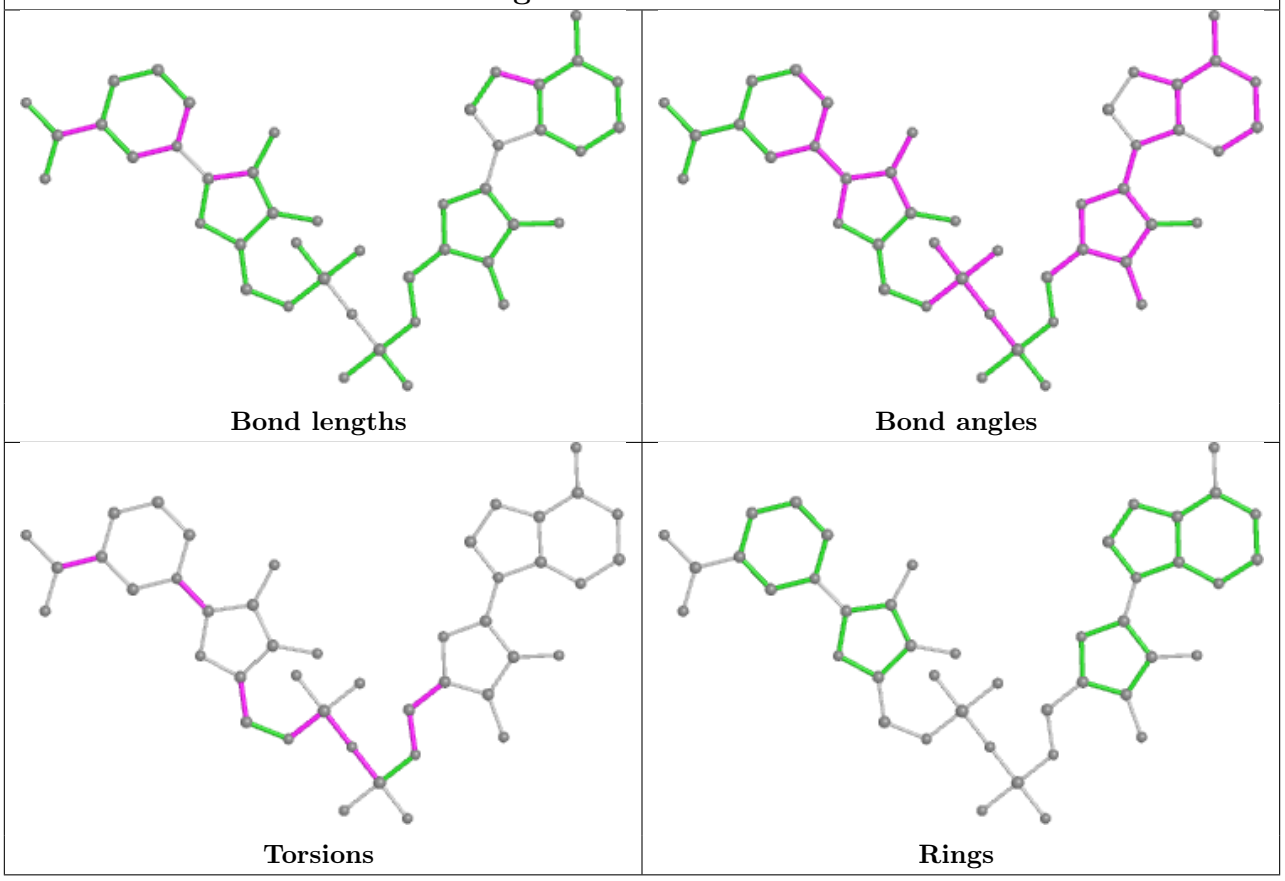


Torsions



Rings

Ligand NAD E 1308



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	268/268 (100%)	-0.46	2 (0%)	87	84	18, 43, 80, 104	0
1	B	268/268 (100%)	-0.44	3 (1%)	80	75	12, 43, 76, 104	0
1	C	268/268 (100%)	-0.09	6 (2%)	62	52	25, 47, 79, 109	0
1	D	268/268 (100%)	-0.03	6 (2%)	62	52	18, 50, 78, 102	0
1	E	268/268 (100%)	-0.55	0	100	100	17, 44, 62, 84	0
1	F	268/268 (100%)	-0.09	7 (2%)	56	46	19, 47, 78, 110	0
All	All	1608/1608 (100%)	-0.28	24 (1%)	73	68	12, 46, 76, 110	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	205	GLY	4.1
1	F	201	ALA	3.7
1	F	198	ALA	3.6
1	F	196	THR	3.2
1	C	45	ARG	3.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

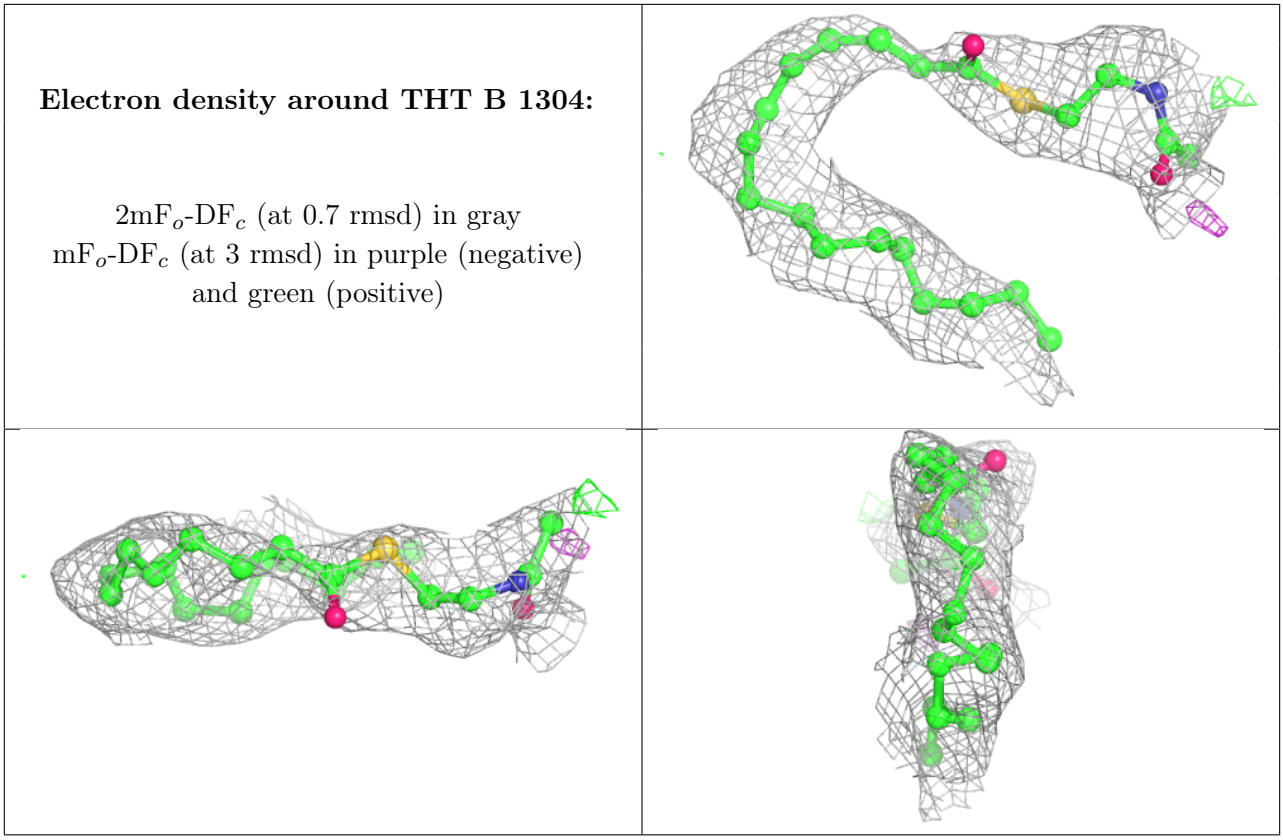
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	THT	B	1304	24/24	0.82	0.20	61,74,89,91	0
3	THT	F	1310	24/24	0.83	0.27	49,76,100,101	0
3	THT	C	1306	24/24	0.85	0.23	45,76,103,107	0
3	THT	A	1302	24/24	0.87	0.20	48,78,85,88	0
2	NAD	F	1309	44/44	0.90	0.19	57,69,75,78	0
2	NAD	D	1307	44/44	0.91	0.18	49,74,83,86	0
2	NAD	A	1301	44/44	0.92	0.17	55,67,75,77	0
2	NAD	B	1303	44/44	0.93	0.17	47,65,74,78	0
2	NAD	C	1305	44/44	0.93	0.17	57,66,76,80	0
2	NAD	E	1308	44/44	0.95	0.14	34,54,70,72	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.

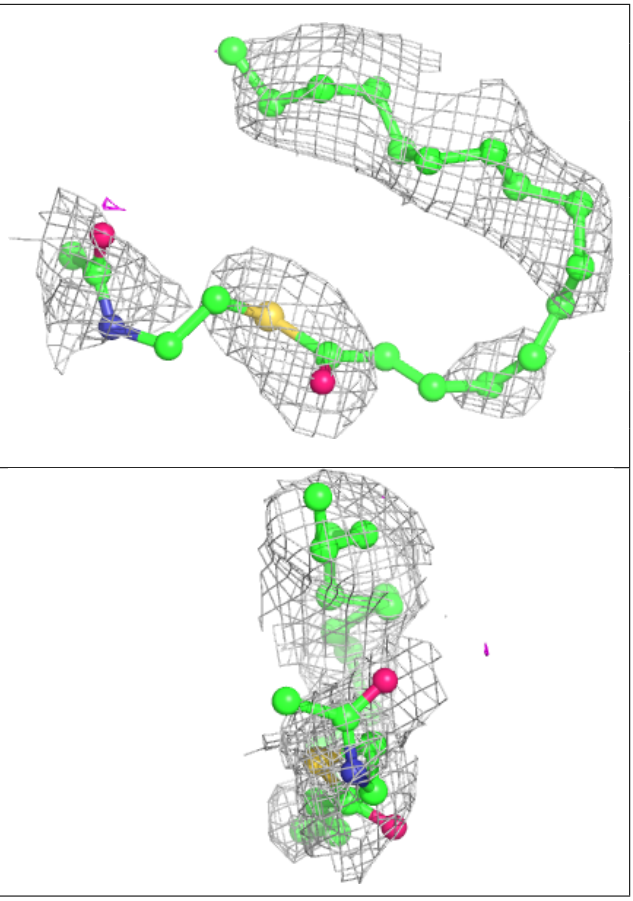
Electron density around THT B 1304:

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



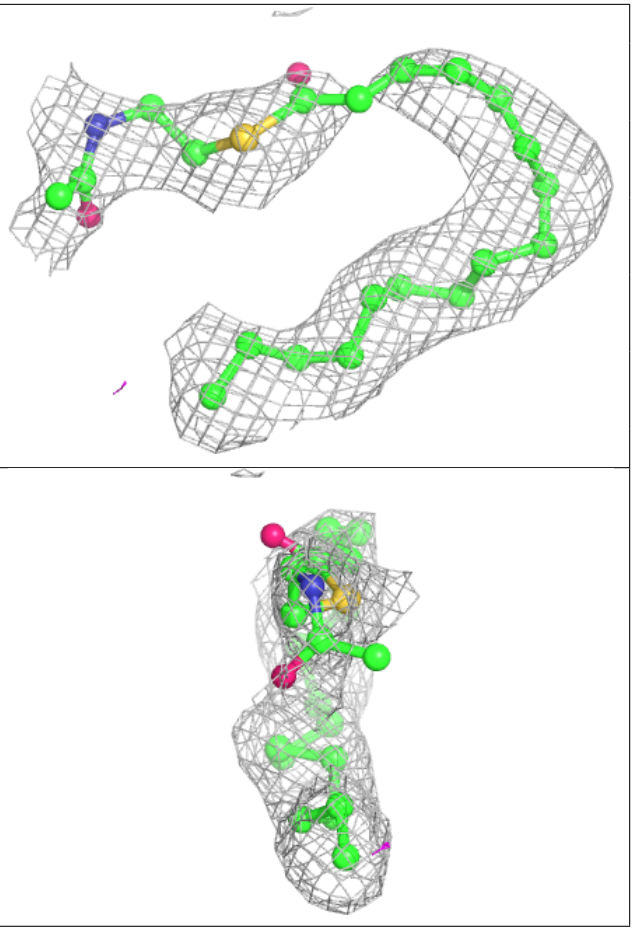
Electron density around THT F 1310:

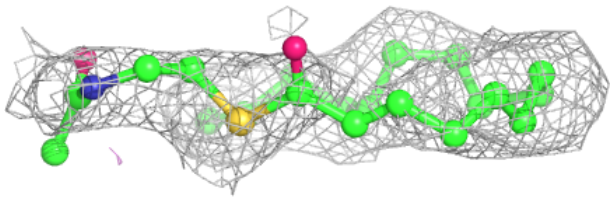
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around THT C 1306:

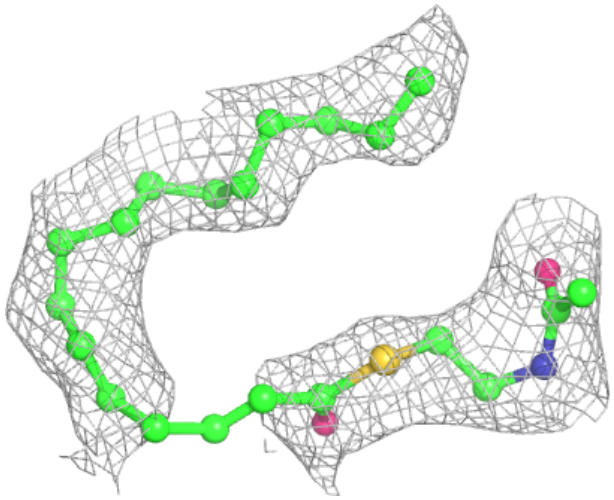
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

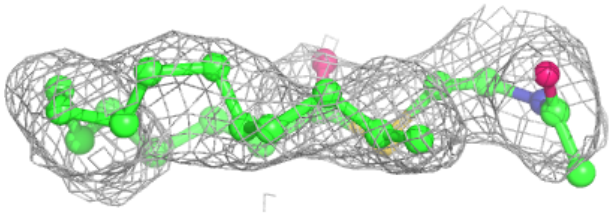


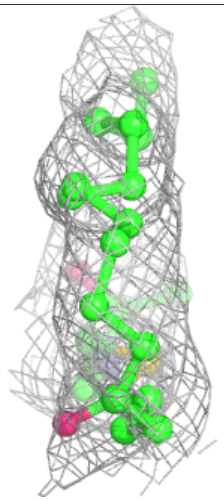


Electron density around THT A 1302:

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

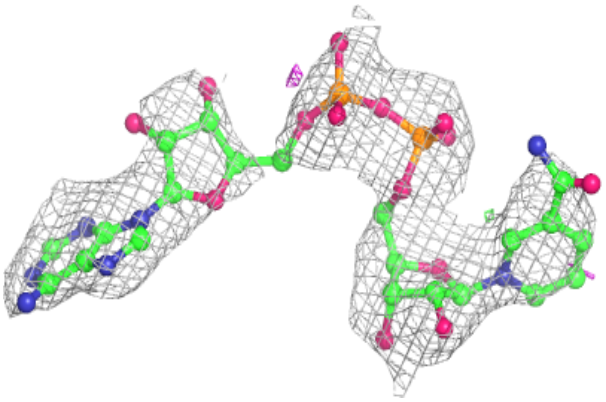


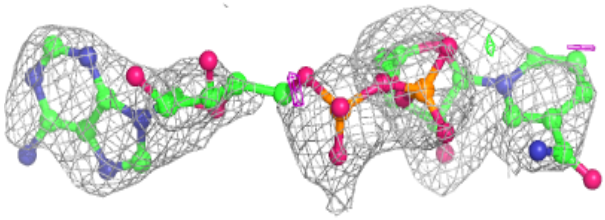


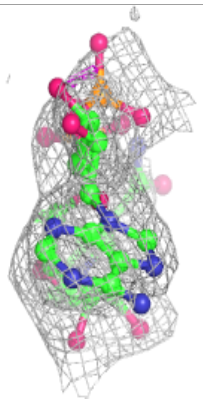


Electron density around NAD F 1309:

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

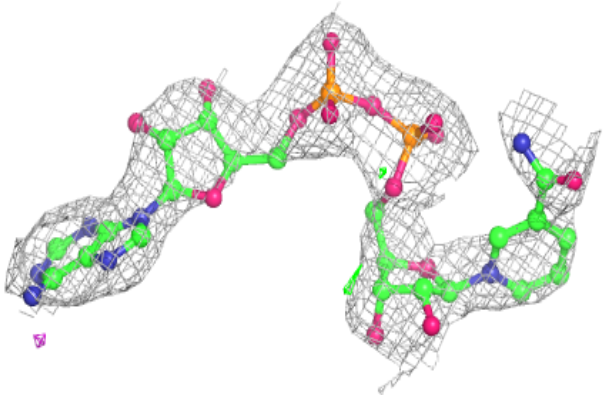


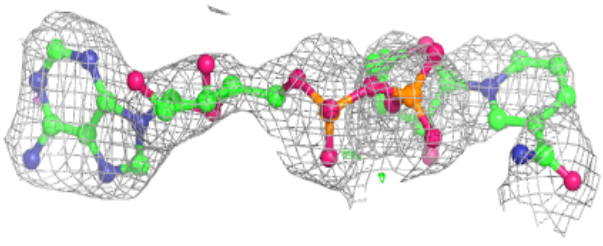


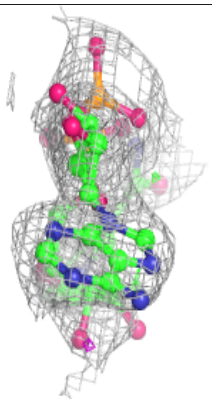


Electron density around NAD D 1307:

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

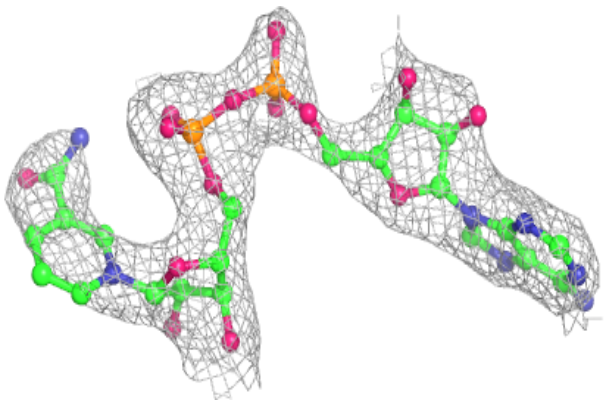


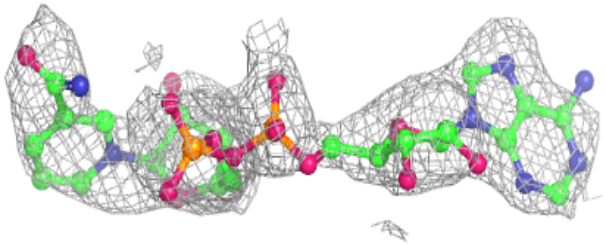


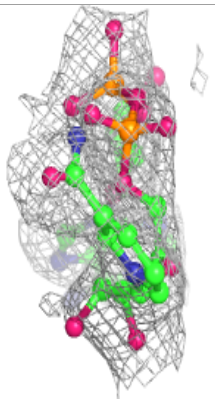


Electron density around NAD A 1301:

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

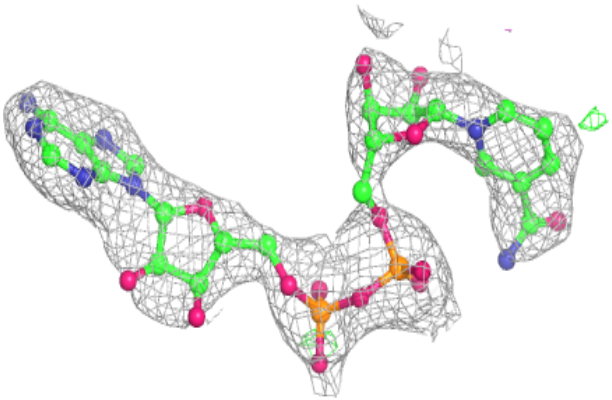


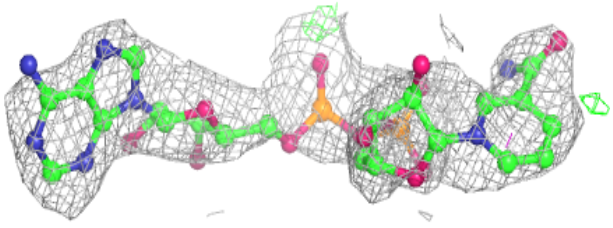


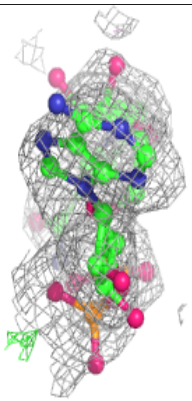


Electron density around NAD B 1303:

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

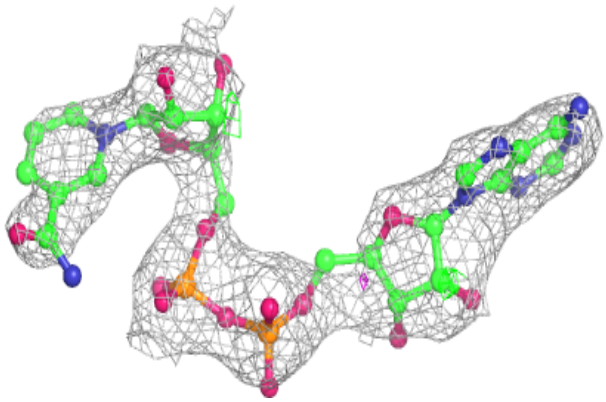


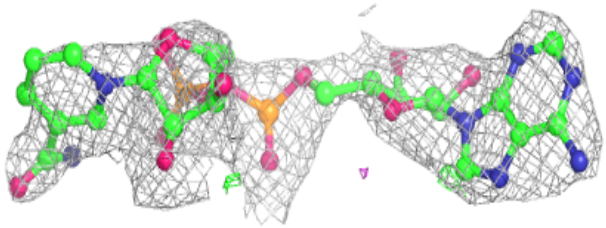


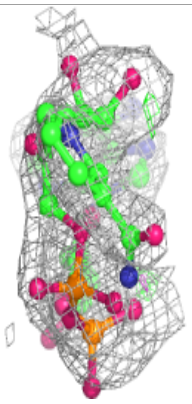


Electron density around NAD C 1305:

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

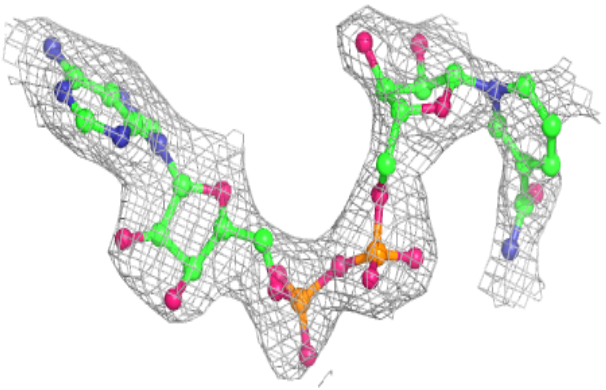


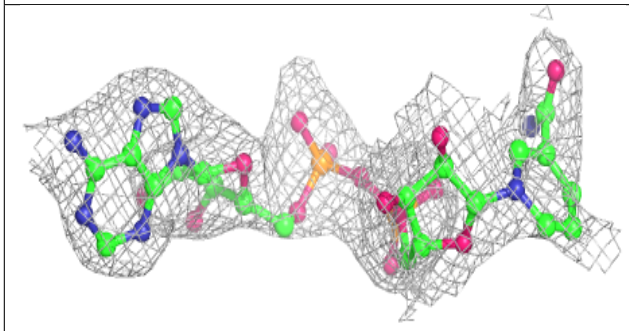


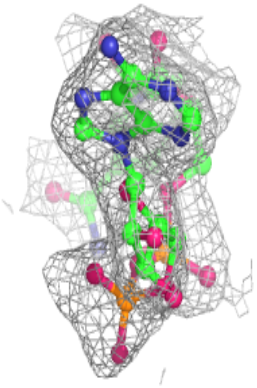


Electron density around NAD E 1308:

$2mF_o$-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.