Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 06:30 PM EDT

PDB ID	:	4XGN
Title	:	Crystal structure of 3-hydroxyacyl-CoA dehydrogenase in complex with NAD from Burkholderia thailandensis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2014-12-31
Resolution	:	1.65 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

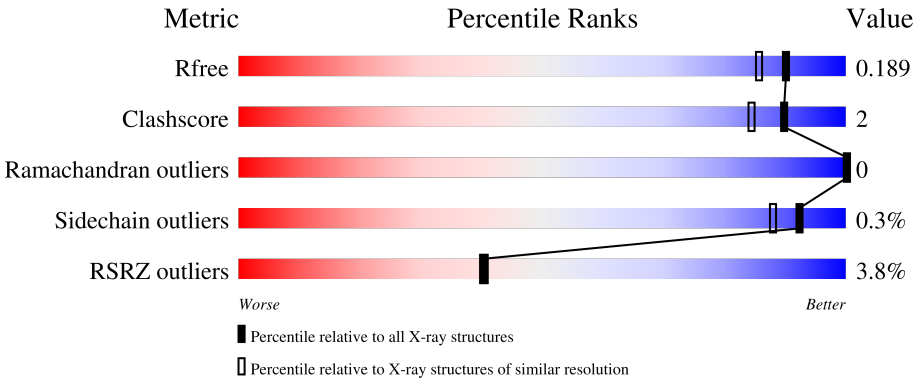
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	260	5% 94%
1	B	260	3% 93%
1	C	260	5% 92% 6%
1	D	260	5% 94%
1	E	260	2% 92% 6%

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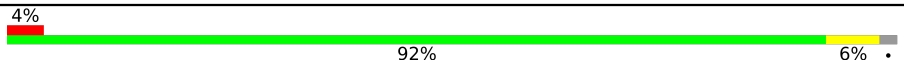
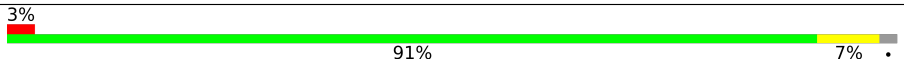
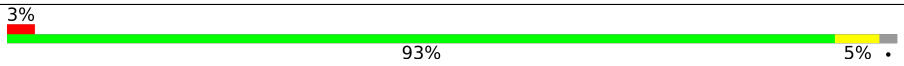
Mol	Chain	Length	Quality of chain
1	F	260	
1	G	260	
1	H	260	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17056 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 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	2	0
			1823	1150	325	335	13			
1	B	255	Total	C	N	O	S	0	3	0
			1837	1160	326	338	13			
1	C	255	Total	C	N	O	S	0	4	0
			1843	1166	328	336	13			
1	D	254	Total	C	N	O	S	0	6	0
			1835	1159	326	336	14			
1	E	253	Total	C	N	O	S	0	5	0
			1827	1156	320	338	13			
1	F	255	Total	C	N	O	S	0	2	0
			1831	1152	328	338	13			
1	G	255	Total	C	N	O	S	0	4	0
			1834	1159	325	337	13			
1	H	255	Total	C	N	O	S	0	4	0
			1835	1159	327	335	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q2T0K5
A	-6	ALA	-	expression tag	UNP Q2T0K5
A	-5	HIS	-	expression tag	UNP Q2T0K5
A	-4	HIS	-	expression tag	UNP Q2T0K5
A	-3	HIS	-	expression tag	UNP Q2T0K5
A	-2	HIS	-	expression tag	UNP Q2T0K5
A	-1	HIS	-	expression tag	UNP Q2T0K5
A	0	HIS	-	expression tag	UNP Q2T0K5
B	-7	MET	-	initiating methionine	UNP Q2T0K5
B	-6	ALA	-	expression tag	UNP Q2T0K5
B	-5	HIS	-	expression tag	UNP Q2T0K5
B	-4	HIS	-	expression tag	UNP Q2T0K5
B	-3	HIS	-	expression tag	UNP Q2T0K5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q2T0K5
B	-1	HIS	-	expression tag	UNP Q2T0K5
B	0	HIS	-	expression tag	UNP Q2T0K5
C	-7	MET	-	initiating methionine	UNP Q2T0K5
C	-6	ALA	-	expression tag	UNP Q2T0K5
C	-5	HIS	-	expression tag	UNP Q2T0K5
C	-4	HIS	-	expression tag	UNP Q2T0K5
C	-3	HIS	-	expression tag	UNP Q2T0K5
C	-2	HIS	-	expression tag	UNP Q2T0K5
C	-1	HIS	-	expression tag	UNP Q2T0K5
C	0	HIS	-	expression tag	UNP Q2T0K5
D	-7	MET	-	initiating methionine	UNP Q2T0K5
D	-6	ALA	-	expression tag	UNP Q2T0K5
D	-5	HIS	-	expression tag	UNP Q2T0K5
D	-4	HIS	-	expression tag	UNP Q2T0K5
D	-3	HIS	-	expression tag	UNP Q2T0K5
D	-2	HIS	-	expression tag	UNP Q2T0K5
D	-1	HIS	-	expression tag	UNP Q2T0K5
D	0	HIS	-	expression tag	UNP Q2T0K5
E	-7	MET	-	initiating methionine	UNP Q2T0K5
E	-6	ALA	-	expression tag	UNP Q2T0K5
E	-5	HIS	-	expression tag	UNP Q2T0K5
E	-4	HIS	-	expression tag	UNP Q2T0K5
E	-3	HIS	-	expression tag	UNP Q2T0K5
E	-2	HIS	-	expression tag	UNP Q2T0K5
E	-1	HIS	-	expression tag	UNP Q2T0K5
E	0	HIS	-	expression tag	UNP Q2T0K5
F	-7	MET	-	initiating methionine	UNP Q2T0K5
F	-6	ALA	-	expression tag	UNP Q2T0K5
F	-5	HIS	-	expression tag	UNP Q2T0K5
F	-4	HIS	-	expression tag	UNP Q2T0K5
F	-3	HIS	-	expression tag	UNP Q2T0K5
F	-2	HIS	-	expression tag	UNP Q2T0K5
F	-1	HIS	-	expression tag	UNP Q2T0K5
F	0	HIS	-	expression tag	UNP Q2T0K5
G	-7	MET	-	initiating methionine	UNP Q2T0K5
G	-6	ALA	-	expression tag	UNP Q2T0K5
G	-5	HIS	-	expression tag	UNP Q2T0K5
G	-4	HIS	-	expression tag	UNP Q2T0K5
G	-3	HIS	-	expression tag	UNP Q2T0K5
G	-2	HIS	-	expression tag	UNP Q2T0K5
G	-1	HIS	-	expression tag	UNP Q2T0K5

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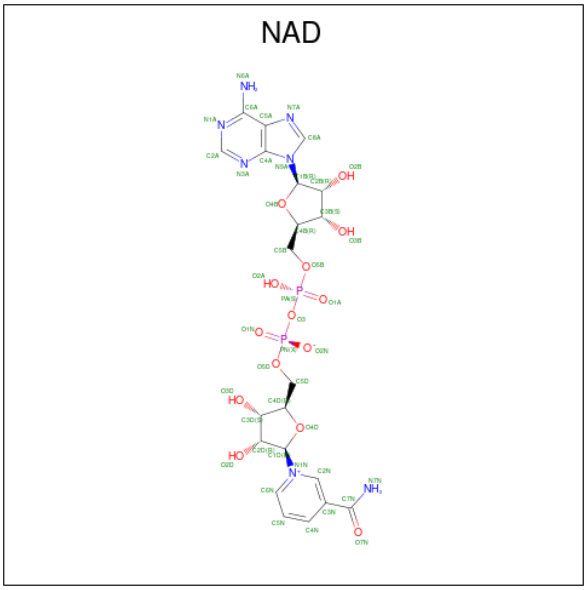
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q2T0K5
H	-7	MET	-	initiating methionine	UNP Q2T0K5
H	-6	ALA	-	expression tag	UNP Q2T0K5
H	-5	HIS	-	expression tag	UNP Q2T0K5
H	-4	HIS	-	expression tag	UNP Q2T0K5
H	-3	HIS	-	expression tag	UNP Q2T0K5
H	-2	HIS	-	expression tag	UNP Q2T0K5
H	-1	HIS	-	expression tag	UNP Q2T0K5
H	0	HIS	-	expression tag	UNP Q2T0K5

- 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		

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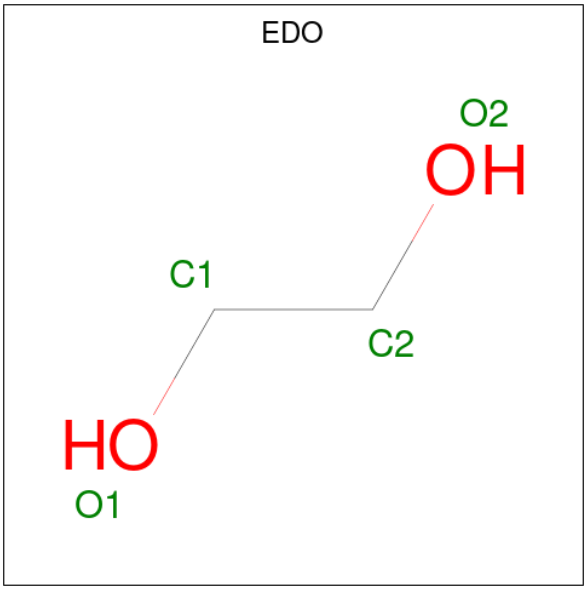
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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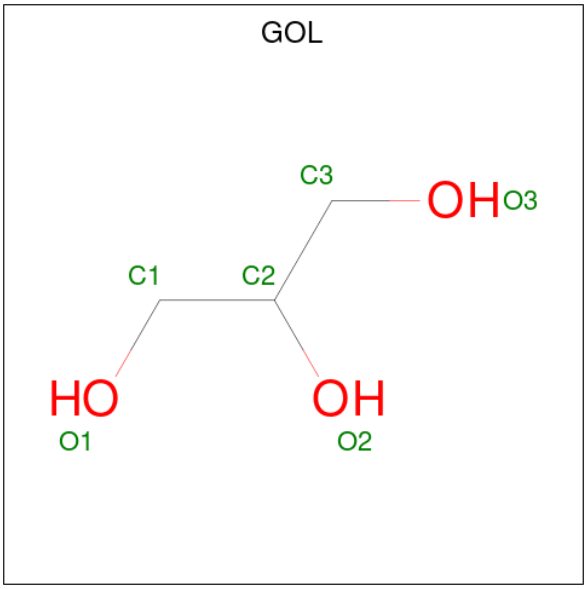
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 8 4 4	0	1
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 8 4 4	0	1
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 12 6 6	0	1
4	D	1	Total C O 12 6 6	0	1
4	G	1	Total C O 12 6 6	0	1
4	H	1	Total C O 12 6 6	0	1

- Molecule 5 is water.

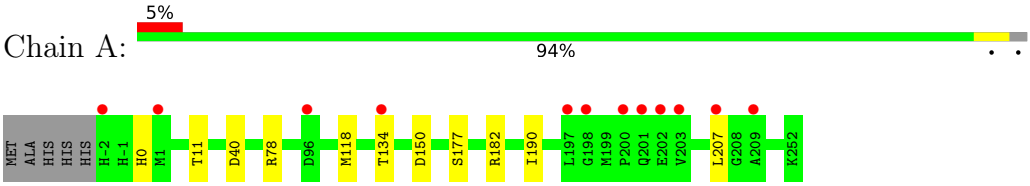
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	260	Total O 260 260	0	0
5	B	244	Total O 244 244	0	0
5	C	249	Total O 249 249	0	0
5	D	223	Total O 223 223	0	0
5	E	218	Total O 218 218	0	0
5	F	231	Total O 231 231	0	0
5	G	235	Total O 235 235	0	0
5	H	263	Total O 263 263	0	0

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.

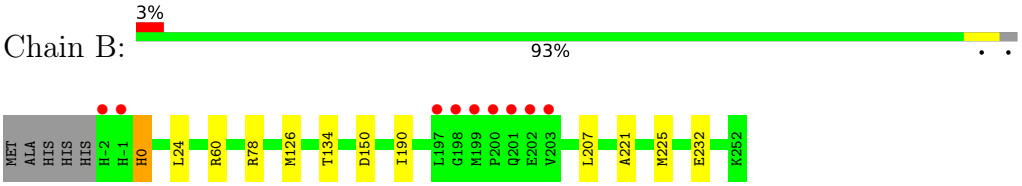
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain A:



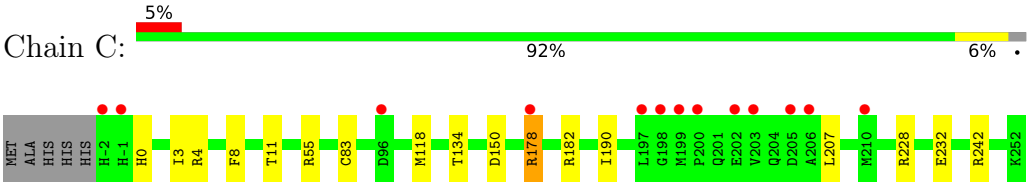
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain B:



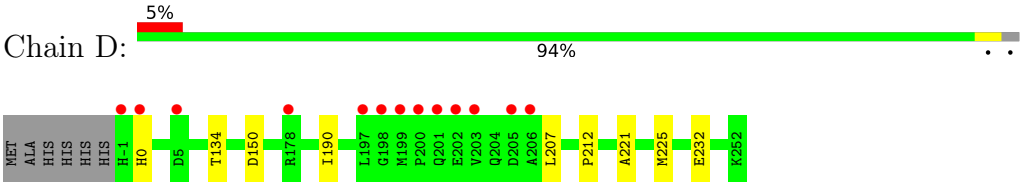
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain C:



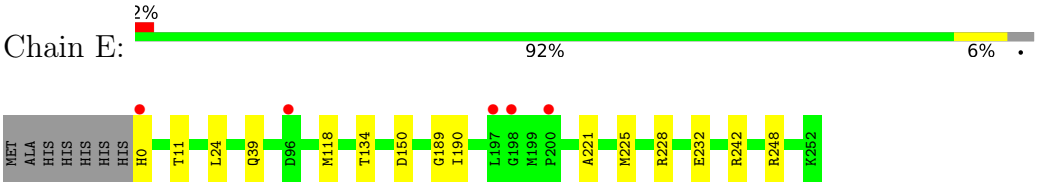
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain D:



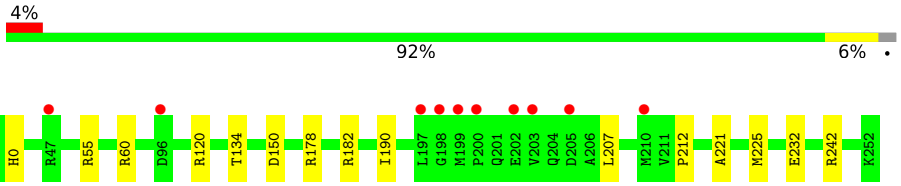
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain E:



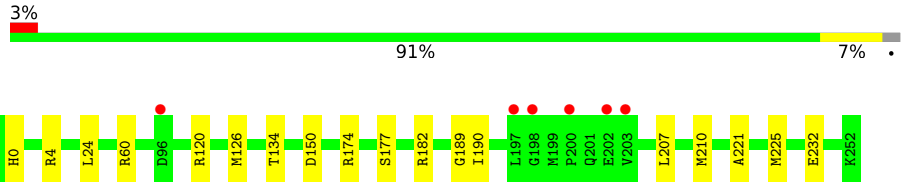
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain F:



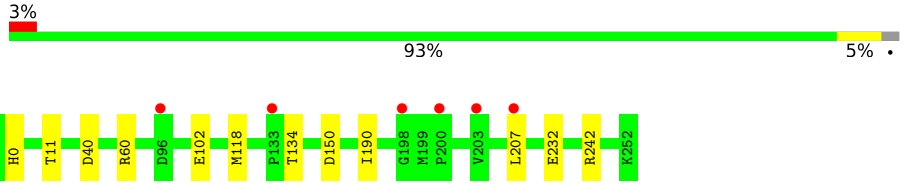
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain G:



• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.22Å 77.10Å 109.35Å 103.26° 93.98° 109.68°	Depositor
Resolution (Å)	50.00 – 1.65 42.22 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-1.65) 97.1 (42.22-1.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.154 , 0.177 0.169 , 0.189	Depositor DCC
R_{free} test set	12256 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17056	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.67% 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: EDO, NAD, GOL

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	0.67	0/1855	0.87	5/2520 (0.2%)
1	B	0.67	0/1872	0.89	6/2540 (0.2%)
1	C	0.63	0/1882	0.90	9/2554 (0.4%)
1	D	0.64	0/1879	0.83	2/2552 (0.1%)
1	E	0.64	0/1868	0.84	4/2540 (0.2%)
1	F	0.66	0/1864	0.90	6/2532 (0.2%)
1	G	0.65	0/1872	0.92	8/2543 (0.3%)
1	H	0.65	0/1874	0.88	6/2545 (0.2%)
All	All	0.65	0/14966	0.88	46/20326 (0.2%)

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	F	0	1

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	60	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	G	60	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	C	178	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	D	150	ASP	CB-CG-OD1	8.04	125.53	118.30
1	E	150	ASP	CB-CG-OD1	7.45	125.01	118.30
1	F	150	ASP	CB-CG-OD1	7.43	124.99	118.30
1	C	242	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	F	55	ARG	NE-CZ-NH2	7.33	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	60	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	60	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	C	150	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	150	ASP	CB-CG-OD1	7.04	124.63	118.30
1	C	182	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	E	150	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	F	242	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	B	150	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	F	178	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	H	40	ASP	CB-CG-OD1	6.65	124.29	118.30
1	G	150	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	G	126	MET	CG-SD-CE	-6.46	89.87	100.20
1	F	182	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	H	60	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	150	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	D	150	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	G	182	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	H	150	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	60	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	C	4	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	150	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	E	242	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	C	4	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	126	MET	CG-SD-CE	-5.69	91.10	100.20
1	A	78	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	G	120	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	55	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	E	248	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	150	ASP	CB-CG-OD1	5.49	123.24	118.30
1	F	60	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	H	150	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	G	174	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	78	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	H	242	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	40	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	4	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	182	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	178	ARG	NE-CZ-NH1	-5.09	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	120	ARG	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	1823	0	1869	4	0
1	B	1837	0	1895	7	0
1	C	1843	0	1907	9	0
1	D	1835	0	1886	8	0
1	E	1827	0	1881	9	0
1	F	1831	0	1867	6	0
1	G	1834	0	1886	9	0
1	H	1835	0	1885	7	0
2	A	44	0	25	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	1	0
2	H	44	0	26	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
3	E	8	0	12	0	0
3	F	12	0	18	0	0
3	G	12	0	18	0	0
3	H	8	0	12	0	0
4	C	12	0	16	0	0
4	D	12	0	16	0	0
4	G	12	0	16	0	0
4	H	12	0	16	0	0
5	A	260	0	0	0	0
5	B	244	0	0	2	0
5	C	249	0	0	1	0
5	D	223	0	0	0	0
5	E	218	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	231	0	0	0	0
5	G	235	0	0	2	0
5	H	263	0	0	1	0
All	All	17056	0	15449	56	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 2.

All (56) 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:G:24[A]:LEU:HD12	5:G:626:HOH:O	1.62	0.98
1:B:24[B]:LEU:HD12	5:B:637:HOH:O	1.82	0.79
1:B:0:HIS:HB3	1:B:232:GLU:O	1.89	0.73
1:A:0:HIS:HA	1:A:134:THR:HG21	1.74	0.69
1:E:0:HIS:HB2	1:E:232:GLU:O	1.90	0.69
1:D:190:ILE:HD13	1:D:207:LEU:HG	1.73	0.68
1:F:190[B]:ILE:HD13	1:F:207:LEU:HG	1.76	0.67
1:B:24[B]:LEU:CD1	5:B:637:HOH:O	2.43	0.64
1:D:0:HIS:HA	1:D:134:THR:HG21	1.81	0.62
1:C:190[B]:ILE:HD13	1:C:207:LEU:HG	1.81	0.62
1:G:0:HIS:HA	1:G:134:THR:HG21	1.83	0.59
1:E:0:HIS:HA	1:E:134:THR:HG21	1.84	0.59
1:G:24[A]:LEU:CD1	5:G:626:HOH:O	2.30	0.59
1:A:190:ILE:HD13	1:A:207:LEU:HG	1.84	0.58
1:F:0:HIS:HA	1:F:134:THR:HG21	1.85	0.58
1:B:0:HIS:HA	1:B:134:THR:HG21	1.86	0.57
1:G:0:HIS:HB3	1:G:232:GLU:O	2.05	0.57
1:E:225:MET:HE1	1:H:232:GLU:O	2.07	0.55
1:D:0:HIS:CB	1:D:232:GLU:O	2.55	0.54
1:G:221:ALA:O	1:G:225:MET:HG3	2.07	0.54
1:B:190[A]:ILE:HD13	1:B:207:LEU:HG	1.88	0.54
1:C:0:HIS:HB3	1:C:232:GLU:O	2.08	0.53
1:E:0:HIS:CB	1:E:232:GLU:O	2.57	0.52
1:D:0:HIS:CA	1:D:134:THR:HG21	2.40	0.52
1:H:190[A]:ILE:HD13	1:H:207:LEU:HG	1.93	0.51
1:D:0:HIS:HB2	1:D:232:GLU:O	2.11	0.50
1:G:190[A]:ILE:HD13	1:G:207:LEU:HG	1.93	0.50
1:H:0:HIS:HB3	1:H:232:GLU:O	2.12	0.49
1:B:221:ALA:O	1:B:225:MET:HG3	2.12	0.49
1:B:0:HIS:CB	1:B:232:GLU:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:0:HIS:HB3	1:F:232:GLU:O	2.13	0.48
1:H:102:GLU:HG2	5:H:427:HOH:O	2.12	0.47
1:C:3[B]:ILE:HD12	1:C:8:PHE:CZ	2.50	0.47
1:E:189:GLY:O	1:E:190[A]:ILE:HD13	2.15	0.47
1:G:0:HIS:CB	1:G:232:GLU:O	2.63	0.46
1:E:0:HIS:CA	1:E:134:THR:HG21	2.45	0.45
1:H:11:THR:HG21	1:H:118:MET:HG3	1.99	0.44
1:F:212:PRO:O	1:G:177:SER:HB2	2.17	0.44
1:F:221:ALA:O	1:F:225:MET:HG3	2.17	0.44
1:C:0:HIS:HA	1:C:134:THR:HG21	2.00	0.44
1:D:221:ALA:O	1:D:225[A]:MET:HG3	2.18	0.43
1:C:11:THR:O	1:C:83:CYS:HB2	2.18	0.43
1:D:0:HIS:HB3	1:D:232:GLU:O	2.18	0.43
1:C:228:ARG:NH1	5:C:550:HOH:O	2.37	0.43
1:H:0:HIS:CB	1:H:232:GLU:O	2.66	0.43
1:E:24[B]:LEU:HD21	1:E:228:ARG:HD2	2.01	0.43
1:F:0:HIS:CB	1:F:232:GLU:O	2.67	0.43
1:E:11:THR:HG21	1:E:118:MET:HG3	2.00	0.42
1:H:0:HIS:HA	1:H:134:THR:HG21	2.01	0.42
1:E:221:ALA:O	1:E:225:MET:HG3	2.19	0.42
1:A:177:SER:HB2	1:D:212:PRO:O	2.20	0.41
1:C:11:THR:HG21	1:C:118:MET:HG3	2.02	0.40
1:A:11:THR:HG21	1:A:118:MET:HG3	2.03	0.40
1:C:0:HIS:CB	1:C:232:GLU:O	2.68	0.40
1:G:189:GLY:O	2:G:302:NAD:H4N	2.21	0.40

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	255/260 (98%)	248 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	256/260 (98%)	250 (98%)	6 (2%)	0	100	100
1	C	257/260 (99%)	251 (98%)	6 (2%)	0	100	100
1	D	258/260 (99%)	250 (97%)	8 (3%)	0	100	100
1	E	256/260 (98%)	249 (97%)	7 (3%)	0	100	100
1	F	255/260 (98%)	249 (98%)	6 (2%)	0	100	100
1	G	257/260 (99%)	251 (98%)	6 (2%)	0	100	100
1	H	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
All	All	2051/2080 (99%)	1998 (97%)	53 (3%)	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	177/187 (95%)	177 (100%)	0	100	100
1	B	180/187 (96%)	179 (99%)	1 (1%)	86	76
1	C	181/187 (97%)	180 (99%)	1 (1%)	86	76
1	D	179/187 (96%)	179 (100%)	0	100	100
1	E	180/187 (96%)	179 (99%)	1 (1%)	86	76
1	F	178/187 (95%)	178 (100%)	0	100	100
1	G	179/187 (96%)	178 (99%)	1 (1%)	86	76
1	H	179/187 (96%)	179 (100%)	0	100	100
All	All	1433/1496 (96%)	1429 (100%)	4 (0%)	92	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	HIS
1	C	178	ARG

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Mol	Chain	Res	Type
1	E	39	GLN
1	G	210	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	D	250	GLN
1	F	250	GLN
1	G	250	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

33 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	$\#\|Z\| > 2$
4	GOL	G	301[B]	-	5,5,5	0.29	0	5,5,5	1.41	1 (20%)
4	GOL	H	301[A]	-	5,5,5	0.48	0	5,5,5	1.16	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	H	302	-	42,48,48	3.99	13 (30%)	50,73,73	1.92	8 (16%)
3	EDO	A	302	-	3,3,3	0.37	0	2,2,2	0.31	0
4	GOL	C	303[B]	-	5,5,5	0.37	0	5,5,5	1.22	1 (20%)
3	EDO	H	303	-	3,3,3	0.77	0	2,2,2	0.15	0
4	GOL	D	301[B]	-	5,5,5	0.34	0	5,5,5	0.72	0
3	EDO	C	302	-	3,3,3	0.66	0	2,2,2	0.17	0
3	EDO	A	301	-	3,3,3	0.73	0	2,2,2	0.10	0
3	EDO	D	303	-	3,3,3	0.49	0	2,2,2	0.27	0
2	NAD	B	300	-	42,48,48	3.50	11 (26%)	50,73,73	1.62	7 (14%)
3	EDO	B	302	-	3,3,3	0.42	0	2,2,2	0.42	0
4	GOL	H	301[B]	-	5,5,5	0.26	0	5,5,5	0.92	0
3	EDO	F	302[A]	-	3,3,3	0.42	0	2,2,2	0.21	0
2	NAD	A	300	-	42,48,48	4.07	14 (33%)	50,73,73	1.89	10 (20%)
3	EDO	G	304[A]	-	3,3,3	0.38	0	2,2,2	0.30	0
4	GOL	G	301[A]	-	5,5,5	0.33	0	5,5,5	0.70	0
3	EDO	E	302	-	3,3,3	0.39	0	2,2,2	0.31	0
2	NAD	G	302	-	42,48,48	3.76	11 (26%)	50,73,73	1.62	7 (14%)
3	EDO	D	304	-	3,3,3	0.42	0	2,2,2	0.08	0
3	EDO	G	303	-	3,3,3	0.66	0	2,2,2	0.20	0
4	GOL	C	303[A]	-	5,5,5	0.27	0	5,5,5	0.69	0
2	NAD	C	301	-	42,48,48	3.75	11 (26%)	50,73,73	1.70	8 (16%)
4	GOL	D	301[A]	-	5,5,5	0.35	0	5,5,5	1.03	0
3	EDO	F	301	-	3,3,3	0.63	0	2,2,2	0.35	0
3	EDO	B	301	-	3,3,3	0.53	0	2,2,2	0.11	0
2	NAD	D	302	-	42,48,48	4.07	9 (21%)	50,73,73	1.75	12 (24%)
2	NAD	F	300	-	42,48,48	3.60	12 (28%)	50,73,73	1.70	9 (18%)
3	EDO	H	304	-	3,3,3	0.41	0	2,2,2	0.26	0
2	NAD	E	300	-	42,48,48	3.79	9 (21%)	50,73,73	1.92	11 (22%)
3	EDO	F	302[B]	-	3,3,3	0.42	0	2,2,2	0.42	0
3	EDO	G	304[B]	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	E	301	-	3,3,3	0.46	0	2,2,2	0.02	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	301[B]	-	-	4/4/4/4	-
4	GOL	H	301[A]	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	H	302	-	-	7/26/62/62	0/5/5/5
3	EDO	A	302	-	-	1/1/1/1	-
4	GOL	C	303[B]	-	-	1/4/4/4	-
3	EDO	H	303	-	-	0/1/1/1	-
4	GOL	D	301[B]	-	-	3/4/4/4	-
3	EDO	C	302	-	-	0/1/1/1	-
3	EDO	A	301	-	-	0/1/1/1	-
3	EDO	D	303	-	-	0/1/1/1	-
2	NAD	B	300	-	-	8/26/62/62	0/5/5/5
3	EDO	B	302	-	-	1/1/1/1	-
4	GOL	H	301[B]	-	-	3/4/4/4	-
3	EDO	F	302[A]	-	-	0/1/1/1	-
2	NAD	A	300	-	-	8/26/62/62	0/5/5/5
3	EDO	G	304[A]	-	-	0/1/1/1	-
4	GOL	G	301[A]	-	-	2/4/4/4	-
3	EDO	E	302	-	-	0/1/1/1	-
2	NAD	G	302	-	-	6/26/62/62	0/5/5/5
3	EDO	D	304	-	-	0/1/1/1	-
3	EDO	G	303	-	-	0/1/1/1	-
4	GOL	C	303[A]	-	-	4/4/4/4	-
2	NAD	C	301	-	-	7/26/62/62	0/5/5/5
4	GOL	D	301[A]	-	-	4/4/4/4	-
3	EDO	F	301	-	-	1/1/1/1	-
3	EDO	B	301	-	-	0/1/1/1	-
2	NAD	D	302	-	-	7/26/62/62	0/5/5/5
2	NAD	F	300	-	-	7/26/62/62	0/5/5/5
3	EDO	H	304	-	-	0/1/1/1	-
2	NAD	E	300	-	-	6/26/62/62	0/5/5/5
3	EDO	F	302[B]	-	-	1/1/1/1	-
3	EDO	G	304[B]	-	-	0/1/1/1	-
3	EDO	E	301	-	-	0/1/1/1	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	NAD	C2D-C1D	-14.27	1.32	1.53
2	D	302	NAD	C2D-C1D	-13.44	1.33	1.53
2	C	301	NAD	C2D-C1D	-13.43	1.33	1.53
2	A	300	NAD	C2B-C1B	-13.35	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	302	NAD	C2B-C1B	-12.92	1.34	1.53
2	G	302	NAD	C2D-C1D	-12.58	1.34	1.53
2	C	301	NAD	C2B-C1B	-12.53	1.34	1.53
2	H	302	NAD	C2D-C1D	-12.49	1.34	1.53
2	F	300	NAD	C2B-C1B	-12.40	1.34	1.53
2	F	300	NAD	C2D-C1D	-12.32	1.35	1.53
2	B	300	NAD	C2D-C1D	-12.20	1.35	1.53
2	D	302	NAD	O4D-C1D	12.01	1.57	1.41
2	E	300	NAD	C2D-C1D	-11.82	1.35	1.53
2	D	302	NAD	C2B-C1B	-11.79	1.35	1.53
2	G	302	NAD	C2B-C1B	-11.63	1.36	1.53
2	B	300	NAD	C2B-C1B	-11.53	1.36	1.53
2	E	300	NAD	C2B-C1B	-11.25	1.36	1.53
2	H	302	NAD	O4D-C1D	11.18	1.56	1.41
2	E	300	NAD	O4D-C1D	10.98	1.56	1.41
2	A	300	NAD	O4D-C1D	10.57	1.55	1.41
2	G	302	NAD	O4D-C1D	10.28	1.55	1.41
2	D	302	NAD	O4B-C1B	9.58	1.54	1.41
2	C	301	NAD	O4D-C1D	9.27	1.54	1.41
2	E	300	NAD	O4B-C1B	9.20	1.53	1.41
2	F	300	NAD	O4D-C1D	9.08	1.53	1.41
2	G	302	NAD	O4B-C1B	8.72	1.53	1.41
2	B	300	NAD	O4D-C1D	8.63	1.53	1.41
2	H	302	NAD	O4B-C1B	8.10	1.52	1.41
2	A	300	NAD	O4B-C1B	7.87	1.52	1.41
2	C	301	NAD	O4B-C1B	7.64	1.51	1.41
2	B	300	NAD	O4B-C1B	7.17	1.51	1.41
2	F	300	NAD	O4B-C1B	6.79	1.50	1.41
2	D	302	NAD	O4B-C4B	-5.89	1.31	1.45
2	E	300	NAD	O4B-C4B	-5.83	1.32	1.45
2	H	302	NAD	O4B-C4B	-5.58	1.32	1.45
2	H	302	NAD	C7N-N7N	5.06	1.42	1.33
2	A	300	NAD	C7N-N7N	4.97	1.42	1.33
2	A	300	NAD	O4B-C4B	-4.94	1.33	1.45
2	D	302	NAD	C7N-N7N	4.73	1.42	1.33
2	E	300	NAD	C7N-N7N	4.69	1.41	1.33
2	C	301	NAD	O4B-C4B	-4.58	1.34	1.45
2	E	300	NAD	O4D-C4D	-4.53	1.34	1.45
2	D	302	NAD	O4D-C4D	-4.47	1.35	1.45
2	F	300	NAD	O4B-C4B	-4.44	1.35	1.45
2	G	302	NAD	O4B-C4B	-4.29	1.35	1.45
2	C	301	NAD	C2N-N1N	4.25	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	302	NAD	C7N-N7N	4.23	1.41	1.33
2	D	302	NAD	C2A-N3A	4.16	1.38	1.32
2	G	302	NAD	O4D-C4D	-4.08	1.35	1.45
2	C	301	NAD	C7N-N7N	3.86	1.40	1.33
2	F	300	NAD	C7N-N7N	3.85	1.40	1.33
2	B	300	NAD	C7N-N7N	3.85	1.40	1.33
2	B	300	NAD	C2N-N1N	3.80	1.39	1.35
2	A	300	NAD	O4D-C4D	-3.53	1.37	1.45
2	H	302	NAD	C6A-N6A	3.50	1.46	1.34
2	H	302	NAD	O4D-C4D	-3.42	1.37	1.45
2	B	300	NAD	O4D-C4D	-3.37	1.37	1.45
2	F	300	NAD	C2N-N1N	3.30	1.39	1.35
2	H	302	NAD	C2N-N1N	3.27	1.38	1.35
2	A	300	NAD	O2D-C2D	3.20	1.50	1.43
2	F	300	NAD	C2A-N3A	3.18	1.37	1.32
2	G	302	NAD	C2A-N3A	3.16	1.37	1.32
2	H	302	NAD	O2D-C2D	3.14	1.50	1.43
2	H	302	NAD	C2A-N3A	3.14	1.37	1.32
2	F	300	NAD	O4D-C4D	-3.10	1.38	1.45
2	A	300	NAD	C2A-N3A	3.06	1.37	1.32
2	C	301	NAD	C2A-N3A	3.00	1.36	1.32
2	G	302	NAD	O2D-C2D	3.00	1.50	1.43
2	F	300	NAD	O2B-C2B	2.88	1.49	1.43
2	B	300	NAD	O4B-C4B	-2.87	1.38	1.45
2	C	301	NAD	O4D-C4D	-2.75	1.38	1.45
2	A	300	NAD	O3D-C3D	-2.72	1.36	1.43
2	G	302	NAD	C2N-N1N	2.58	1.38	1.35
2	D	302	NAD	C2A-N1A	2.57	1.38	1.33
2	F	300	NAD	O3D-C3D	-2.52	1.37	1.43
2	A	300	NAD	C6A-N6A	2.50	1.43	1.34
2	A	300	NAD	C2N-N1N	2.48	1.38	1.35
2	G	302	NAD	O3D-C3D	-2.38	1.37	1.43
2	C	301	NAD	C6A-N6A	2.33	1.42	1.34
2	H	302	NAD	O3D-C3D	-2.28	1.37	1.43
2	B	300	NAD	O3D-C3D	-2.26	1.37	1.43
2	B	300	NAD	C2A-N1A	2.25	1.38	1.33
2	B	300	NAD	O2D-C2D	2.24	1.48	1.43
2	A	300	NAD	C5A-C4A	-2.19	1.35	1.40
2	E	300	NAD	C3N-C7N	2.16	1.53	1.50
2	E	300	NAD	C2A-N1A	2.12	1.37	1.33
2	A	300	NAD	O2B-C2B	2.08	1.47	1.43
2	C	301	NAD	O2B-C2B	2.08	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	302	NAD	C2A-N1A	2.06	1.37	1.33
2	F	300	NAD	O2D-C2D	2.06	1.47	1.43

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	300	NAD	C5A-C6A-N6A	6.47	130.19	120.35
2	H	302	NAD	N3A-C2A-N1A	-6.43	118.62	128.68
2	E	300	NAD	N3A-C2A-N1A	-6.03	119.25	128.68
2	C	301	NAD	C5A-C6A-N6A	5.90	129.31	120.35
2	H	302	NAD	C6N-N1N-C2N	-5.79	116.70	121.97
2	A	300	NAD	N3A-C2A-N1A	-5.60	119.93	128.68
2	A	300	NAD	C5A-C6A-N6A	5.57	128.82	120.35
2	D	302	NAD	N3A-C2A-N1A	-5.48	120.11	128.68
2	H	302	NAD	C5A-C6A-N6A	5.21	128.27	120.35
2	E	300	NAD	C6N-N1N-C2N	-5.06	117.36	121.97
2	G	302	NAD	N3A-C2A-N1A	-4.96	120.93	128.68
2	B	300	NAD	N3A-C2A-N1A	-4.63	121.45	128.68
2	D	302	NAD	C5A-C6A-N6A	4.49	127.17	120.35
2	A	300	NAD	O4B-C1B-C2B	-4.45	100.42	106.93
2	G	302	NAD	C5A-C6A-N6A	4.23	126.79	120.35
2	G	302	NAD	C6N-N1N-C2N	-4.21	118.13	121.97
2	B	300	NAD	C6N-N1N-C2N	-4.20	118.14	121.97
2	B	300	NAD	C5A-C6A-N6A	4.20	126.73	120.35
2	C	301	NAD	N3A-C2A-N1A	-4.19	122.14	128.68
2	E	300	NAD	C5A-C6A-N6A	4.16	126.68	120.35
2	F	300	NAD	N6A-C6A-N1A	-4.02	110.22	118.57
2	C	301	NAD	C6N-N1N-C2N	-3.74	118.56	121.97
2	F	300	NAD	C6N-N1N-C2N	-3.72	118.58	121.97
2	F	300	NAD	N3A-C2A-N1A	-3.67	122.94	128.68
2	A	300	NAD	C6N-N1N-C2N	-3.62	118.67	121.97
2	H	302	NAD	O4B-C1B-C2B	-3.59	101.67	106.93
2	A	300	NAD	C3B-C2B-C1B	3.58	106.37	100.98
2	E	300	NAD	O4B-C1B-C2B	-3.56	101.73	106.93
2	G	302	NAD	O4B-C1B-C2B	-3.51	101.80	106.93
2	B	300	NAD	O4B-C1B-C2B	-3.50	101.81	106.93
2	C	301	NAD	C3B-C2B-C1B	3.46	106.18	100.98
2	H	302	NAD	C3B-C2B-C1B	3.38	106.06	100.98
2	C	301	NAD	N6A-C6A-N1A	-3.32	111.68	118.57
2	D	302	NAD	C6N-N1N-C2N	-3.31	118.96	121.97
2	D	302	NAD	N6A-C6A-N1A	-3.17	111.98	118.57
2	E	300	NAD	C3B-C2B-C1B	3.14	105.71	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	NAD	N6A-C6A-N1A	-3.08	112.17	118.57
2	D	302	NAD	C3B-C2B-C1B	2.96	105.44	100.98
2	H	302	NAD	N6A-C6A-N1A	-2.87	112.62	118.57
2	E	300	NAD	O4B-C4B-C3B	2.83	110.71	105.11
2	D	302	NAD	O4B-C1B-C2B	-2.80	102.84	106.93
2	F	300	NAD	O7N-C7N-N7N	-2.79	118.61	122.58
2	H	302	NAD	C3N-C2N-N1N	2.78	123.14	120.43
4	G	301[B]	GOL	O1-C1-C2	-2.77	96.90	110.20
2	D	302	NAD	O4D-C1D-C2D	-2.74	102.92	106.93
2	G	302	NAD	C3B-C2B-C1B	2.69	105.02	100.98
2	E	300	NAD	C3N-C7N-N7N	2.68	120.97	117.75
2	E	300	NAD	C2N-N1N-C1D	2.65	125.03	119.14
2	B	300	NAD	N6A-C6A-N1A	-2.60	113.17	118.57
2	B	300	NAD	C3B-C2B-C1B	2.59	104.88	100.98
2	D	302	NAD	C3N-C7N-N7N	2.56	120.82	117.75
2	F	300	NAD	O4B-C1B-C2B	-2.55	103.19	106.93
2	B	300	NAD	O4D-C1D-C2D	-2.50	103.27	106.93
2	E	300	NAD	C3N-C2N-N1N	2.47	122.84	120.43
2	C	301	NAD	O4B-C1B-C2B	-2.46	103.34	106.93
2	H	302	NAD	C2N-N1N-C1D	2.44	124.57	119.14
2	A	300	NAD	O4D-C1D-C2D	-2.44	103.37	106.93
2	A	300	NAD	C3N-C7N-N7N	2.37	120.59	117.75
2	F	300	NAD	C3B-C2B-C1B	2.34	104.50	100.98
2	E	300	NAD	N6A-C6A-N1A	-2.30	113.79	118.57
2	E	300	NAD	C2B-C3B-C4B	-2.27	98.23	102.64
2	C	301	NAD	O4D-C1D-C2D	-2.22	103.69	106.93
2	F	300	NAD	O4D-C1D-C2D	-2.18	103.74	106.93
2	A	300	NAD	PN-O3-PA	-2.16	125.43	132.83
2	C	301	NAD	C2D-C3D-C4D	-2.15	98.46	102.64
2	D	302	NAD	O7N-C7N-N7N	-2.13	119.55	122.58
4	C	303[B]	GOL	O1-C1-C2	-2.13	100.00	110.20
2	G	302	NAD	N6A-C6A-N1A	-2.12	114.17	118.57
2	D	302	NAD	C1B-N9A-C4A	-2.12	122.91	126.64
4	H	301[A]	GOL	O3-C3-C2	-2.10	100.14	110.20
2	D	302	NAD	C2N-N1N-C1D	2.09	123.78	119.14
2	D	302	NAD	O4B-C4B-C3B	2.09	109.24	105.11
2	G	302	NAD	O4D-C1D-C2D	-2.07	103.90	106.93
2	F	300	NAD	C3N-C7N-N7N	2.07	120.24	117.75
2	A	300	NAD	O4B-C4B-C5B	-2.02	102.72	109.37

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NAD	C5D-O5D-PN-O3
2	A	300	NAD	C5D-O5D-PN-O1N
2	A	300	NAD	C5D-O5D-PN-O2N
2	A	300	NAD	O4D-C1D-N1N-C2N
2	B	300	NAD	C5D-O5D-PN-O3
2	B	300	NAD	O4D-C1D-N1N-C2N
2	C	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	O4D-C1D-N1N-C2N
2	D	302	NAD	C5D-O5D-PN-O1N
2	D	302	NAD	C5D-O5D-PN-O2N
2	D	302	NAD	O4D-C1D-N1N-C2N
2	E	300	NAD	C5D-O5D-PN-O1N
2	E	300	NAD	C5D-O5D-PN-O2N
2	E	300	NAD	O4D-C1D-N1N-C2N
2	F	300	NAD	C5D-O5D-PN-O1N
2	F	300	NAD	C5D-O5D-PN-O2N
2	F	300	NAD	O4D-C1D-N1N-C2N
2	G	302	NAD	C5D-O5D-PN-O1N
2	G	302	NAD	C5D-O5D-PN-O2N
2	G	302	NAD	O4D-C1D-N1N-C2N
2	H	302	NAD	PN-O3-PA-O5B
2	H	302	NAD	C5D-O5D-PN-O3
2	H	302	NAD	C5D-O5D-PN-O1N
2	H	302	NAD	C5D-O5D-PN-O2N
2	H	302	NAD	O4D-C1D-N1N-C2N
4	C	303[A]	GOL	C1-C2-C3-O3
4	C	303[A]	GOL	O2-C2-C3-O3
4	D	301[B]	GOL	O1-C1-C2-C3
4	G	301[A]	GOL	C1-C2-C3-O3
4	G	301[B]	GOL	O1-C1-C2-C3
4	H	301[A]	GOL	O1-C1-C2-O2
4	H	301[A]	GOL	O1-C1-C2-C3
4	H	301[B]	GOL	C1-C2-C3-O3
4	D	301[B]	GOL	O1-C1-C2-O2
4	G	301[A]	GOL	O2-C2-C3-O3
4	C	303[A]	GOL	O1-C1-C2-C3
4	D	301[A]	GOL	O1-C1-C2-C3
4	D	301[B]	GOL	C1-C2-C3-O3
4	G	301[B]	GOL	C1-C2-C3-O3
4	H	301[B]	GOL	O2-C2-C3-O3
4	C	303[A]	GOL	O1-C1-C2-O2
4	G	301[B]	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	F	302[B]	EDO	O1-C1-C2-O2
2	A	300	NAD	PN-O3-PA-O5B
2	B	300	NAD	PN-O3-PA-O5B
2	G	302	NAD	C5D-O5D-PN-O3
4	D	301[A]	GOL	O1-C1-C2-O2
4	G	301[B]	GOL	O1-C1-C2-O2
2	A	300	NAD	PA-O3-PN-O2N
2	B	300	NAD	PA-O3-PN-O2N
2	C	301	NAD	PA-O3-PN-O2N
2	D	302	NAD	PA-O3-PN-O2N
2	F	300	NAD	PA-O3-PN-O2N
2	B	300	NAD	C5D-O5D-PN-O1N
2	E	300	NAD	PA-O3-PN-O2N
2	G	302	NAD	PA-O3-PN-O2N
2	H	302	NAD	PA-O3-PN-O2N
2	B	300	NAD	O4B-C4B-C5B-O5B
2	A	300	NAD	O4B-C4B-C5B-O5B
2	F	300	NAD	O4B-C4B-C5B-O5B
2	H	302	NAD	O4B-C4B-C5B-O5B
2	G	302	NAD	O4B-C4B-C5B-O5B
3	A	302	EDO	O1-C1-C2-O2
3	B	302	EDO	O1-C1-C2-O2
3	F	301	EDO	O1-C1-C2-O2
2	B	300	NAD	C2D-C1D-N1N-C6N
2	C	301	NAD	C5D-O5D-PN-O3
2	D	302	NAD	C5D-O5D-PN-O3
2	E	300	NAD	C5D-O5D-PN-O3
2	F	300	NAD	C5D-O5D-PN-O3
2	C	301	NAD	O4B-C4B-C5B-O5B
2	D	302	NAD	O4B-C4B-C5B-O5B
2	E	300	NAD	O4B-C4B-C5B-O5B
2	A	300	NAD	PA-O3-PN-O1N
2	B	300	NAD	PA-O3-PN-O1N
2	C	301	NAD	PA-O3-PN-O1N
2	D	302	NAD	PA-O3-PN-O1N
2	F	300	NAD	PA-O3-PN-O1N
4	C	303[B]	GOL	O1-C1-C2-C3
4	D	301[A]	GOL	C1-C2-C3-O3
4	D	301[A]	GOL	O2-C2-C3-O3
4	H	301[B]	GOL	O1-C1-C2-O2

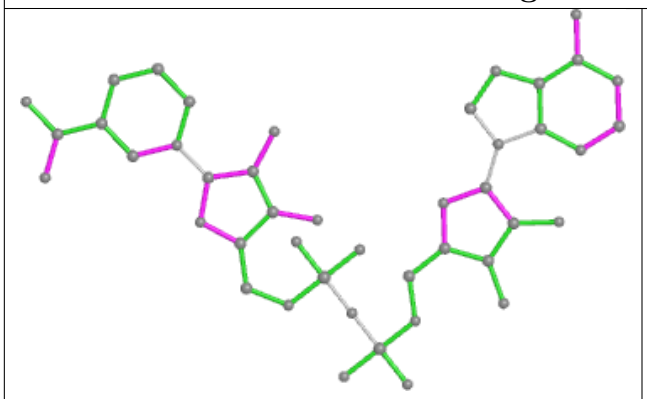
There are no ring outliers.

1 monomer is involved in 1 short contact:

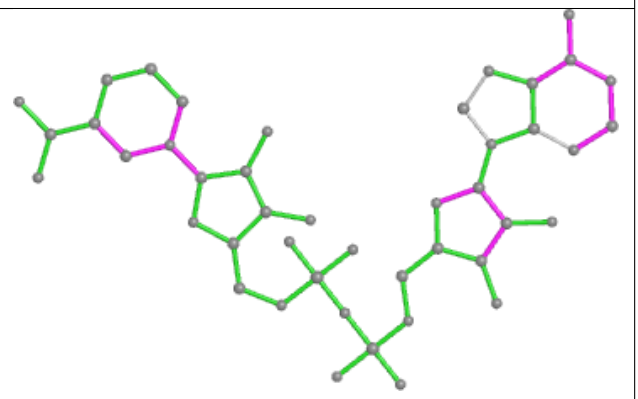
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	302	NAD	1	0

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.

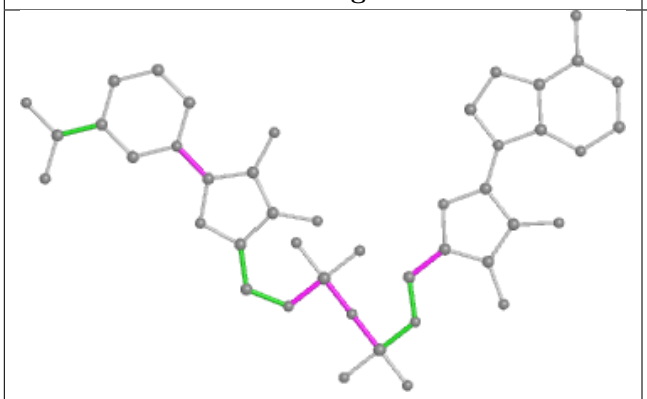
Ligand NAD H 302



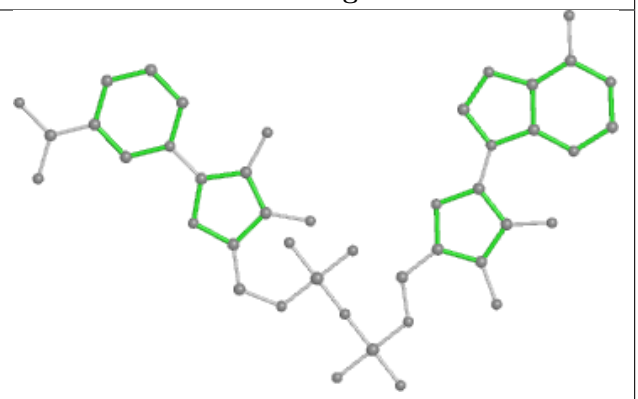
Bond lengths



Bond angles

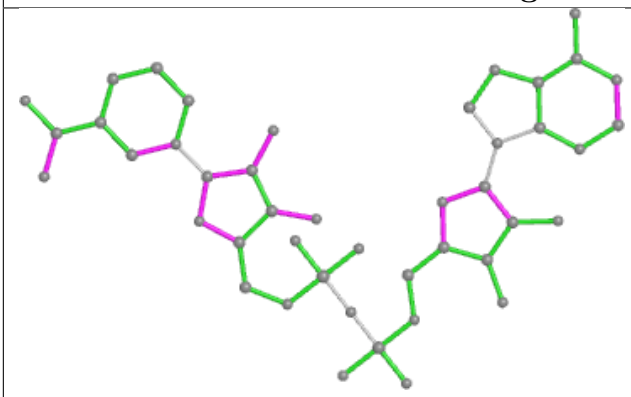


Torsions

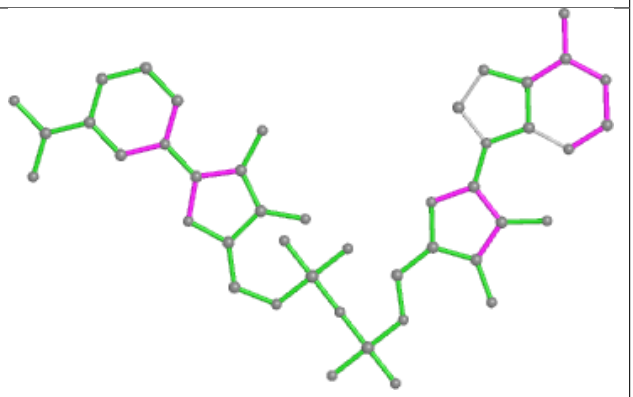


Rings

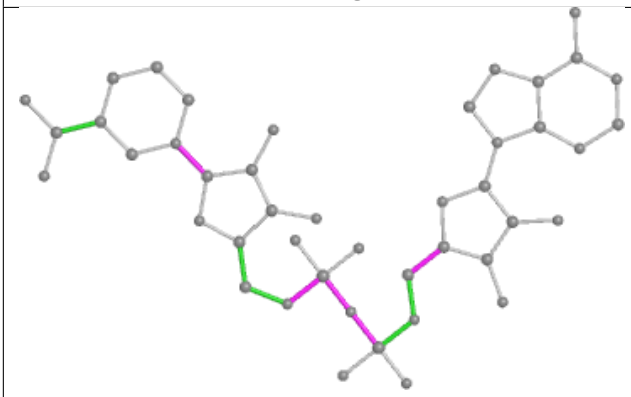
Ligand NAD B 300



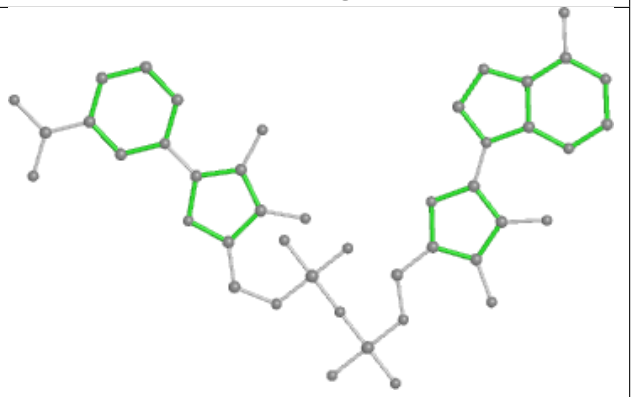
Bond lengths



Bond angles

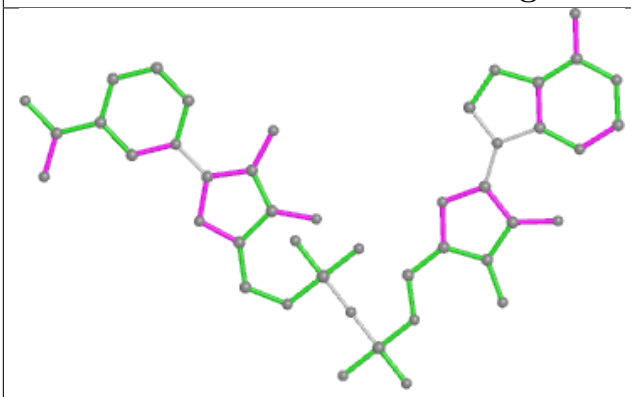


Torsions

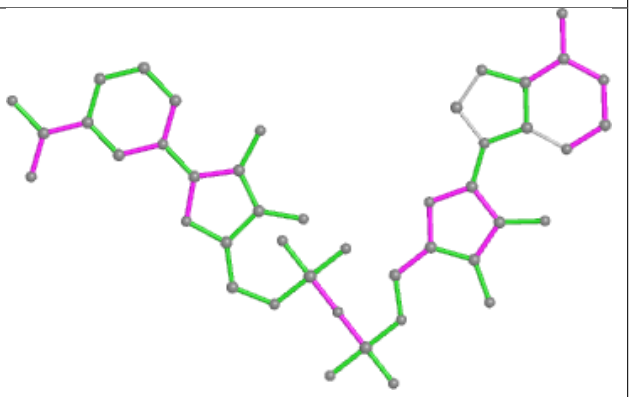


Rings

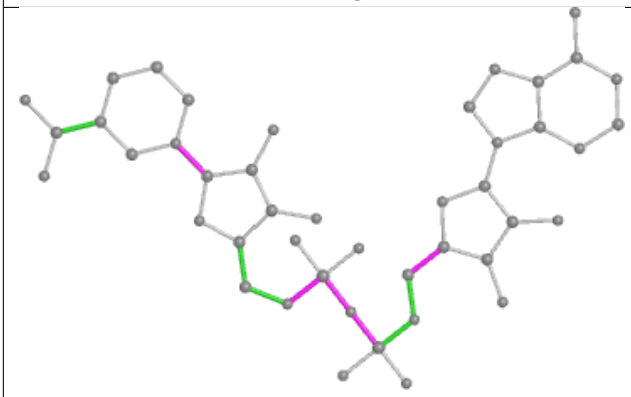
Ligand NAD A 300



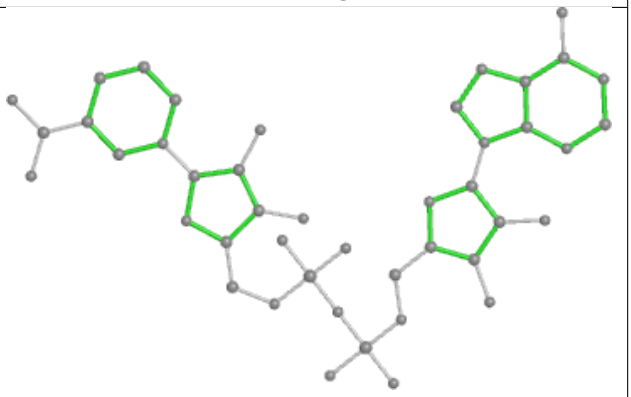
Bond lengths



Bond angles

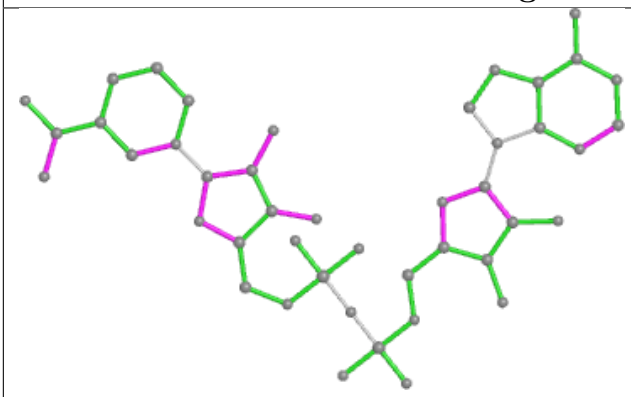


Torsions

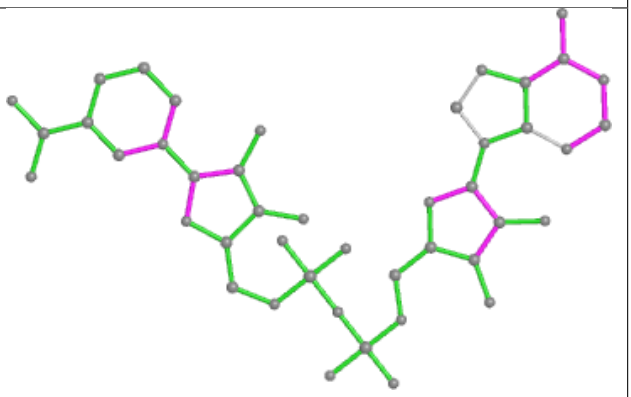


Rings

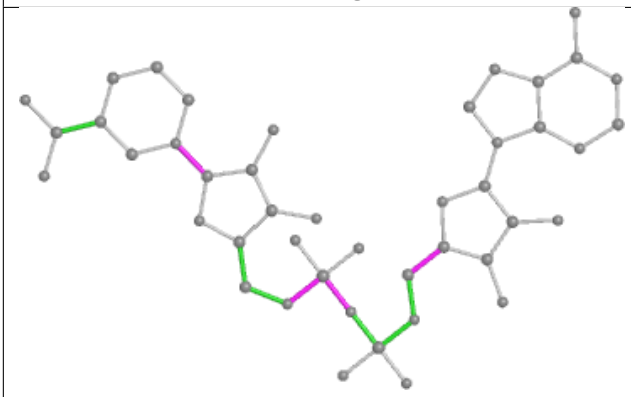
Ligand NAD G 302



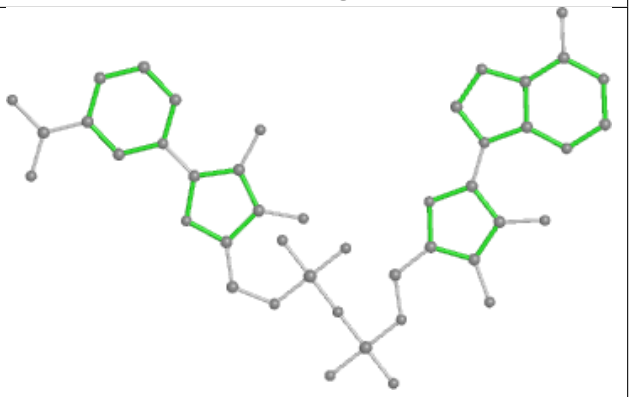
Bond lengths



Bond angles

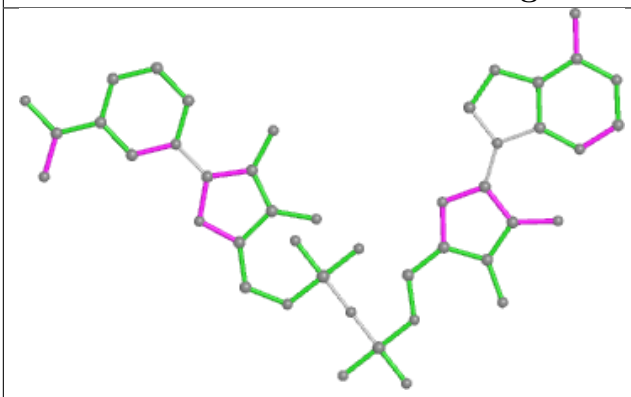


Torsions

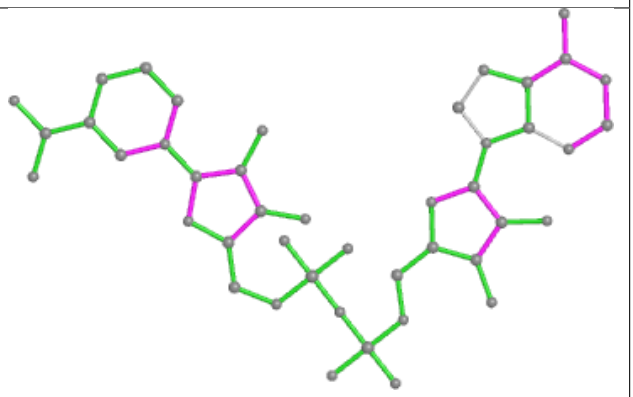


Rings

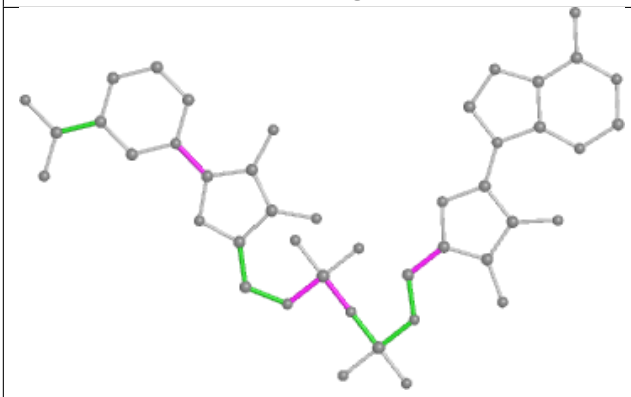
Ligand NAD C 301



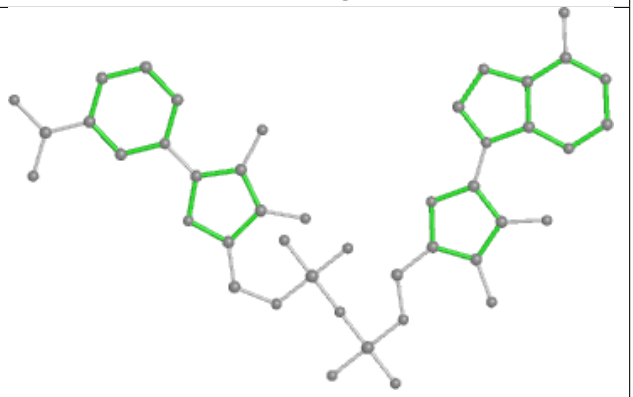
Bond lengths



Bond angles

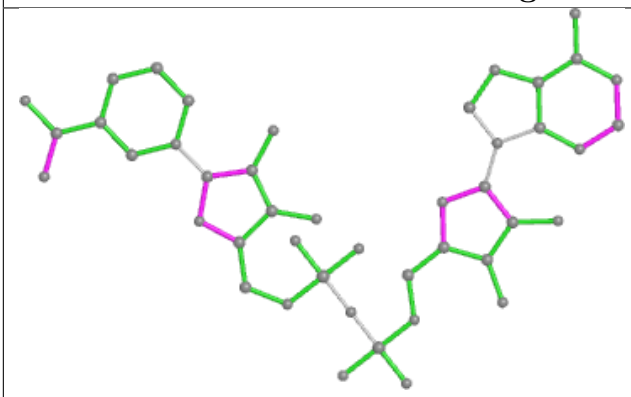


Torsions

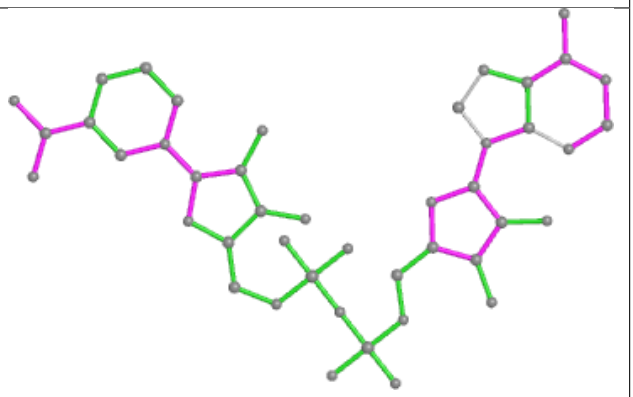


Rings

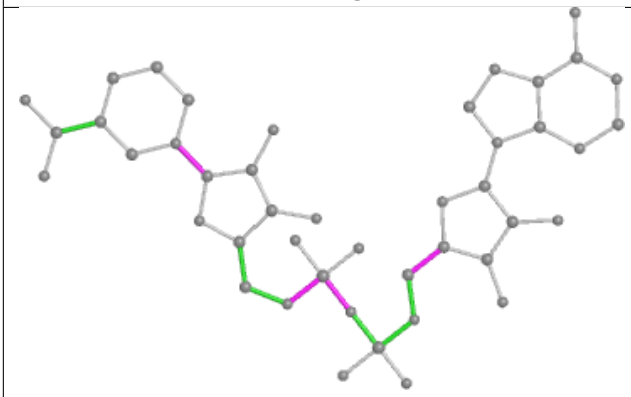
Ligand NAD D 302



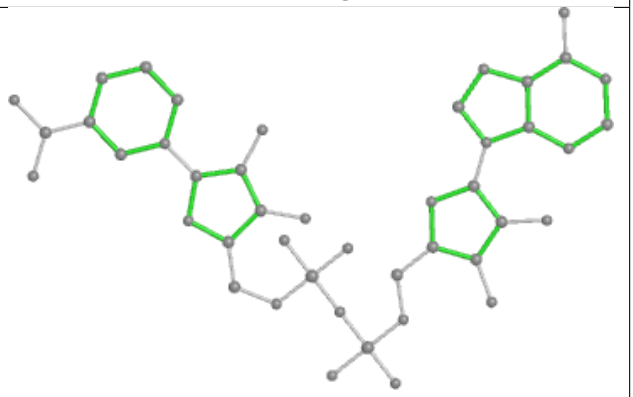
Bond lengths



Bond angles

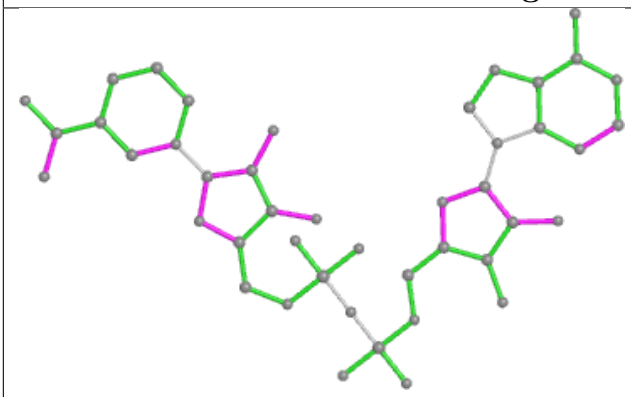


Torsions

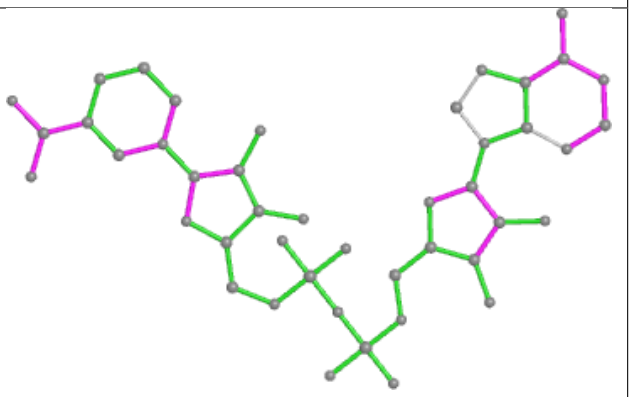


Rings

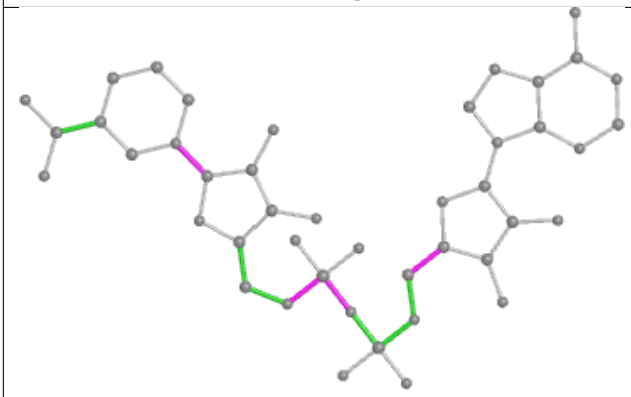
Ligand NAD F 300



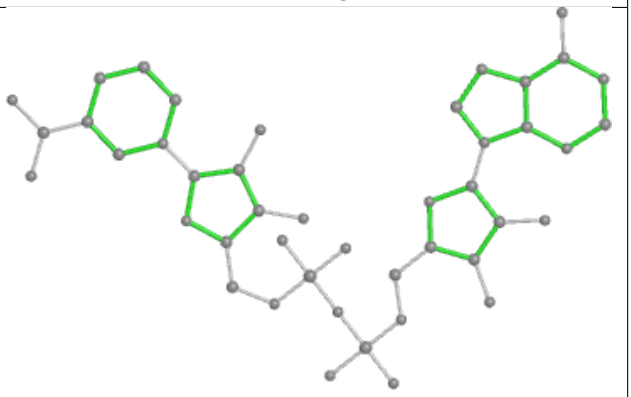
Bond lengths



Bond angles

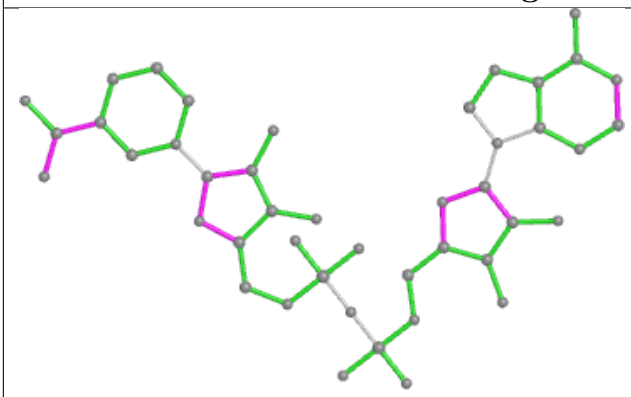


Torsions

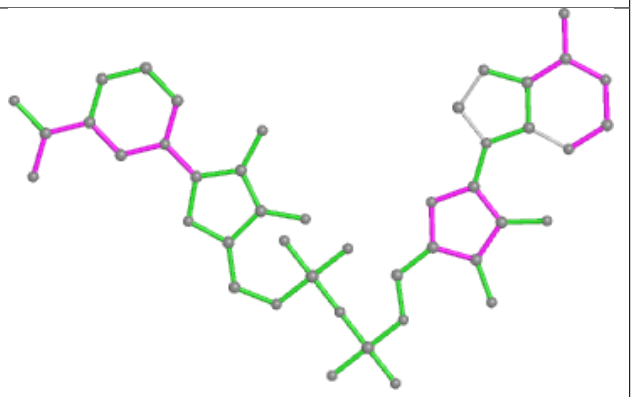


Rings

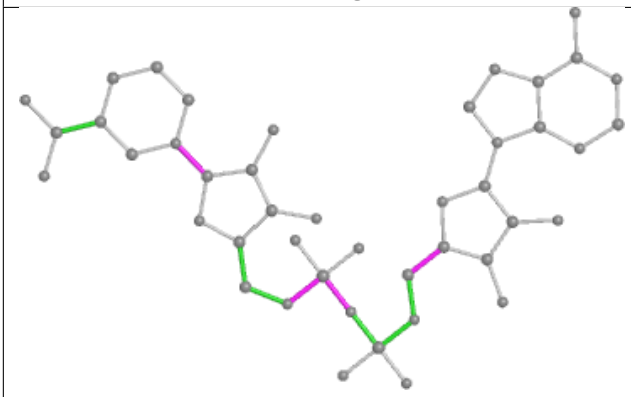
Ligand NAD E 300



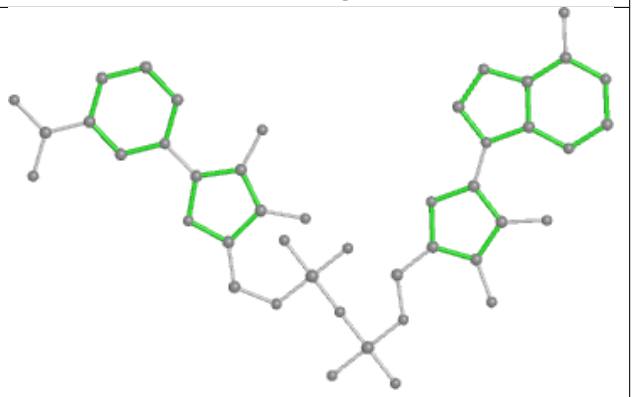
Bond lengths



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	255/260 (98%)	0.12	12 (4%)	31	30	8, 15, 31, 45	0
1	B	255/260 (98%)	0.06	9 (3%)	44	45	8, 13, 31, 46	0
1	C	255/260 (98%)	0.02	13 (5%)	28	27	8, 14, 33, 41	0
1	D	254/260 (97%)	0.09	13 (5%)	28	27	8, 15, 35, 51	0
1	E	253/260 (97%)	-0.10	5 (1%)	65	67	8, 15, 30, 46	0
1	F	255/260 (98%)	0.01	11 (4%)	35	34	8, 14, 34, 56	0
1	G	255/260 (98%)	-0.03	7 (2%)	54	55	9, 14, 32, 46	0
1	H	255/260 (98%)	0.02	8 (3%)	49	49	8, 14, 30, 47	0
All	All	2037/2080 (97%)	0.02	78 (3%)	40	40	8, 14, 33, 56	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	198	GLY	6.3
1	B	198	GLY	5.7
1	A	-2	HIS	5.6
1	A	200	PRO	5.0
1	D	198	GLY	4.7
1	D	200	PRO	4.5
1	F	203	VAL	4.5
1	D	197	LEU	4.5
1	F	200	PRO	4.4
1	H	-2	HIS	4.4
1	G	198	GLY	4.4
1	H	198	GLY	4.4
1	C	197	LEU	4.3
1	A	203	VAL	3.9
1	H	200	PRO	3.8
1	E	197	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	201	GLN	3.6
1	A	198	GLY	3.6
1	A	197	LEU	3.5
1	D	0	HIS	3.4
1	C	198	GLY	3.4
1	D	206	ALA	3.4
1	E	198	GLY	3.3
1	F	197	LEU	3.3
1	A	202	GLU	3.3
1	C	200	PRO	3.2
1	B	203	VAL	3.2
1	D	203	VAL	3.2
1	G	200	PRO	3.1
1	B	-2	HIS	3.1
1	C	-1	HIS	3.0
1	B	200	PRO	3.0
1	E	0	HIS	3.0
1	B	197	LEU	3.0
1	H	203	VAL	3.0
1	F	202	GLU	2.9
1	H	96	ASP	2.9
1	D	199	MET	2.9
1	F	199	MET	2.9
1	F	205	ASP	2.8
1	A	201	GLN	2.8
1	D	205	ASP	2.8
1	G	197	LEU	2.8
1	A	96	ASP	2.7
1	C	-2	HIS	2.7
1	H	-1	HIS	2.7
1	G	203	VAL	2.7
1	D	-1	HIS	2.6
1	G	-2	HIS	2.5
1	A	134	THR	2.5
1	B	201	GLN	2.5
1	D	202	GLU	2.5
1	F	-1	HIS	2.4
1	F	96	ASP	2.4
1	F	47	ARG	2.4
1	B	-1	HIS	2.4
1	B	199	MET	2.3
1	C	96	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	209	ALA	2.3
1	B	202	GLU	2.3
1	H	133	PRO	2.3
1	G	202	GLU	2.3
1	C	205	ASP	2.3
1	A	1	MET	2.3
1	C	206	ALA	2.2
1	C	203	VAL	2.2
1	A	207	LEU	2.2
1	C	199	MET	2.2
1	G	96	ASP	2.2
1	D	178	ARG	2.2
1	C	210	MET	2.2
1	H	207	LEU	2.1
1	C	178	ARG	2.1
1	D	5	ASP	2.1
1	E	96	ASP	2.1
1	F	210	MET	2.1
1	C	202	GLU	2.0
1	E	200	PRO	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 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
4	GOL	H	301[A]	6/6	0.79	0.27	13,14,14,16	6
4	GOL	H	301[B]	6/6	0.79	0.27	13,15,16,17	6
4	GOL	C	303[A]	6/6	0.80	0.30	15,15,16,16	6

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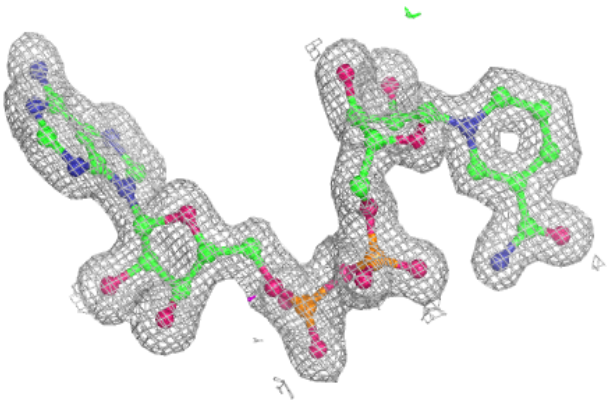
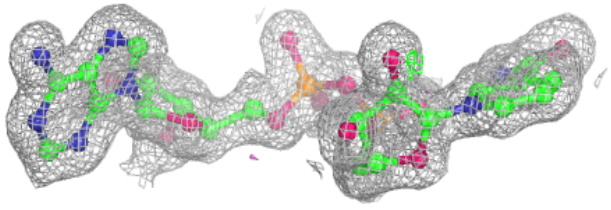
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	C	303[B]	6/6	0.80	0.30	11,11,13,14	6
4	GOL	D	301[A]	6/6	0.85	0.30	11,11,12,13	6
4	GOL	D	301[B]	6/6	0.85	0.30	16,16,17,17	6
4	GOL	G	301[B]	6/6	0.86	0.24	11,12,12,13	6
3	EDO	A	302	4/4	0.86	0.20	23,28,31,34	0
4	GOL	G	301[A]	6/6	0.86	0.24	14,15,16,16	6
3	EDO	D	304	4/4	0.87	0.17	25,30,32,34	0
3	EDO	E	302	4/4	0.88	0.23	27,30,32,33	0
3	EDO	C	302	4/4	0.89	0.13	19,21,22,22	0
3	EDO	F	302[A]	4/4	0.89	0.19	23,24,24,25	4
3	EDO	F	302[B]	4/4	0.89	0.19	22,23,24,24	4
3	EDO	H	304	4/4	0.89	0.22	25,29,31,34	0
3	EDO	B	302	4/4	0.90	0.13	23,27,28,32	0
3	EDO	G	304[B]	4/4	0.93	0.17	22,24,24,24	4
3	EDO	G	304[A]	4/4	0.93	0.17	22,23,23,23	4
3	EDO	H	303	4/4	0.94	0.10	17,18,18,19	0
3	EDO	D	303	4/4	0.94	0.07	21,21,22,22	0
3	EDO	B	301	4/4	0.95	0.08	18,19,19,19	0
3	EDO	F	301	4/4	0.95	0.09	19,20,20,20	0
3	EDO	G	303	4/4	0.95	0.08	20,20,20,20	0
3	EDO	E	301	4/4	0.96	0.08	19,20,20,20	0
3	EDO	A	301	4/4	0.96	0.07	18,19,19,19	0
2	NAD	C	301	44/44	0.97	0.07	12,13,14,16	0
2	NAD	D	302	44/44	0.97	0.07	12,13,14,15	0
2	NAD	F	300	44/44	0.97	0.07	13,13,14,15	0
2	NAD	G	302	44/44	0.97	0.07	12,13,14,14	0
2	NAD	H	302	44/44	0.97	0.06	12,12,13,14	0
2	NAD	B	300	44/44	0.97	0.07	11,12,13,13	0
2	NAD	A	300	44/44	0.98	0.06	11,12,13,13	0
2	NAD	E	300	44/44	0.98	0.06	11,12,14,14	0

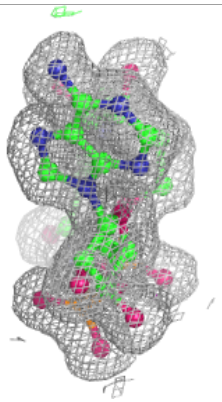
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

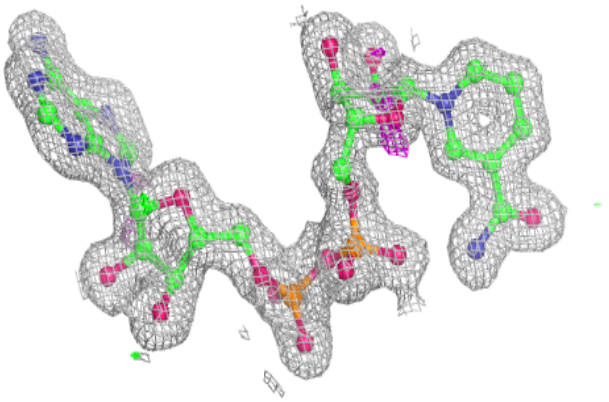


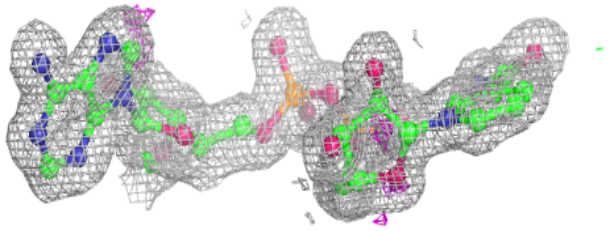


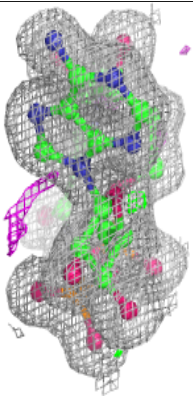


Electron density around NAD D 302:

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

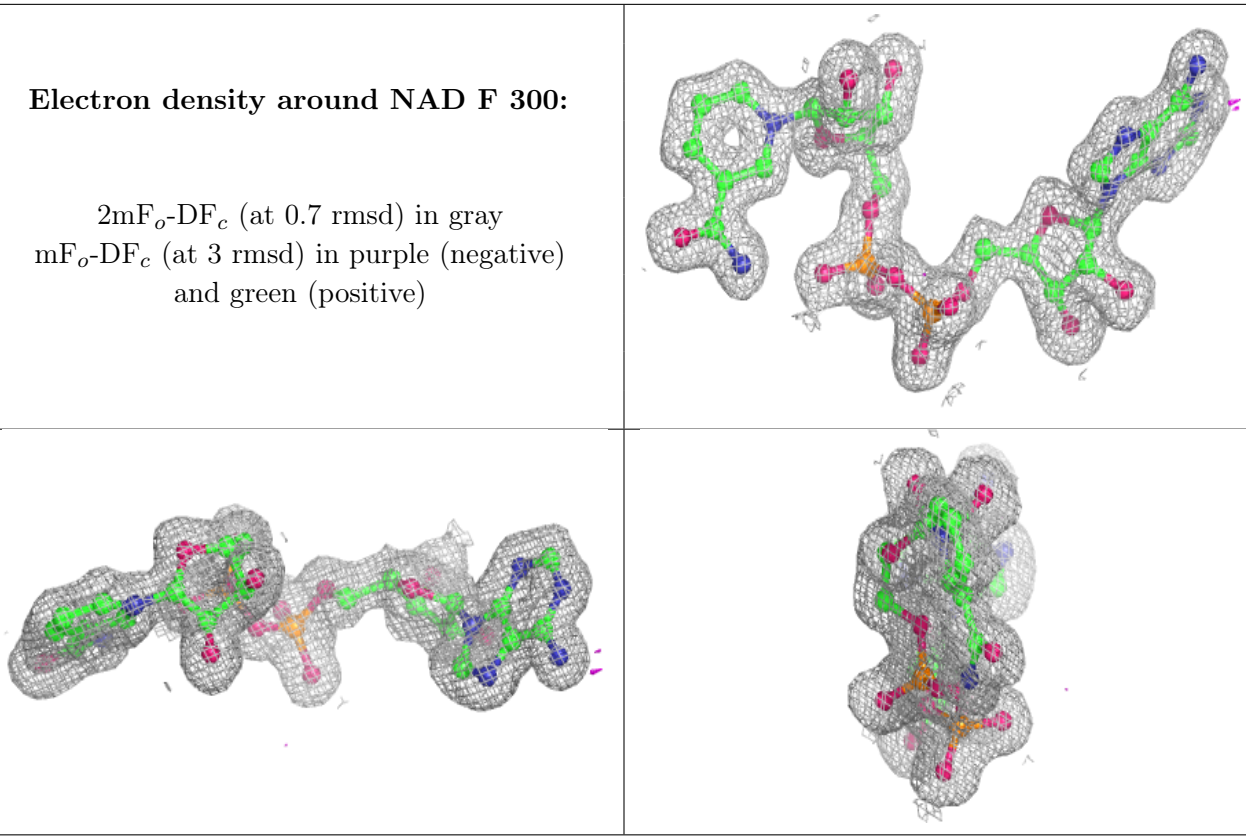






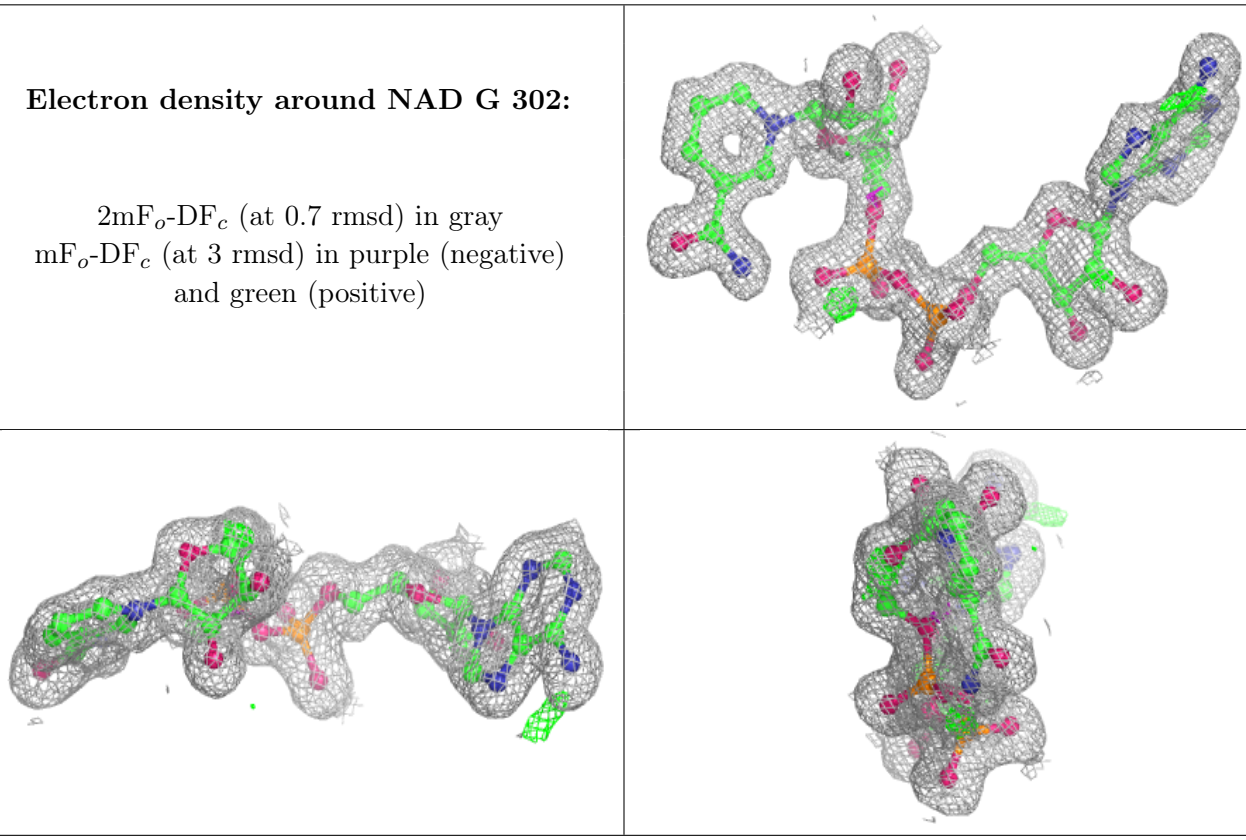
Electron density around NAD F 300:

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



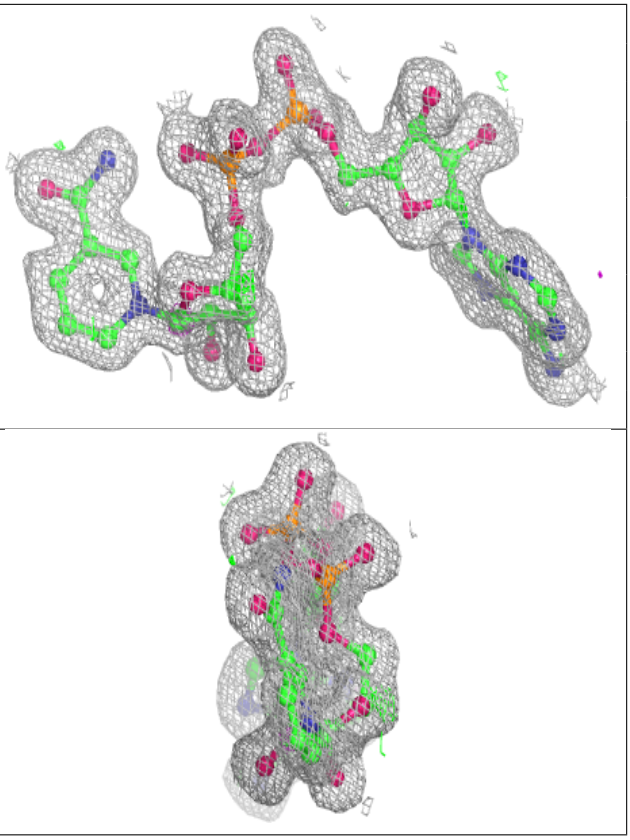
Electron density around NAD G 302:

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



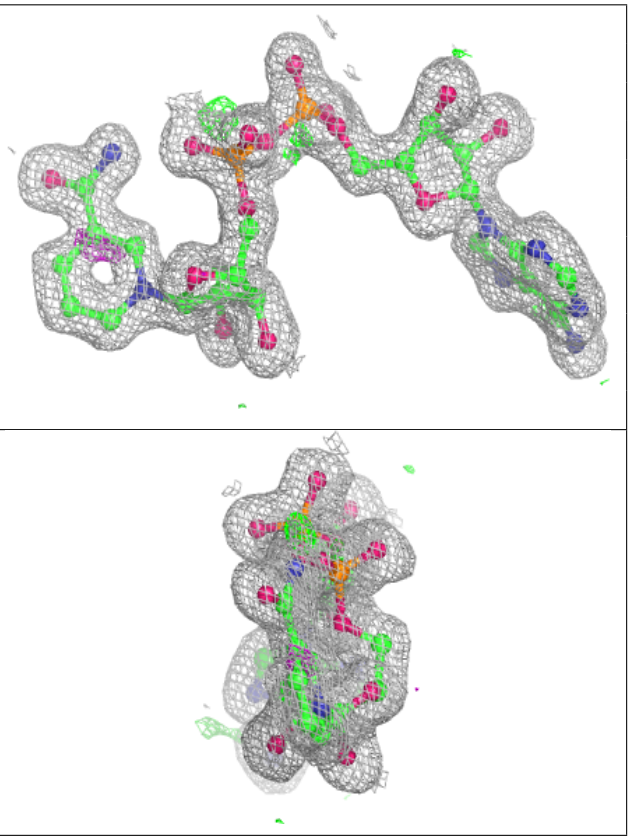
Electron density around NAD H 302:

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



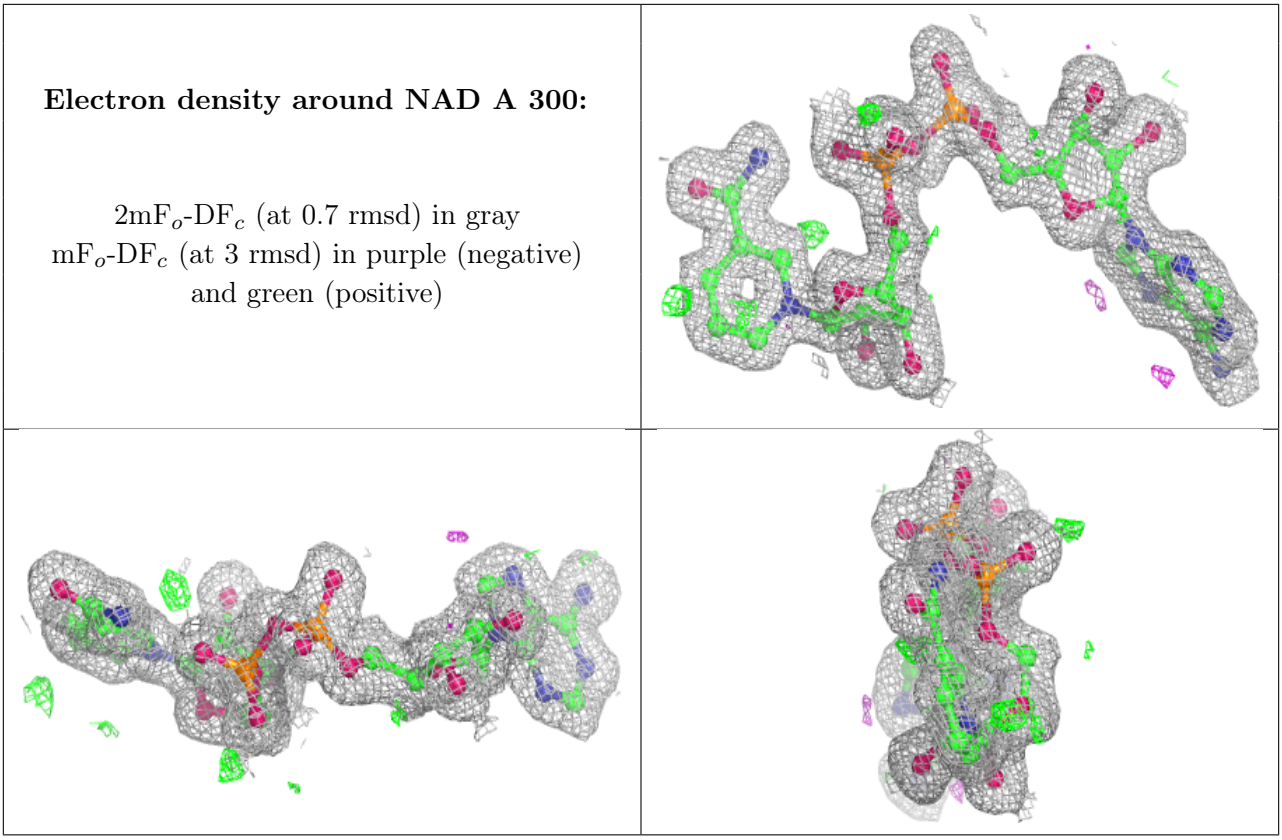
Electron density around NAD B 300:

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



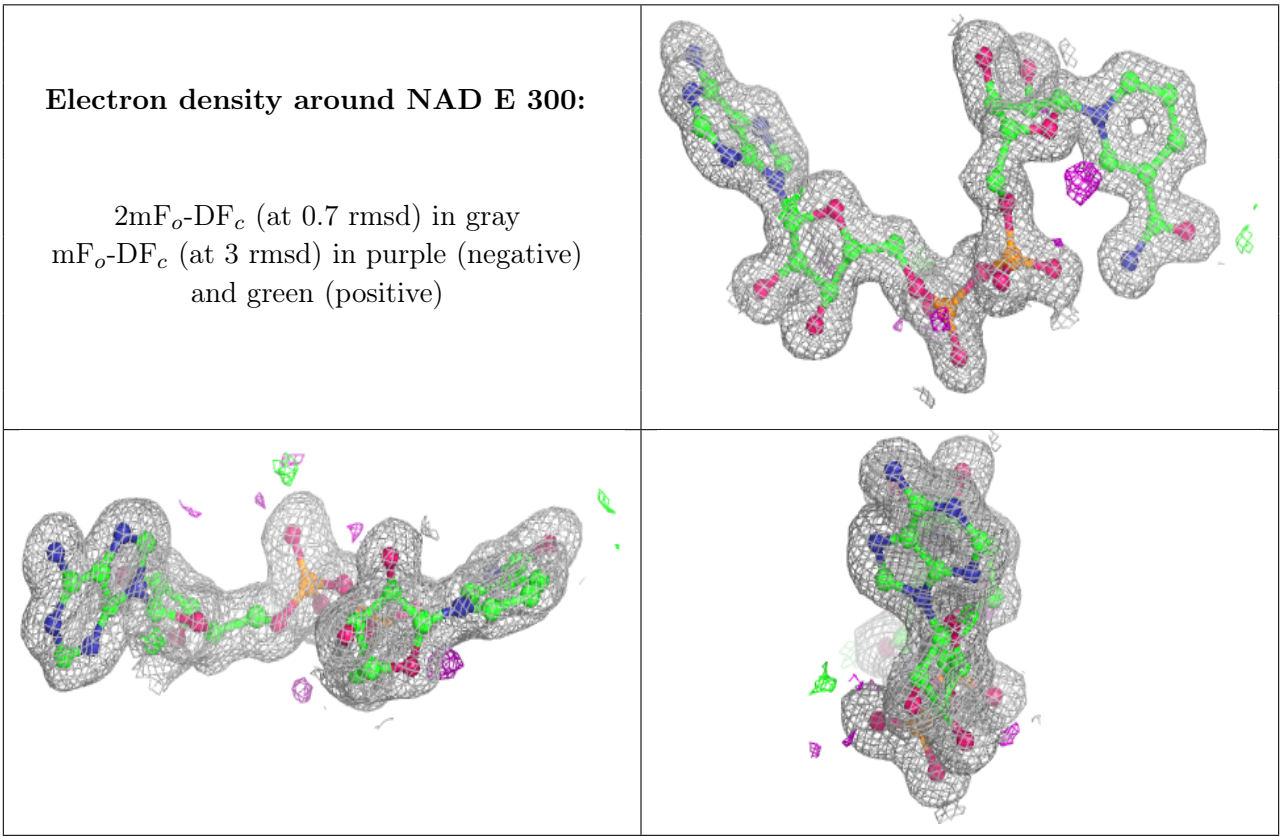
Electron density around NAD A 300:

$2mF_o$-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 300:

$2mF_o$-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.