



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 02:31 pm BST

PDB ID : 6JYG  
Title : Crystal Structure of L-threonine dehydrogenase from *Phytophthora infestans*  
Authors : Yoneda, K.; Sakuraba, H.; Ohshima, T.  
Deposited on : 2019-04-26  
Resolution : 2.31 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](mailto: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.

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

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

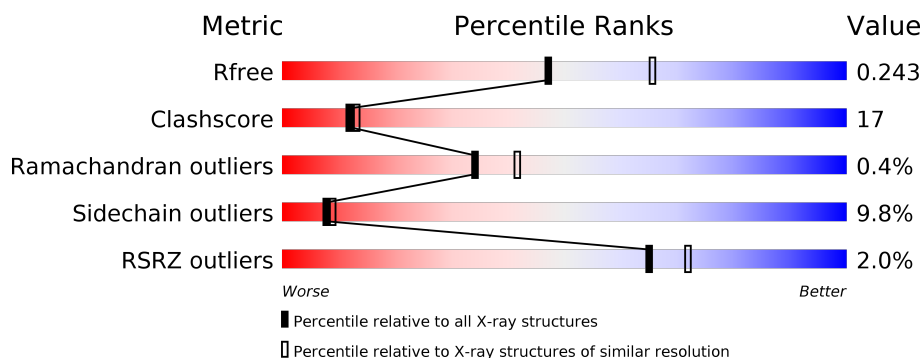
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	345	<div> <div style="width: 58%;"></div> <div style="width: 24%;"></div> <div style="width: 5%;"></div> <div style="width: 11%;"></div> </div>
1	B	345	<div> <div style="width: 54%;"></div> <div style="width: 28%;"></div> <div style="width: 6%;"></div> <div style="width: 11%;"></div> </div>
1	C	345	<div> <div style="width: 58%;"></div> <div style="width: 23%;"></div> <div style="width: 6%;"></div> <div style="width: 11%;"></div> </div>
1	D	345	<div> <div style="width: 63%;"></div> <div style="width: 21%;"></div> <div style="width: 1%;"></div> <div style="width: 11%;"></div> </div>
1	E	345	<div> <div style="width: 58%;"></div> <div style="width: 23%;"></div> <div style="width: 6%;"></div> <div style="width: 12%;"></div> </div>
1	F	345	<div> <div style="width: 58%;"></div> <div style="width: 26%;"></div> <div style="width: 5%;"></div> <div style="width: 11%;"></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PE8	A	402	-	-	X	X
3	PE8	D	402	-	-	X	X

## 2 Entry composition [i](#)

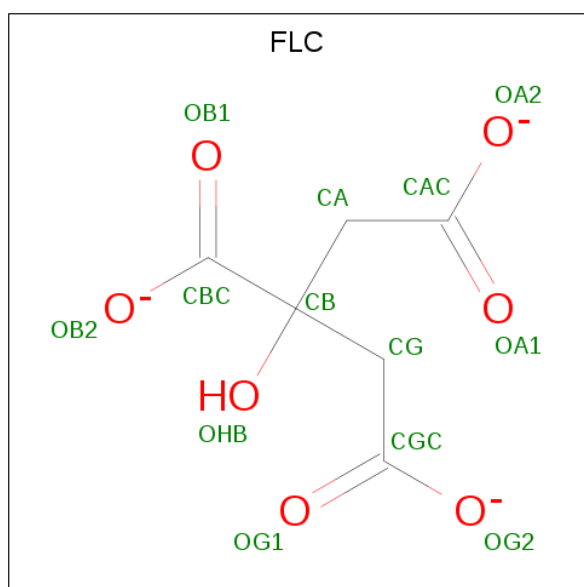
There are 5 unique types of molecules in this entry. The entry contains 15108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-threonine 3-dehydrogenase, putative.

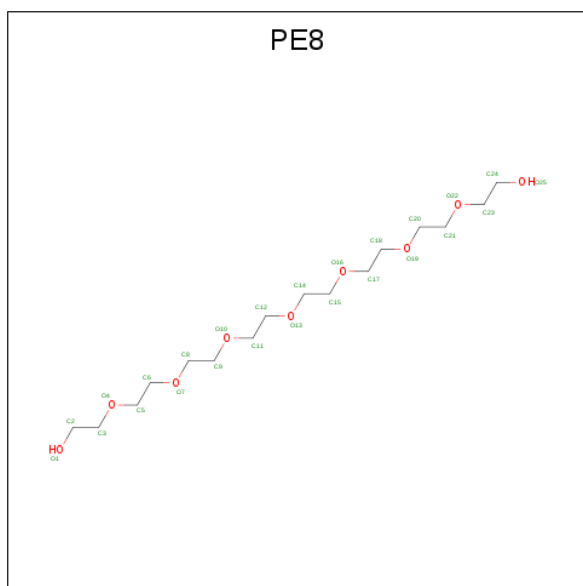
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2395	1518	397	462	18			
1	B	306	Total	C	N	O	S	0	0	0
			2395	1518	397	462	18			
1	C	306	Total	C	N	O	S	0	0	0
			2395	1518	397	462	18			
1	D	307	Total	C	N	O	S	0	0	0
			2406	1524	401	463	18			
1	E	304	Total	C	N	O	S	0	0	0
			2378	1506	394	460	18			
1	F	307	Total	C	N	O	S	0	0	0
			2406	1524	401	463	18			

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



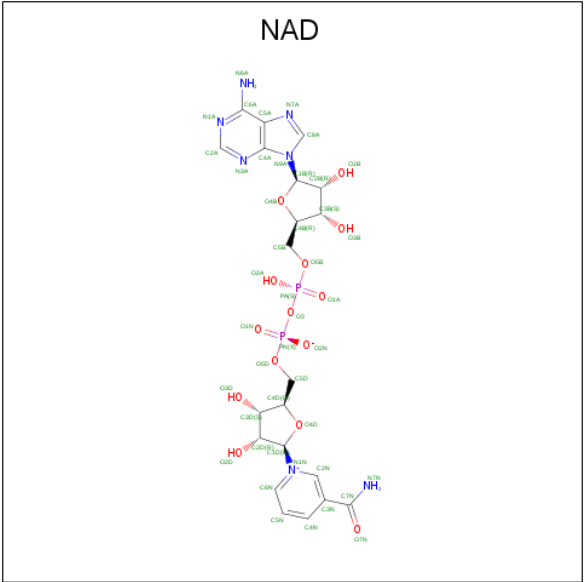
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula:  $C_{16}H_{34}O_9$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	16	9		
3	D	1	Total	C	O	0	0
			25	16	9		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by author).



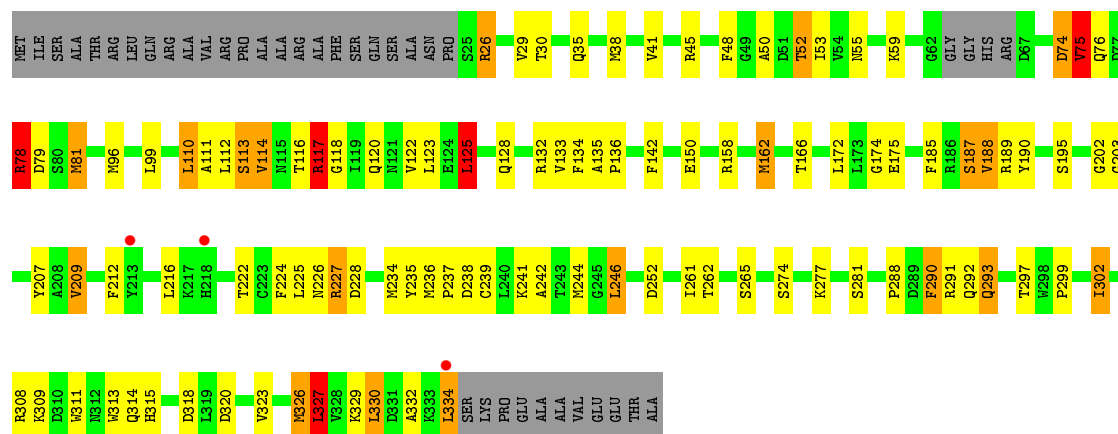
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

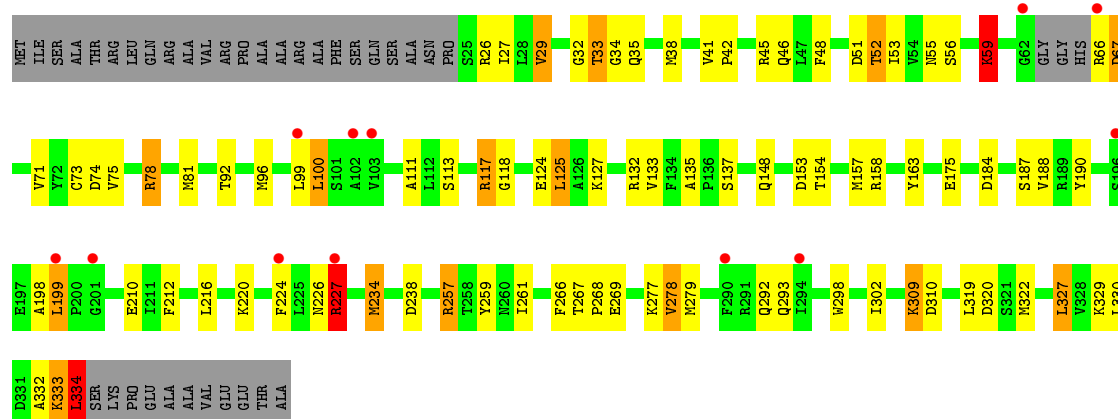
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	56	Total	O	0	0
			56	56		
5	C	58	Total	O	0	0
			58	58		
5	D	46	Total	O	0	0
			46	46		
5	E	58	Total	O	0	0
			58	58		
5	F	54	Total	O	0	0
			54	54		

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

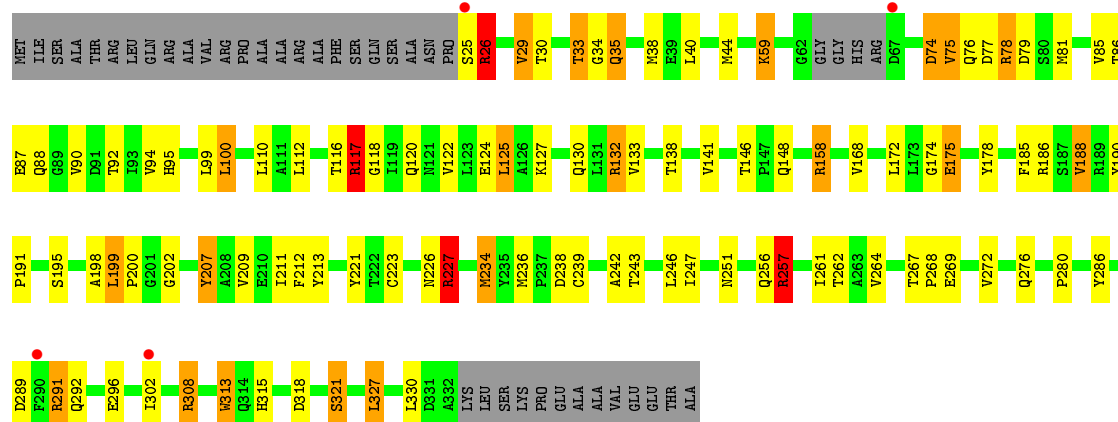
- Chain C:  58% 23% 6% 11%



• Molecule 1: L-threonine 3-dehydrogenase, putative

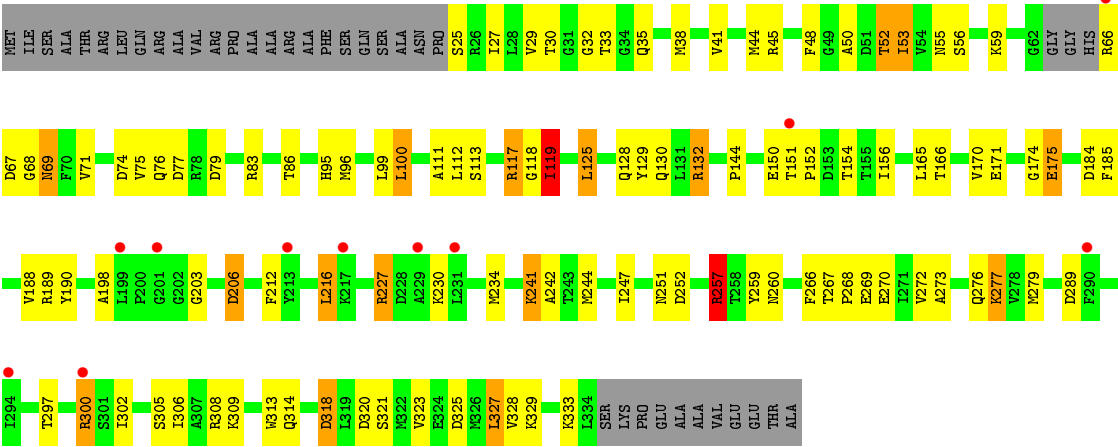


• Molecule 1: L-threonine 3-dehydrogenase, putative



• Molecule 1: L-threonine 3-dehydrogenase, putative





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.21Å 98.86Å 152.51Å 90.00° 106.72° 90.00°	Depositor
Resolution (Å)	49.28 – 2.31 49.28 – 2.31	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.28-2.31) 93.1 (49.28-2.31)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.32Å)	Xtriage
Refinement program	REFMAC, CNS 1.3	Depositor
R, $R_{free}$	0.238 , 0.242 0.239 , 0.243	Depositor DCC
$R_{free}$ test set	5028 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3805e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: FLC, PE8, 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	1.28	7/2446 (0.3%)	1.37	29/3322 (0.9%)
1	B	1.28	5/2446 (0.2%)	1.36	21/3322 (0.6%)
1	C	1.26	3/2446 (0.1%)	1.28	19/3322 (0.6%)
1	D	1.17	2/2457 (0.1%)	1.22	10/3336 (0.3%)
1	E	1.25	4/2429 (0.2%)	1.33	25/3300 (0.8%)
1	F	1.18	2/2457 (0.1%)	1.33	23/3336 (0.7%)
All	All	1.24	23/14681 (0.2%)	1.32	127/19938 (0.6%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	83	ARG	CZ-NH1	7.40	1.42	1.33
1	A	129	TYR	CE1-CZ	7.33	1.48	1.38
1	A	72	TYR	CE1-CZ	-7.08	1.29	1.38
1	A	235	TYR	CB-CG	6.40	1.61	1.51
1	C	162	MET	C-O	6.35	1.35	1.23

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	257	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	F	257	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	E	257	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	D	74	ASP	CB-CG-OD1	11.87	128.98	118.30
1	A	257	ARG	NE-CZ-NH1	9.94	125.27	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2395	0	2352	83	0
1	B	2395	0	2352	81	0
1	C	2395	0	2352	101	0
1	D	2406	0	2365	75	0
1	E	2378	0	2328	94	0
1	F	2406	0	2365	78	0
2	A	13	0	5	3	0
2	B	13	0	5	3	0
2	C	13	0	5	1	0
2	D	13	0	5	1	0
2	E	26	0	10	4	0
2	F	13	0	5	3	0
3	A	25	0	34	13	0
3	D	25	0	34	11	0
4	A	44	0	26	6	0
4	B	44	0	26	7	0
4	C	44	0	26	4	0
4	D	44	0	26	4	0
4	E	44	0	26	6	0
4	F	44	0	26	8	0
5	A	56	0	0	5	0
5	B	56	0	0	3	0
5	C	58	0	0	8	0
5	D	46	0	0	0	0
5	E	58	0	0	4	0
5	F	54	0	0	5	0
All	All	15108	0	14373	504	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 504 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:H	1:C:227:ARG:CD	1.55	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:LYS:HB2	3:D:402:PE8:H232	1.30	1.10
1:C:227:ARG:HD2	1:C:227:ARG:H	0.93	1.05
1:C:227:ARG:HD2	1:C:227:ARG:N	1.71	1.04
1:D:117:ARG:HG2	1:D:117:ARG:HH11	1.20	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	302/345 (88%)	280 (93%)	22 (7%)	0	100	100
1	B	302/345 (88%)	287 (95%)	15 (5%)	0	100	100
1	C	302/345 (88%)	282 (93%)	20 (7%)	0	100	100
1	D	303/345 (88%)	288 (95%)	11 (4%)	4 (1%)	12	12
1	E	300/345 (87%)	284 (95%)	14 (5%)	2 (1%)	22	26
1	F	303/345 (88%)	281 (93%)	20 (7%)	2 (1%)	22	26
All	All	1812/2070 (88%)	1702 (94%)	102 (6%)	8 (0%)	34	41

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	67	ASP
1	D	227	ARG
1	E	26	ARG
1	F	69	ASN
1	D	184	ASP

### 5.3.2 Protein sidechains ⓘ

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	265/293 (90%)	240 (91%)	25 (9%)	8	10
1	B	265/293 (90%)	236 (89%)	29 (11%)	6	7
1	C	265/293 (90%)	237 (89%)	28 (11%)	6	7
1	D	266/293 (91%)	237 (89%)	29 (11%)	6	7
1	E	263/293 (90%)	238 (90%)	25 (10%)	8	9
1	F	266/293 (91%)	246 (92%)	20 (8%)	13	16
All	All	1590/1758 (90%)	1434 (90%)	156 (10%)	8	9

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	246	LEU
1	D	52	THR
1	F	188	VAL
1	C	265	SER
1	C	327	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	292	GLN
1	D	35	GLN
1	F	121	ASN
1	C	312	ASN
1	D	76	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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	NAD	F	402	-	42,48,48	1.12	4 (9%)	50,73,73	1.57	9 (18%)
2	FLC	A	401	-	3,12,12	1.22	0	3,17,17	1.79	2 (66%)
2	FLC	E	402	-	3,12,12	0.59	0	3,17,17	3.56	3 (100%)
4	NAD	B	402	-	42,48,48	1.50	6 (14%)	50,73,73	1.59	14 (28%)
4	NAD	D	403	-	42,48,48	1.07	3 (7%)	50,73,73	1.48	5 (10%)
2	FLC	D	401	-	3,12,12	1.28	0	3,17,17	1.77	1 (33%)
2	FLC	F	401	-	3,12,12	1.37	1 (33%)	3,17,17	4.33	1 (33%)
2	FLC	C	401	-	3,12,12	0.82	0	3,17,17	1.77	1 (33%)
2	FLC	E	401	-	3,12,12	0.86	0	3,17,17	3.49	2 (66%)
2	FLC	B	401	-	3,12,12	0.44	0	3,17,17	0.70	0
4	NAD	A	403	-	42,48,48	1.44	5 (11%)	50,73,73	1.45	7 (14%)
3	PE8	D	402	-	24,24,24	0.76	0	23,23,23	0.78	0
4	NAD	E	403	-	42,48,48	1.32	6 (14%)	50,73,73	1.51	11 (22%)
3	PE8	A	402	-	24,24,24	0.79	0	23,23,23	0.86	0
4	NAD	C	402	-	42,48,48	0.94	2 (4%)	50,73,73	1.33	4 (8%)

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	NAD	F	402	-	-	3/26/62/62	0/5/5/5
2	FLC	A	401	-	-	3/6/16/16	-
2	FLC	E	402	-	-	0/6/16/16	-
4	NAD	B	402	-	-	1/26/62/62	0/5/5/5
4	NAD	D	403	-	-	3/26/62/62	0/5/5/5
2	FLC	D	401	-	-	1/6/16/16	-
2	FLC	F	401	-	-	3/6/16/16	-
2	FLC	C	401	-	-	0/6/16/16	-
2	FLC	E	401	-	-	5/6/16/16	-
2	FLC	B	401	-	-	5/6/16/16	-
4	NAD	A	403	-	-	3/26/62/62	0/5/5/5
3	PE8	D	402	-	-	12/22/22/22	-
4	NAD	E	403	-	-	3/26/62/62	0/5/5/5
3	PE8	A	402	-	-	14/22/22/22	-
4	NAD	C	402	-	-	3/26/62/62	0/5/5/5

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	403	NAD	O4D-C1D	4.23	1.47	1.41
4	B	402	NAD	C2A-N3A	3.97	1.38	1.32
4	B	402	NAD	C5A-C4A	3.85	1.51	1.40
4	B	402	NAD	C2N-C3N	3.64	1.44	1.39
4	A	403	NAD	C5A-C4A	3.55	1.50	1.40

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	FLC	CB-CG-CGC	7.27	126.63	114.98
2	E	401	FLC	CB-CA-CAC	5.45	123.71	114.98
4	F	402	NAD	C4A-C5A-N7A	-4.56	104.65	109.40
4	D	403	NAD	N3A-C2A-N1A	-4.52	121.61	128.68
4	C	402	NAD	N3A-C2A-N1A	-4.46	121.70	128.68

There are no chirality outliers.

5 of 59 torsion outliers are listed below:



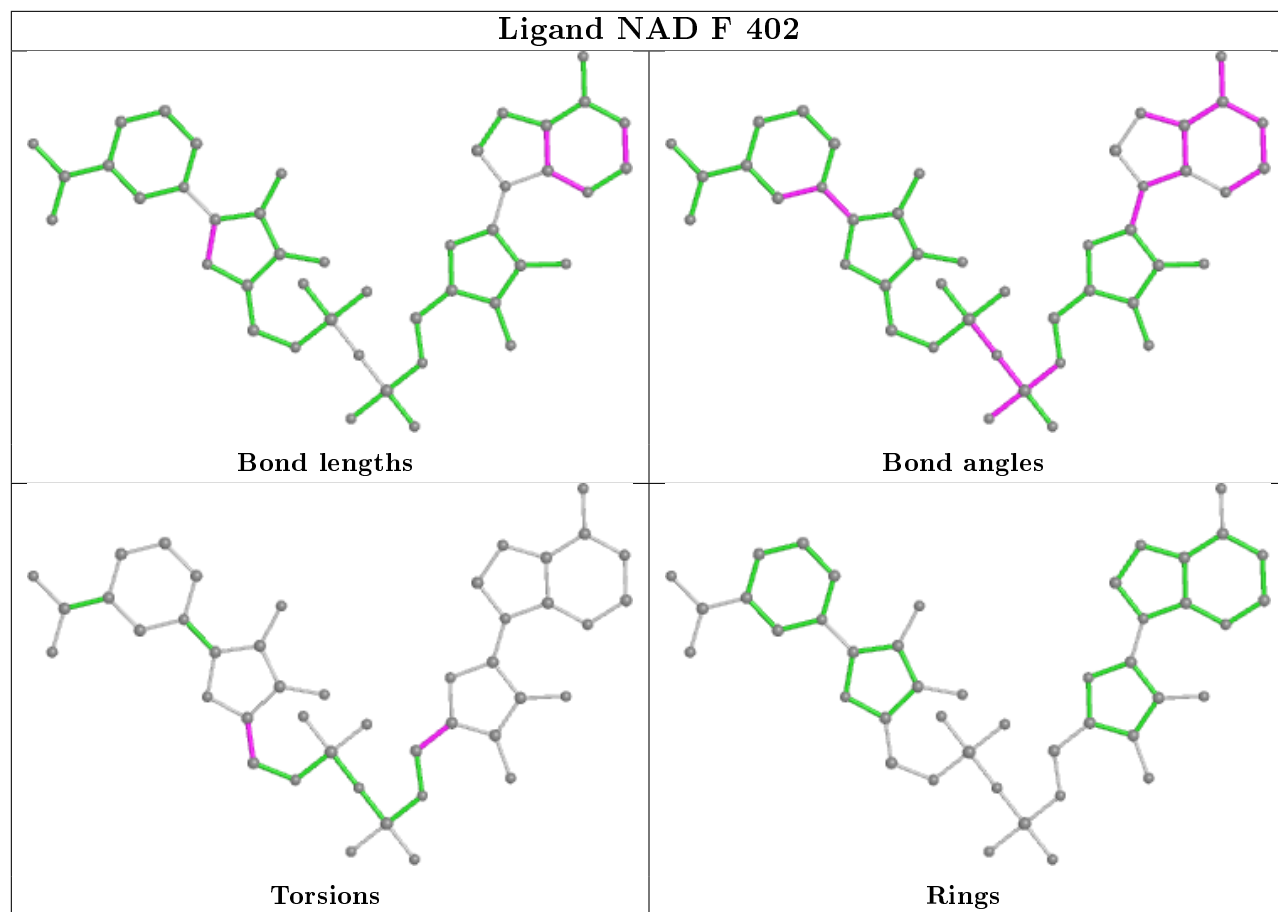
Mol	Chain	Res	Type	Atoms
2	A	401	FLC	CA-CB-CG-CGC
2	A	401	FLC	CBC-CB-CG-CGC
2	A	401	FLC	OHB-CB-CG-CGC
2	E	401	FLC	CAC-CA-CB-CBC
2	E	401	FLC	CBC-CB-CG-CGC

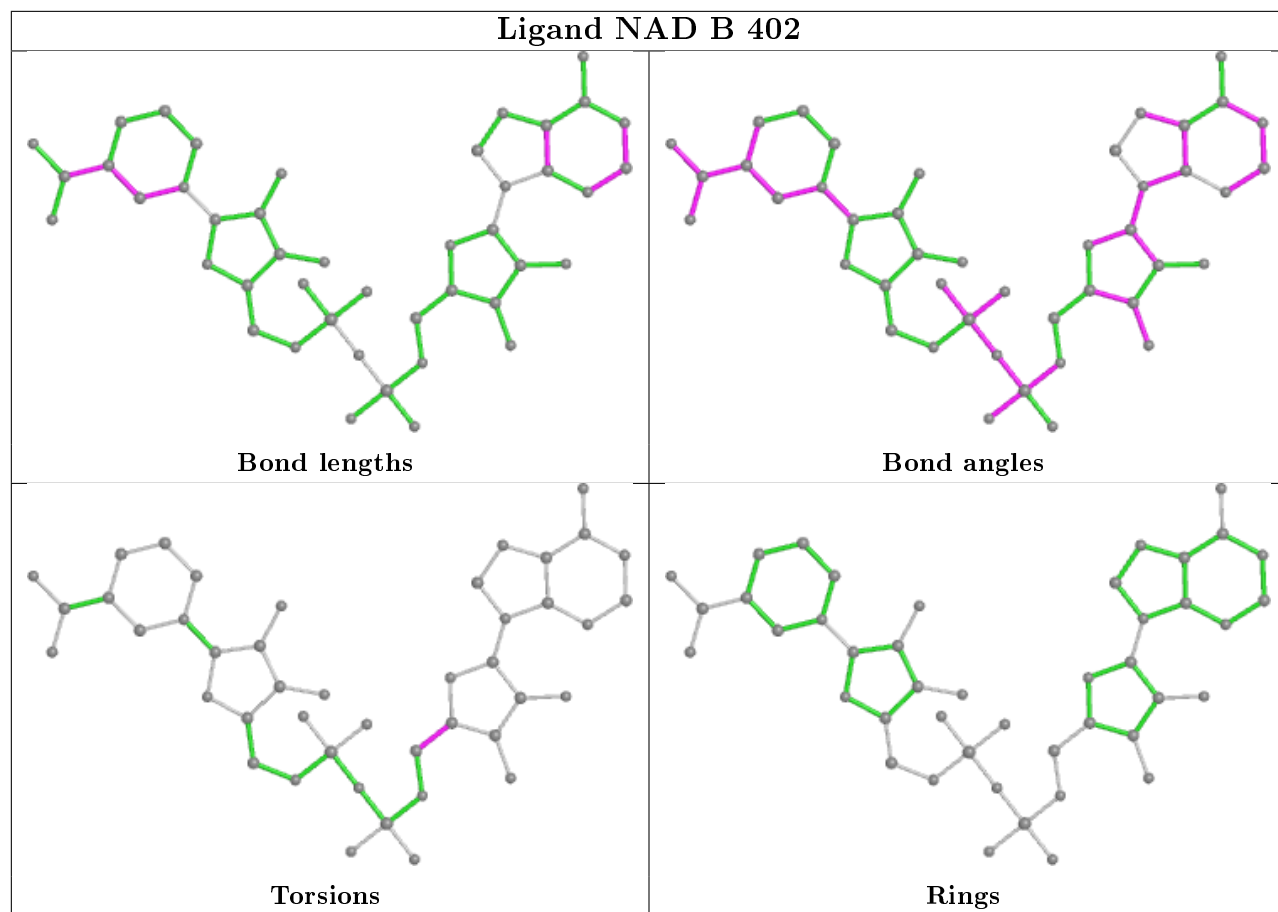
There are no ring outliers.

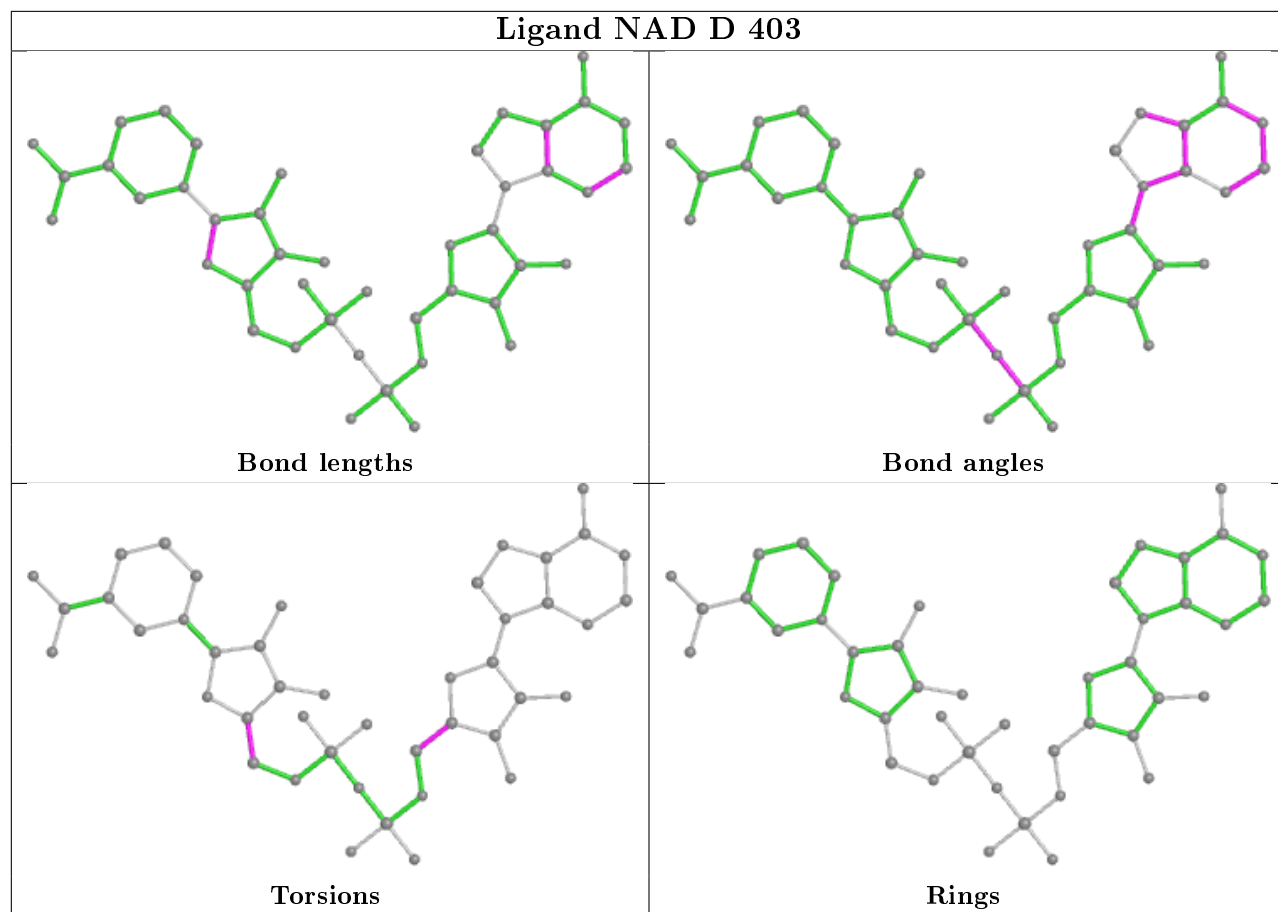
15 monomers are involved in 67 short contacts:

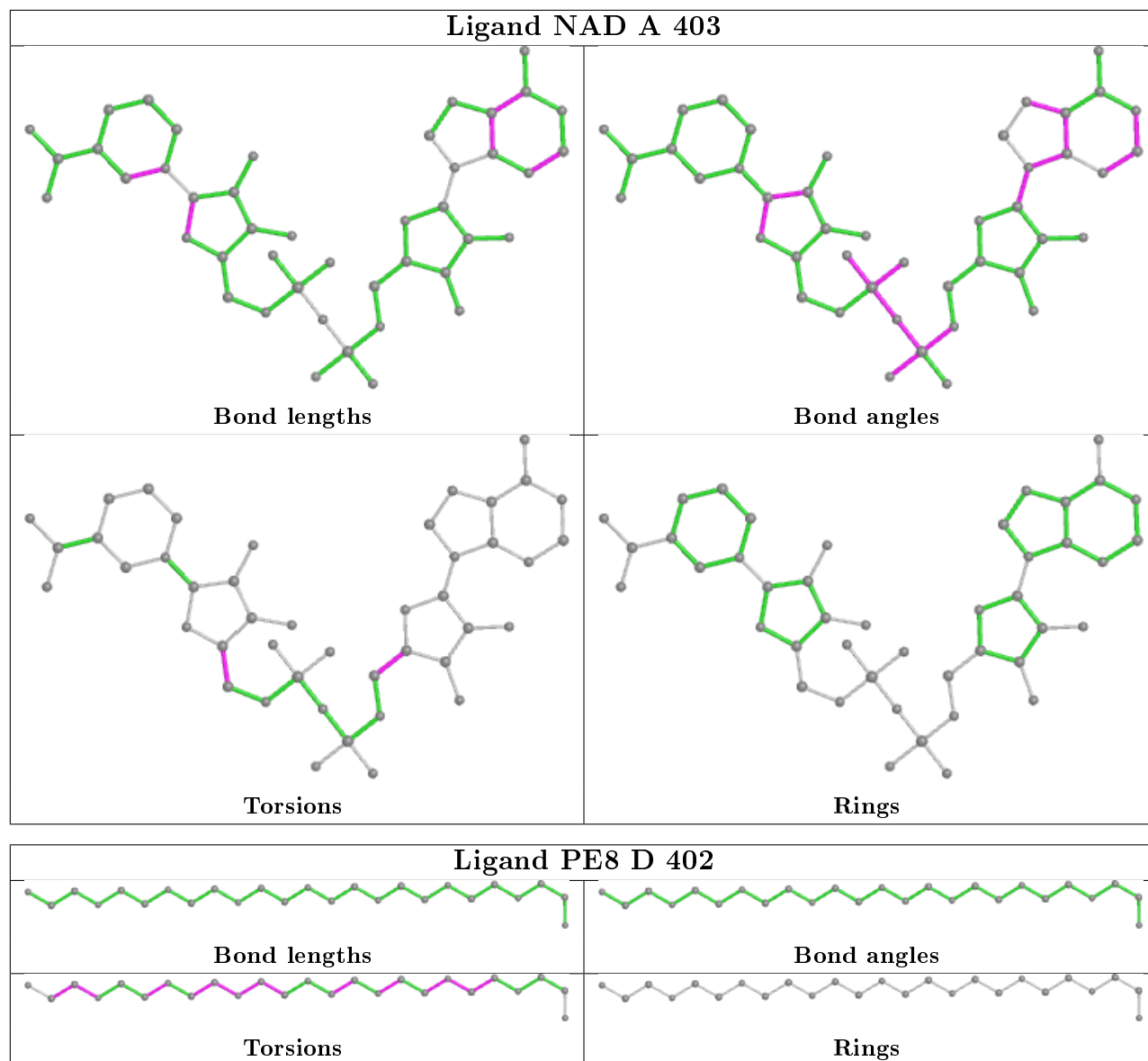
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	402	NAD	8	0
2	A	401	FLC	3	0
2	E	402	FLC	1	0
4	B	402	NAD	7	0
4	D	403	NAD	4	0
2	D	401	FLC	1	0
2	F	401	FLC	3	0
2	C	401	FLC	1	0
2	E	401	FLC	3	0
2	B	401	FLC	3	0
4	A	403	NAD	6	0
3	D	402	PE8	11	0
4	E	403	NAD	6	0
3	A	402	PE8	13	0
4	C	402	NAD	4	0

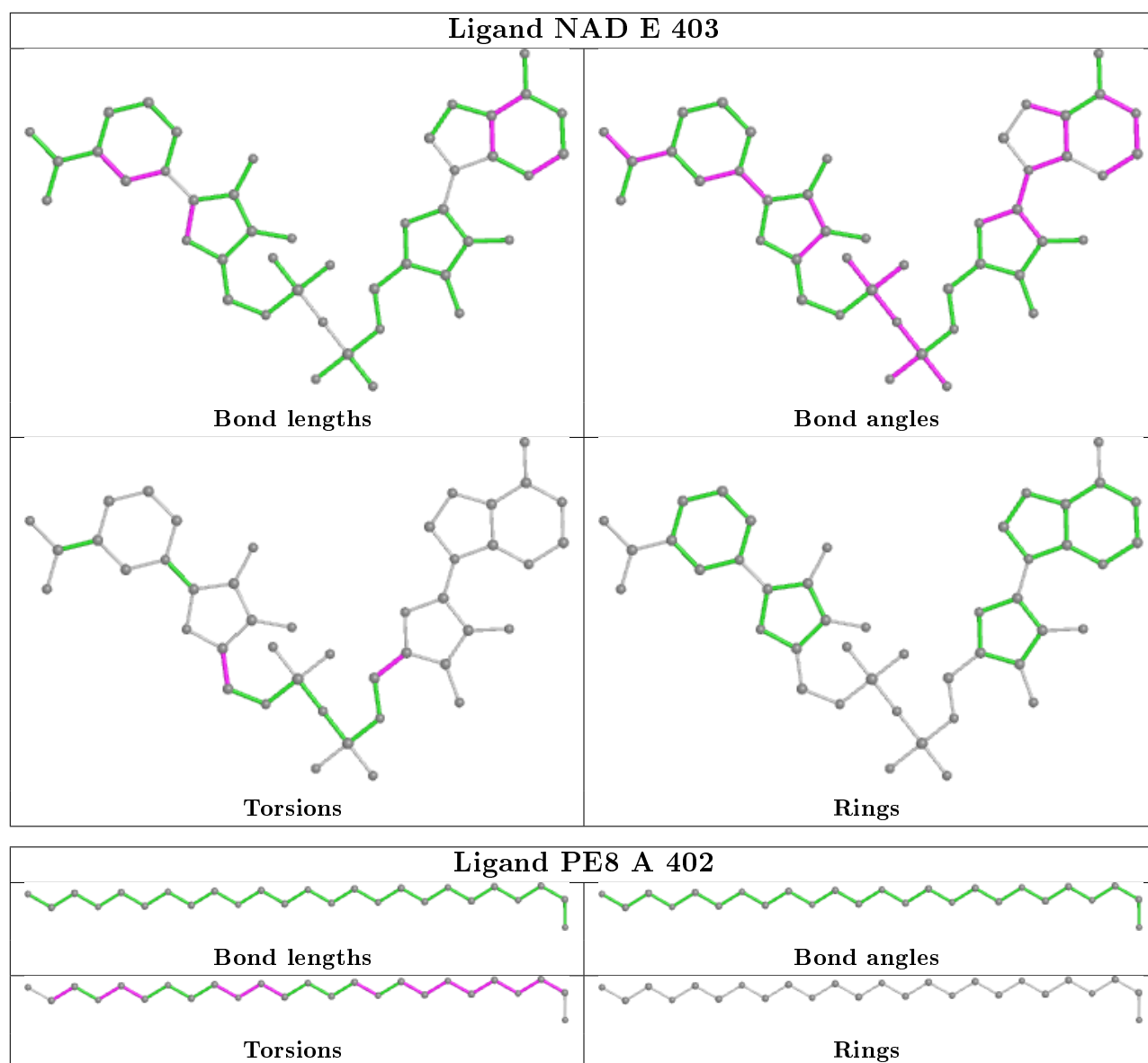
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

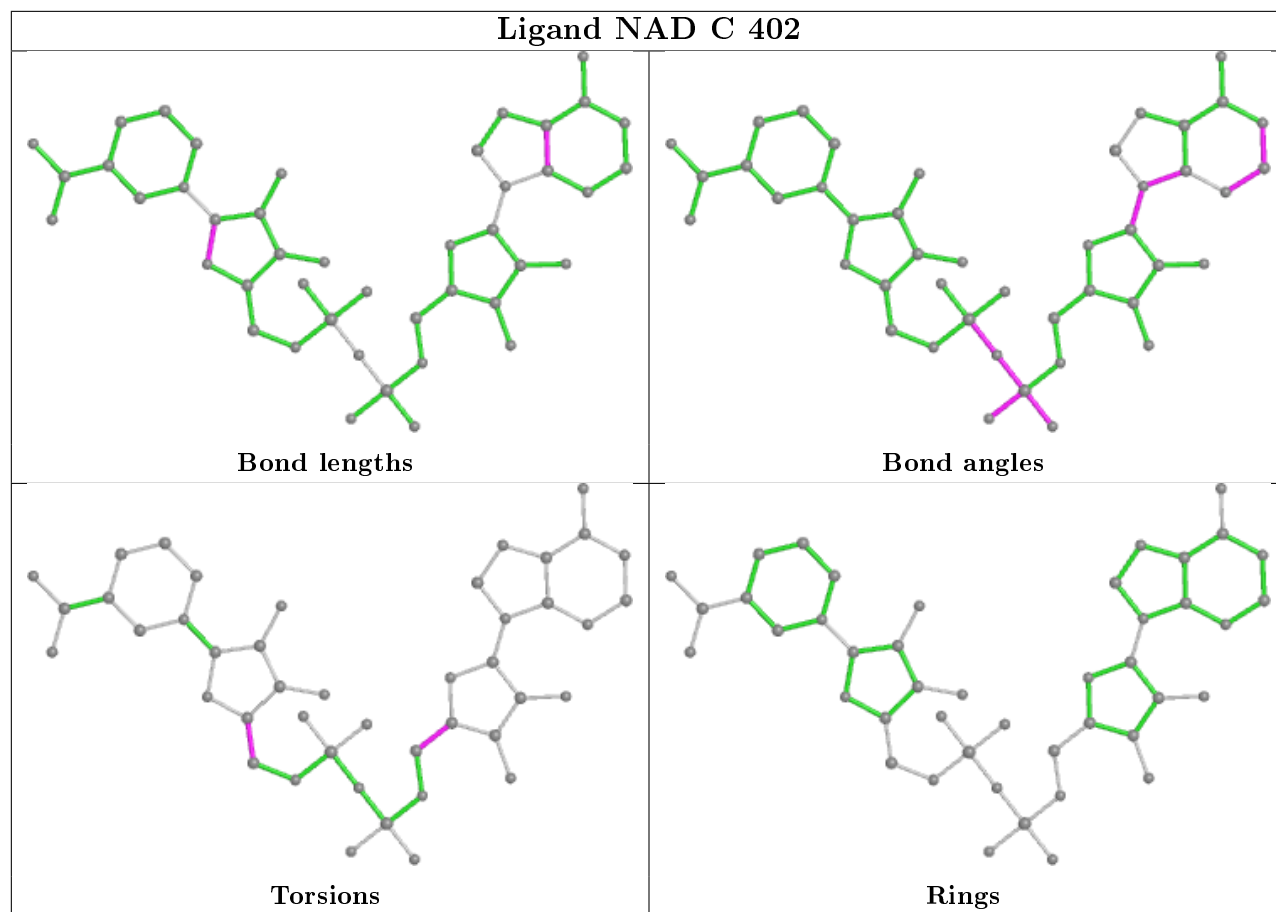












## 5.7 Other polymers [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	306/345 (88%)	-0.08	1 (0%) 94 96	21, 34, 57, 75	0
1	B	306/345 (88%)	-0.06	5 (1%) 72 78	23, 37, 56, 69	0
1	C	306/345 (88%)	0.08	3 (0%) 82 86	20, 37, 57, 81	0
1	D	307/345 (88%)	0.20	12 (3%) 39 46	26, 42, 61, 96	0
1	E	304/345 (88%)	0.07	4 (1%) 77 81	21, 36, 55, 71	0
1	F	307/345 (88%)	0.19	11 (3%) 42 49	25, 41, 62, 90	0
All	All	1836/2070 (88%)	0.07	36 (1%) 65 72	20, 38, 59, 96	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	290	PHE	6.2
1	D	66	ARG	4.3
1	F	229	ALA	3.9
1	E	290	PHE	3.8
1	F	217	LYS	3.3

### 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 carbohydrates in this entry.



## 6.4 Ligands

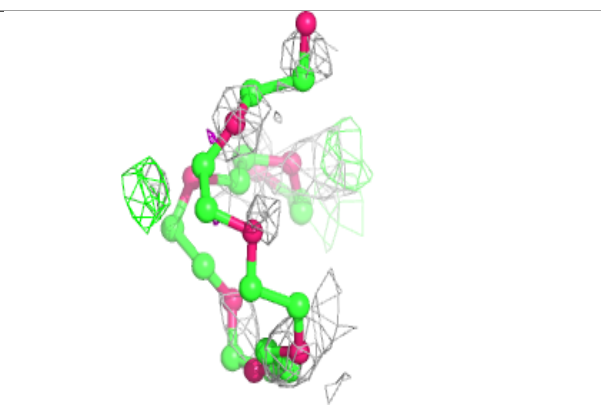
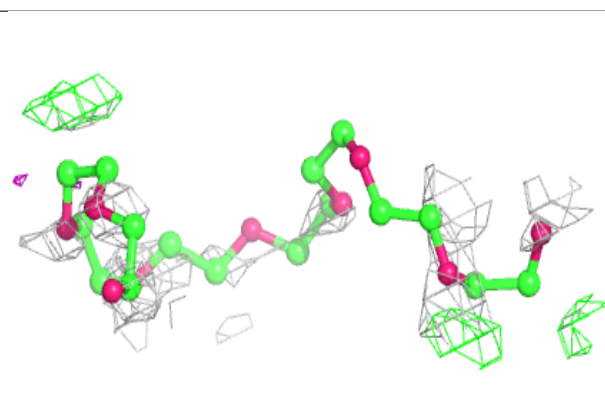
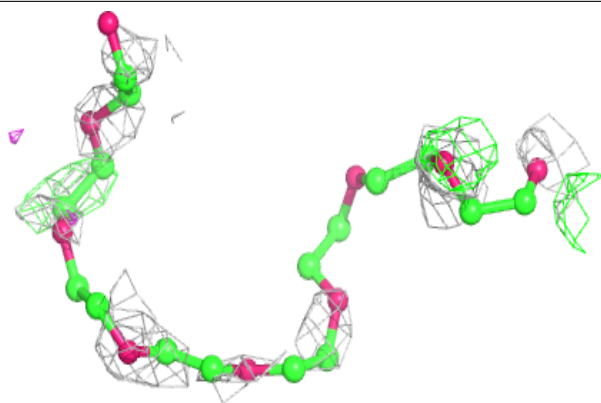
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PE8	D	402	25/25	0.61	0.74	80,93,108,108	0
3	PE8	A	402	25/25	0.68	0.58	60,72,74,76	0
2	FLC	F	401	13/13	0.69	0.27	59,68,74,75	0
2	FLC	C	401	13/13	0.78	0.26	77,82,85,85	0
2	FLC	D	401	13/13	0.80	0.20	65,70,72,74	0
2	FLC	B	401	13/13	0.80	0.20	77,82,87,89	0
2	FLC	E	401	13/13	0.82	0.23	68,75,79,80	0
2	FLC	E	402	13/13	0.82	0.26	63,67,69,70	0
2	FLC	A	401	13/13	0.83	0.21	64,65,69,72	0
4	NAD	E	403	44/44	0.93	0.14	27,34,44,49	0
4	NAD	F	402	44/44	0.94	0.12	24,37,43,49	0
4	NAD	D	403	44/44	0.95	0.13	35,43,58,66	0
4	NAD	B	402	44/44	0.95	0.12	25,37,45,47	0
4	NAD	A	403	44/44	0.95	0.12	27,36,43,49	0
4	NAD	C	402	44/44	0.96	0.12	28,39,59,64	0

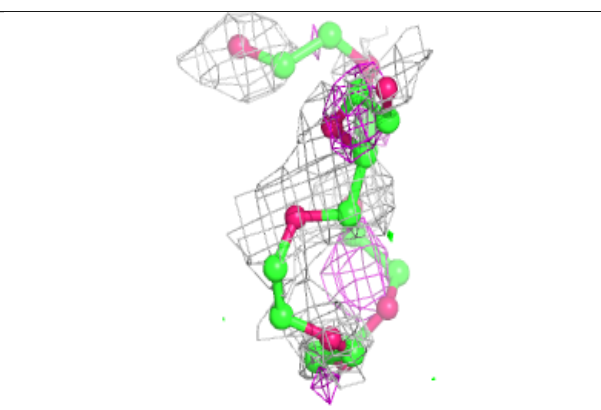
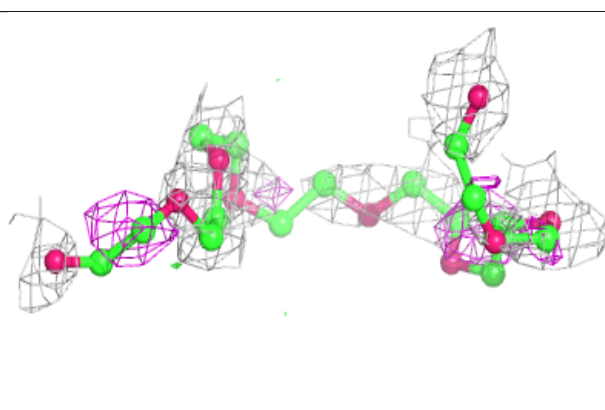
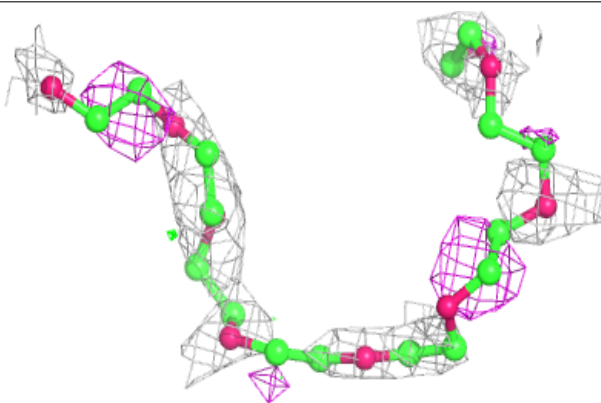
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PE8 D 402:**

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

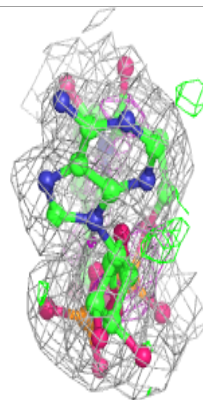
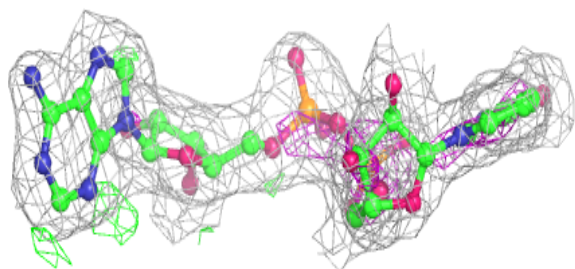
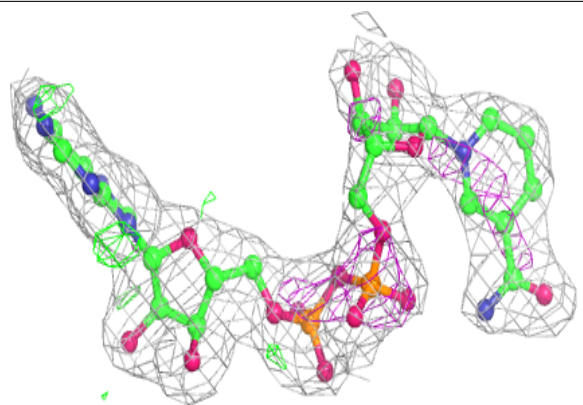
**Electron density around PE8 A 402:**

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

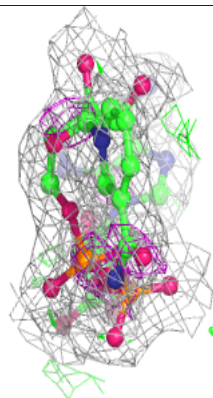
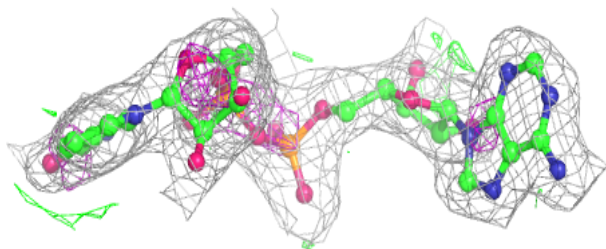
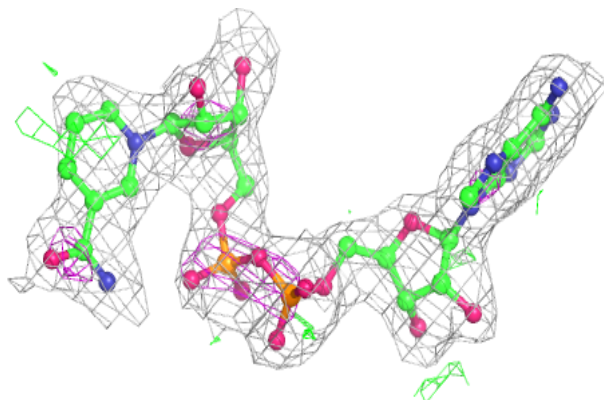


**Electron density around NAD E 403:**

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

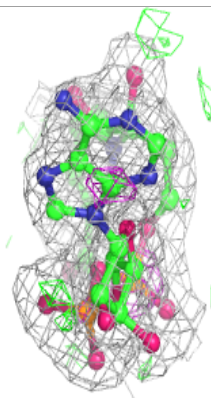
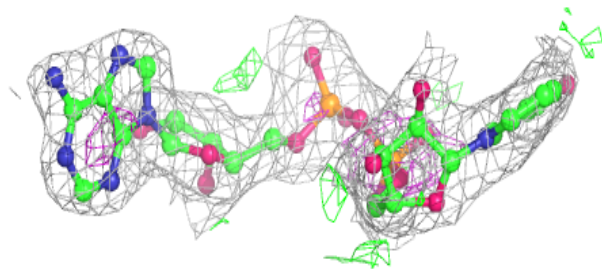
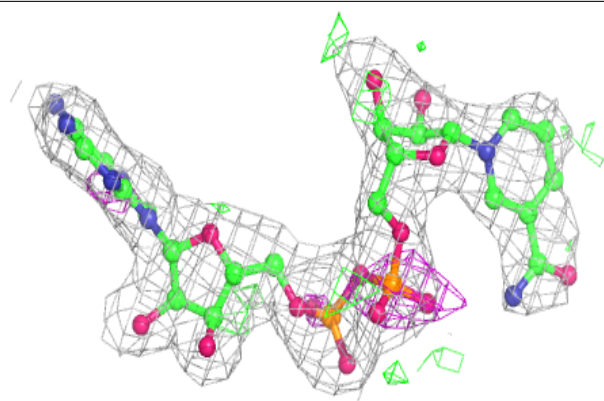
**Electron density around NAD F 402:**

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

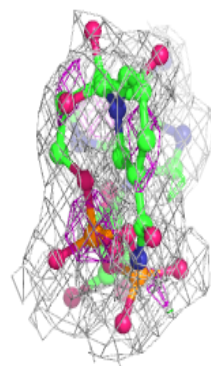
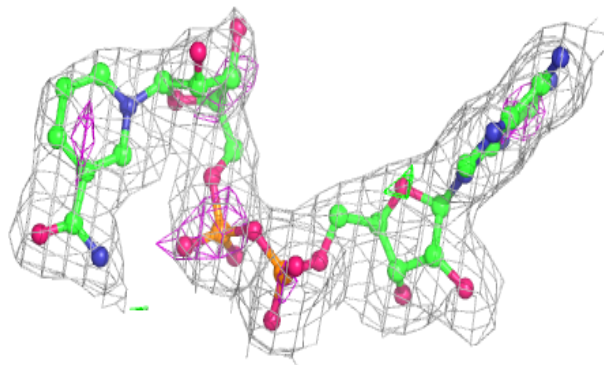


**Electron density around NAD D 403:**

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

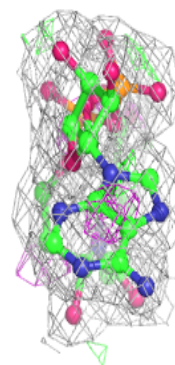
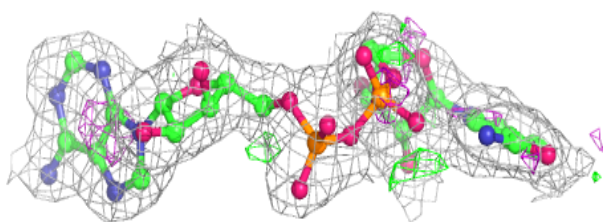
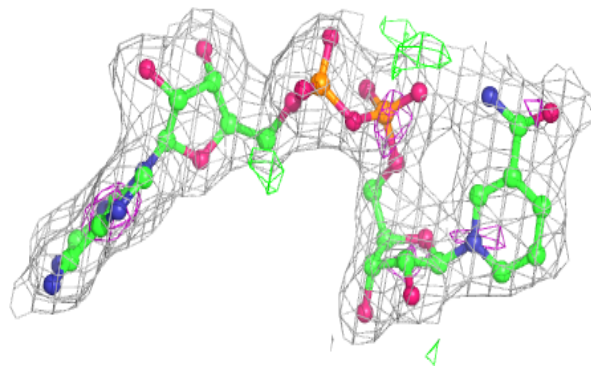
**Electron density around NAD B 402:**

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

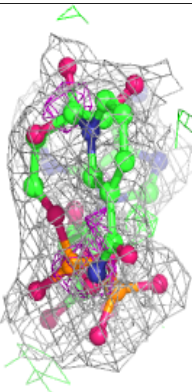
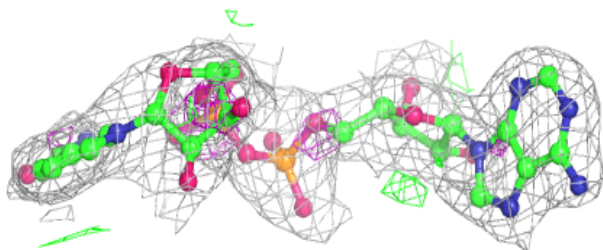
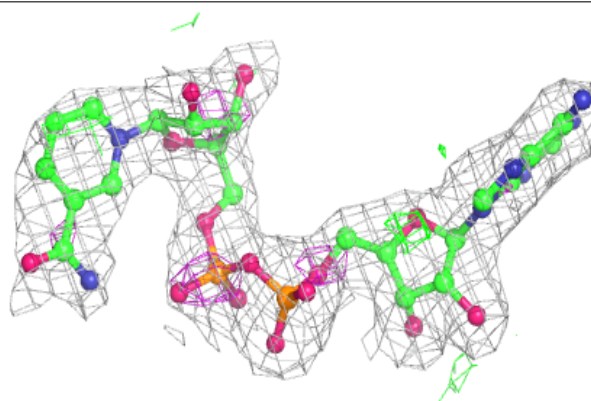


**Electron density around NAD A 403:**

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

**Electron density around NAD C 402:**

$2mF_o-DF_c$  (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.