



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 03:24 AM EDT

PDB ID : 4FBG  
Title : Crystal structure of *Treponema denticola* trans-2-enoyl-CoA reductase in complex with NAD  
Authors : Hu, K.; Zhao, M.; Zhang, T.; Yang, S.; Ding, J.  
Deposited on : 2012-05-23  
Resolution : 3.02 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

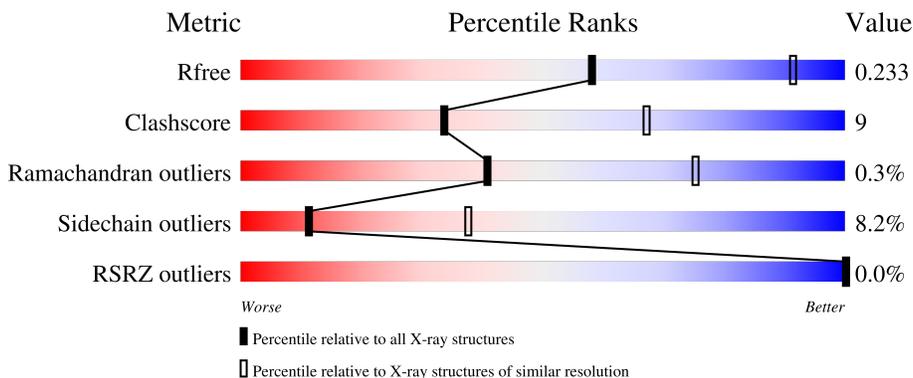
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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  $\geq 3$ , 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	405	73% 22% ..
1	B	405	75% 20% ..
1	C	405	77% 18% ..
1	D	405	78% 20% ..
1	E	405	76% 20% ..

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Mol	Chain	Length	Quality of chain
1	F	405	 75% 20% ..
1	G	405	 72% 24% ..
1	H	405	 74% 22% ..
1	I	405	 77% 20% ..
1	J	405	 80% 17% ..
1	K	405	 72% 23% ..
1	L	405	 72% 24% ..
1	M	405	 76% 20% ..
1	N	405	 76% 20% ..
1	O	405	 76% 19% ..
1	P	405	 73% 23% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	K	1001	-	-	-	X
2	NAD	M	1001	-	-	-	X

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 49790 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 Putative reductase TDE\_0597.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	399	Total 3096	C 1957	N 527	O 601	S 5	Se 6	0	0	0
1	B	397	Total 3079	C 1946	N 525	O 597	S 5	Se 6	0	0	0
1	C	399	Total 3096	C 1957	N 527	O 601	S 5	Se 6	0	0	0
1	D	401	Total 3116	C 1969	N 533	O 603	S 5	Se 6	0	0	0
1	E	397	Total 3079	C 1946	N 525	O 597	S 5	Se 6	0	0	0
1	F	398	Total 3087	C 1952	N 526	O 598	S 5	Se 6	0	0	0
1	G	398	Total 3087	C 1952	N 526	O 598	S 5	Se 6	0	0	0
1	H	399	Total 3096	C 1957	N 527	O 601	S 5	Se 6	0	0	0
1	I	399	Total 3096	C 1957	N 527	O 601	S 5	Se 6	0	0	0
1	J	397	Total 3079	C 1946	N 525	O 597	S 5	Se 6	0	0	0
1	K	397	Total 3079	C 1946	N 525	O 597	S 5	Se 6	0	0	0
1	L	401	Total 3116	C 1969	N 533	O 603	S 5	Se 6	0	0	0
1	M	397	Total 3079	C 1946	N 525	O 597	S 5	Se 6	0	0	0
1	N	398	Total 3087	C 1952	N 526	O 598	S 5	Se 6	0	0	0
1	O	397	Total 3079	C 1946	N 525	O 597	S 5	Se 6	0	0	0
1	P	398	Total 3087	C 1952	N 526	O 598	S 5	Se 6	0	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	LEU	-	expression tag	UNP Q73Q47
A	399	GLU	-	expression tag	UNP Q73Q47
A	400	HIS	-	expression tag	UNP Q73Q47
A	401	HIS	-	expression tag	UNP Q73Q47
A	402	HIS	-	expression tag	UNP Q73Q47
A	403	HIS	-	expression tag	UNP Q73Q47
A	404	HIS	-	expression tag	UNP Q73Q47
A	405	HIS	-	expression tag	UNP Q73Q47
B	398	LEU	-	expression tag	UNP Q73Q47
B	399	GLU	-	expression tag	UNP Q73Q47
B	400	HIS	-	expression tag	UNP Q73Q47
B	401	HIS	-	expression tag	UNP Q73Q47
B	402	HIS	-	expression tag	UNP Q73Q47
B	403	HIS	-	expression tag	UNP Q73Q47
B	404	HIS	-	expression tag	UNP Q73Q47
B	405	HIS	-	expression tag	UNP Q73Q47
C	398	LEU	-	expression tag	UNP Q73Q47
C	399	GLU	-	expression tag	UNP Q73Q47
C	400	HIS	-	expression tag	UNP Q73Q47
C	401	HIS	-	expression tag	UNP Q73Q47
C	402	HIS	-	expression tag	UNP Q73Q47
C	403	HIS	-	expression tag	UNP Q73Q47
C	404	HIS	-	expression tag	UNP Q73Q47
C	405	HIS	-	expression tag	UNP Q73Q47
D	398	LEU	-	expression tag	UNP Q73Q47
D	399	GLU	-	expression tag	UNP Q73Q47
D	400	HIS	-	expression tag	UNP Q73Q47
D	401	HIS	-	expression tag	UNP Q73Q47
D	402	HIS	-	expression tag	UNP Q73Q47
D	403	HIS	-	expression tag	UNP Q73Q47
D	404	HIS	-	expression tag	UNP Q73Q47
D	405	HIS	-	expression tag	UNP Q73Q47
E	398	LEU	-	expression tag	UNP Q73Q47
E	399	GLU	-	expression tag	UNP Q73Q47
E	400	HIS	-	expression tag	UNP Q73Q47
E	401	HIS	-	expression tag	UNP Q73Q47
E	402	HIS	-	expression tag	UNP Q73Q47
E	403	HIS	-	expression tag	UNP Q73Q47
E	404	HIS	-	expression tag	UNP Q73Q47
E	405	HIS	-	expression tag	UNP Q73Q47
F	398	LEU	-	expression tag	UNP Q73Q47
F	399	GLU	-	expression tag	UNP Q73Q47

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Chain	Residue	Modelled	Actual	Comment	Reference
F	400	HIS	-	expression tag	UNP Q73Q47
F	401	HIS	-	expression tag	UNP Q73Q47
F	402	HIS	-	expression tag	UNP Q73Q47
F	403	HIS	-	expression tag	UNP Q73Q47
F	404	HIS	-	expression tag	UNP Q73Q47
F	405	HIS	-	expression tag	UNP Q73Q47
G	398	LEU	-	expression tag	UNP Q73Q47
G	399	GLU	-	expression tag	UNP Q73Q47
G	400	HIS	-	expression tag	UNP Q73Q47
G	401	HIS	-	expression tag	UNP Q73Q47
G	402	HIS	-	expression tag	UNP Q73Q47
G	403	HIS	-	expression tag	UNP Q73Q47
G	404	HIS	-	expression tag	UNP Q73Q47
G	405	HIS	-	expression tag	UNP Q73Q47
H	398	LEU	-	expression tag	UNP Q73Q47
H	399	GLU	-	expression tag	UNP Q73Q47
H	400	HIS	-	expression tag	UNP Q73Q47
H	401	HIS	-	expression tag	UNP Q73Q47
H	402	HIS	-	expression tag	UNP Q73Q47
H	403	HIS	-	expression tag	UNP Q73Q47
H	404	HIS	-	expression tag	UNP Q73Q47
H	405	HIS	-	expression tag	UNP Q73Q47
I	398	LEU	-	expression tag	UNP Q73Q47
I	399	GLU	-	expression tag	UNP Q73Q47
I	400	HIS	-	expression tag	UNP Q73Q47
I	401	HIS	-	expression tag	UNP Q73Q47
I	402	HIS	-	expression tag	UNP Q73Q47
I	403	HIS	-	expression tag	UNP Q73Q47
I	404	HIS	-	expression tag	UNP Q73Q47
I	405	HIS	-	expression tag	UNP Q73Q47
J	398	LEU	-	expression tag	UNP Q73Q47
J	399	GLU	-	expression tag	UNP Q73Q47
J	400	HIS	-	expression tag	UNP Q73Q47
J	401	HIS	-	expression tag	UNP Q73Q47
J	402	HIS	-	expression tag	UNP Q73Q47
J	403	HIS	-	expression tag	UNP Q73Q47
J	404	HIS	-	expression tag	UNP Q73Q47
J	405	HIS	-	expression tag	UNP Q73Q47
K	398	LEU	-	expression tag	UNP Q73Q47
K	399	GLU	-	expression tag	UNP Q73Q47
K	400	HIS	-	expression tag	UNP Q73Q47
K	401	HIS	-	expression tag	UNP Q73Q47

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Chain	Residue	Modelled	Actual	Comment	Reference
K	402	HIS	-	expression tag	UNP Q73Q47
K	403	HIS	-	expression tag	UNP Q73Q47
K	404	HIS	-	expression tag	UNP Q73Q47
K	405	HIS	-	expression tag	UNP Q73Q47
L	398	LEU	-	expression tag	UNP Q73Q47
L	399	GLU	-	expression tag	UNP Q73Q47
L	400	HIS	-	expression tag	UNP Q73Q47
L	401	HIS	-	expression tag	UNP Q73Q47
L	402	HIS	-	expression tag	UNP Q73Q47
L	403	HIS	-	expression tag	UNP Q73Q47
L	404	HIS	-	expression tag	UNP Q73Q47
L	405	HIS	-	expression tag	UNP Q73Q47
M	398	LEU	-	expression tag	UNP Q73Q47
M	399	GLU	-	expression tag	UNP Q73Q47
M	400	HIS	-	expression tag	UNP Q73Q47
M	401	HIS	-	expression tag	UNP Q73Q47
M	402	HIS	-	expression tag	UNP Q73Q47
M	403	HIS	-	expression tag	UNP Q73Q47
M	404	HIS	-	expression tag	UNP Q73Q47
M	405	HIS	-	expression tag	UNP Q73Q47
N	398	LEU	-	expression tag	UNP Q73Q47
N	399	GLU	-	expression tag	UNP Q73Q47
N	400	HIS	-	expression tag	UNP Q73Q47
N	401	HIS	-	expression tag	UNP Q73Q47
N	402	HIS	-	expression tag	UNP Q73Q47
N	403	HIS	-	expression tag	UNP Q73Q47
N	404	HIS	-	expression tag	UNP Q73Q47
N	405	HIS	-	expression tag	UNP Q73Q47
O	398	LEU	-	expression tag	UNP Q73Q47
O	399	GLU	-	expression tag	UNP Q73Q47
O	400	HIS	-	expression tag	UNP Q73Q47
O	401	HIS	-	expression tag	UNP Q73Q47
O	402	HIS	-	expression tag	UNP Q73Q47
O	403	HIS	-	expression tag	UNP Q73Q47
O	404	HIS	-	expression tag	UNP Q73Q47
O	405	HIS	-	expression tag	UNP Q73Q47
P	398	LEU	-	expression tag	UNP Q73Q47
P	399	GLU	-	expression tag	UNP Q73Q47
P	400	HIS	-	expression tag	UNP Q73Q47
P	401	HIS	-	expression tag	UNP Q73Q47
P	402	HIS	-	expression tag	UNP Q73Q47
P	403	HIS	-	expression tag	UNP Q73Q47

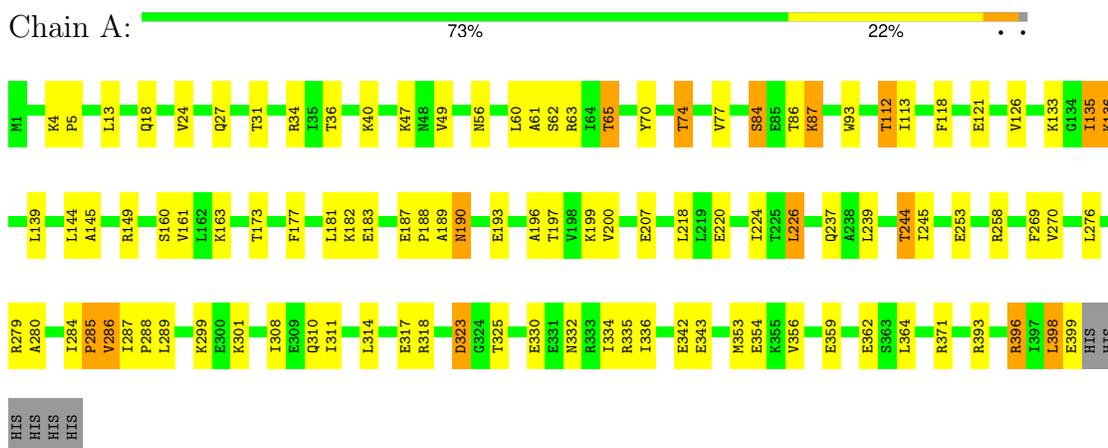
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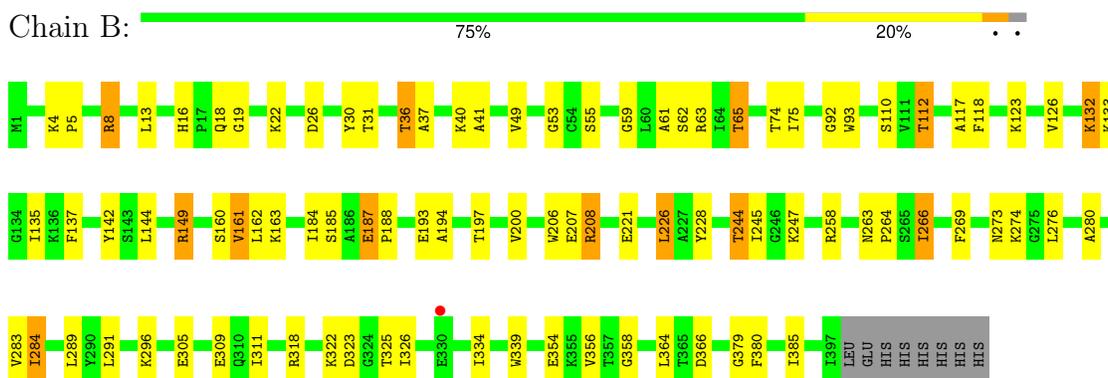
### 3 Residue-property plots

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.

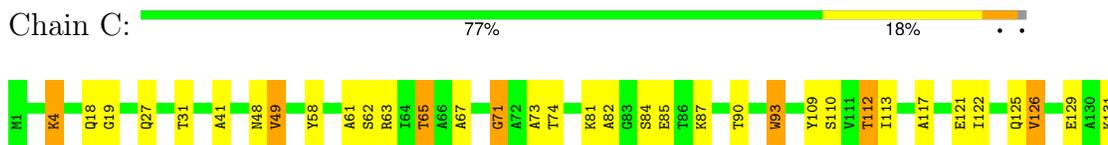
- Molecule 1: Putative reductase TDE\_0597



- Molecule 1: Putative reductase TDE\_0597



- Molecule 1: Putative reductase TDE\_0597

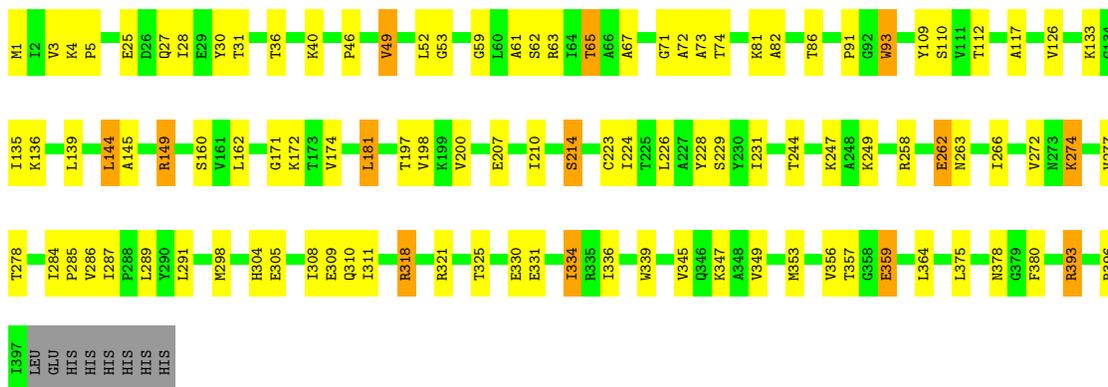






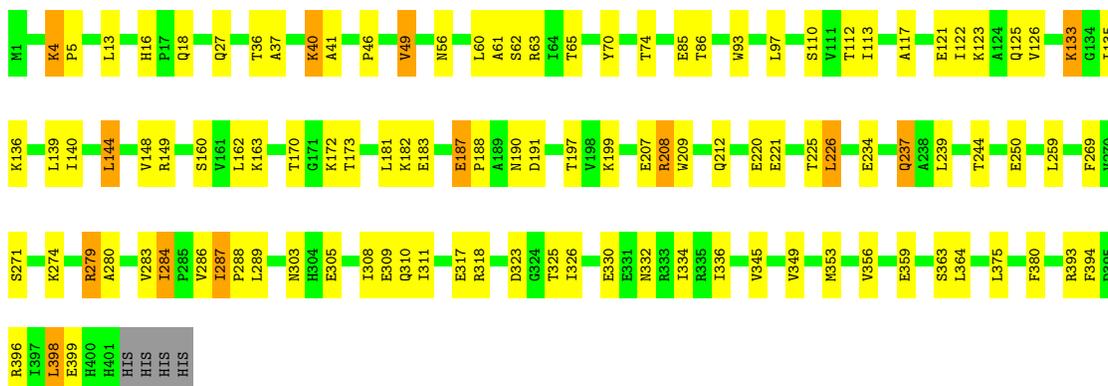
- Molecule 1: Putative reductase TDE\_0597

Chain K:  72% 23% ..



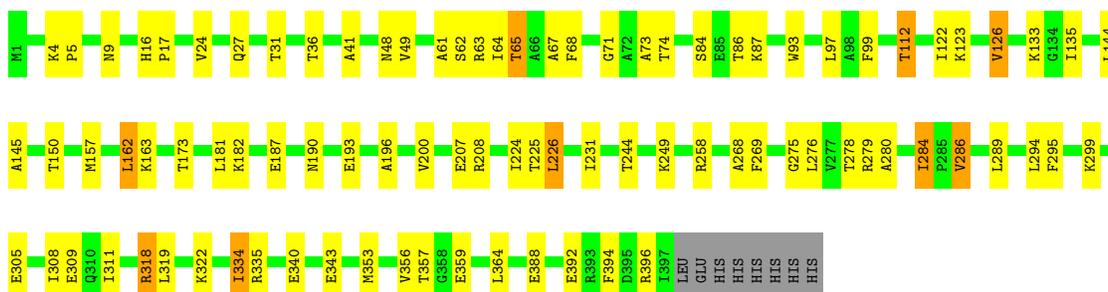
- Molecule 1: Putative reductase TDE\_0597

Chain L:  72% 24% ..



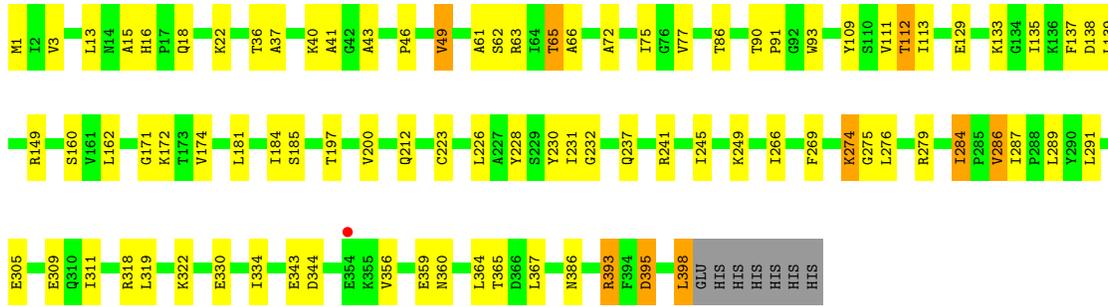
- Molecule 1: Putative reductase TDE\_0597

Chain M:  76% 20% ..

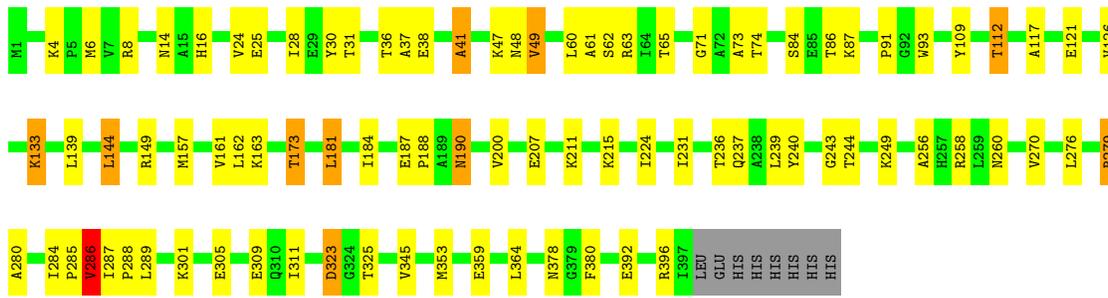
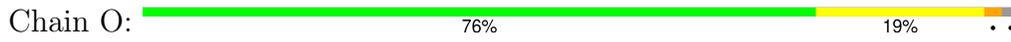


- Molecule 1: Putative reductase TDE\_0597

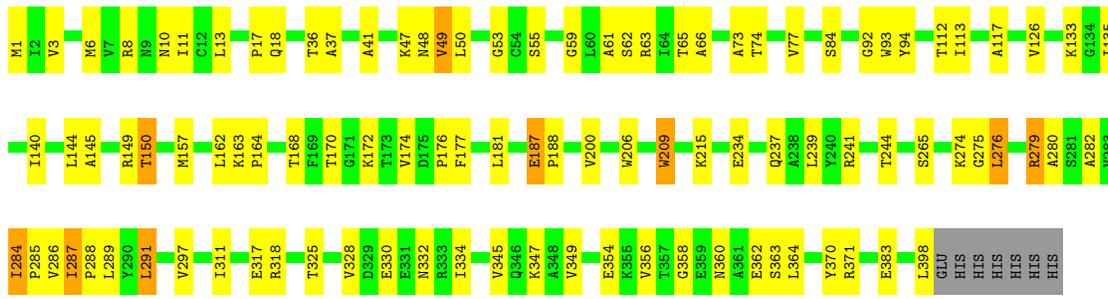
Chain N:  76% 20% ..



● Molecule 1: Putative reductase TDE\_0597



● Molecule 1: Putative reductase TDE\_0597



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.79Å 120.03Å 171.29Å 90.80° 104.96° 112.75°	Depositor
Resolution (Å)	50.00 – 3.02 41.07 – 3.02	Depositor EDS
% Data completeness (in resolution range)	94.8 (50.00-3.02) 94.9 (41.07-3.02)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.235 , 0.292 0.237 , 0.233	Depositor DCC
$R_{free}$ test set	6665 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtrriage
Anisotropy	0.288	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 11.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	49790	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.31 % 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 5.9504e-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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	0.47	2/3146 (0.1%)	0.55	0/4237
1	B	0.48	3/3129 (0.1%)	0.54	0/4214
1	C	0.46	1/3146 (0.0%)	0.55	0/4237
1	D	0.46	1/3168 (0.0%)	0.54	0/4267
1	E	0.48	1/3129 (0.0%)	0.55	1/4214 (0.0%)
1	F	0.48	1/3137 (0.0%)	0.55	0/4225
1	G	0.48	2/3137 (0.1%)	0.55	0/4225
1	H	0.55	3/3146 (0.1%)	0.56	0/4237
1	I	0.51	3/3146 (0.1%)	0.54	0/4237
1	J	0.46	2/3129 (0.1%)	0.54	0/4214
1	K	0.48	2/3129 (0.1%)	0.55	0/4214
1	L	0.47	1/3168 (0.0%)	0.54	0/4267
1	M	0.46	1/3129 (0.0%)	0.53	0/4214
1	N	0.50	1/3137 (0.0%)	0.55	0/4225
1	O	0.57	3/3129 (0.1%)	0.57	1/4214 (0.0%)
1	P	0.49	4/3137 (0.1%)	0.55	0/4225
All	All	0.49	31/50242 (0.1%)	0.55	2/67666 (0.0%)

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	4	LYS	CD-CE	5.90	1.66	1.51
1	A	285	PRO	N-CD	5.58	1.55	1.47
1	I	285	PRO	N-CD	5.57	1.55	1.47
1	O	41	ALA	C-O	5.56	1.33	1.23
1	P	93	TRP	CD2-CE2	5.55	1.48	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	181	LEU	CA-CB-CG	5.82	128.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	364	LEU	CA-CB-CG	5.21	127.29	115.30

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	3096	0	3097	61	0
1	B	3079	0	3080	53	0
1	C	3096	0	3097	60	0
1	D	3116	0	3111	44	0
1	E	3079	0	3080	50	0
1	F	3087	0	3091	58	0
1	G	3087	0	3091	64	0
1	H	3096	0	3097	51	0
1	I	3096	0	3097	45	0
1	J	3079	0	3080	40	0
1	K	3079	0	3080	54	0
1	L	3116	0	3111	62	0
1	M	3079	0	3080	45	0
1	N	3087	0	3091	54	0
1	O	3079	0	3080	47	0
1	P	3087	0	3091	68	0
2	A	44	0	26	2	0
2	E	44	0	26	3	0
2	G	44	0	26	4	0
2	H	44	0	26	2	0
2	I	44	0	26	1	0
2	K	44	0	26	2	0
2	M	44	0	26	4	0
2	P	44	0	26	3	0
All	All	49790	0	49662	847	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 9.

The worst 5 of 847 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:N:393:ARG:HG2	1:N:393:ARG:HH11	1.18	1.08
1:K:63:ARG:HH12	1:K:112:THR:HG22	1.20	1.02
1:G:396:ARG:HG2	1:G:396:ARG:HH11	1.34	0.92
1:B:8:ARG:HG3	1:B:8:ARG:HH11	1.36	0.91
1:K:258:ARG:O	1:K:262:GLU:HG2	1.71	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	397/405 (98%)	370 (93%)	26 (6%)	1 (0%)	41 75
1	B	395/405 (98%)	378 (96%)	16 (4%)	1 (0%)	41 75
1	C	397/405 (98%)	368 (93%)	26 (6%)	3 (1%)	19 55
1	D	399/405 (98%)	378 (95%)	20 (5%)	1 (0%)	41 75
1	E	395/405 (98%)	372 (94%)	22 (6%)	1 (0%)	41 75
1	F	396/405 (98%)	369 (93%)	27 (7%)	0	100 100
1	G	396/405 (98%)	369 (93%)	26 (7%)	1 (0%)	41 75
1	H	397/405 (98%)	365 (92%)	29 (7%)	3 (1%)	19 55
1	I	397/405 (98%)	370 (93%)	26 (6%)	1 (0%)	41 75
1	J	395/405 (98%)	373 (94%)	21 (5%)	1 (0%)	41 75
1	K	395/405 (98%)	366 (93%)	29 (7%)	0	100 100
1	L	399/405 (98%)	367 (92%)	31 (8%)	1 (0%)	41 75
1	M	395/405 (98%)	374 (95%)	20 (5%)	1 (0%)	41 75
1	N	396/405 (98%)	375 (95%)	20 (5%)	1 (0%)	41 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	395/405 (98%)	370 (94%)	23 (6%)	2 (0%)	29	66
1	P	396/405 (98%)	366 (92%)	30 (8%)	0	100	100
All	All	6340/6480 (98%)	5930 (94%)	392 (6%)	18 (0%)	41	75

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	286	VAL
1	E	286	VAL
1	G	286	VAL
1	I	286	VAL
1	M	286	VAL

### 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	325/325 (100%)	291 (90%)	34 (10%)	7	26
1	B	323/325 (99%)	296 (92%)	27 (8%)	11	37
1	C	325/325 (100%)	302 (93%)	23 (7%)	14	44
1	D	327/325 (101%)	300 (92%)	27 (8%)	11	37
1	E	323/325 (99%)	306 (95%)	17 (5%)	22	57
1	F	324/325 (100%)	300 (93%)	24 (7%)	13	42
1	G	324/325 (100%)	298 (92%)	26 (8%)	12	39
1	H	325/325 (100%)	298 (92%)	27 (8%)	11	37
1	I	325/325 (100%)	301 (93%)	24 (7%)	13	42
1	J	323/325 (99%)	304 (94%)	19 (6%)	19	52
1	K	323/325 (99%)	292 (90%)	31 (10%)	8	30
1	L	327/325 (101%)	289 (88%)	38 (12%)	5	22
1	M	323/325 (99%)	296 (92%)	27 (8%)	11	37
1	N	324/325 (100%)	298 (92%)	26 (8%)	12	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	323/325 (99%)	297 (92%)	26 (8%)	12	39
1	P	324/325 (100%)	297 (92%)	27 (8%)	11	37
All	All	5188/5200 (100%)	4765 (92%)	423 (8%)	11	38

5 of 423 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	85	GLU
1	L	133	LYS
1	P	47	LYS
1	J	156	ILE
1	K	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	304	HIS
1	M	304	HIS
1	K	27	GLN
1	L	18	GLN
1	N	212	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	A	1001	-	42,48,48	3.79	12 (28%)	50,73,73	2.32	8 (16%)
2	NAD	G	1001	-	42,48,48	3.64	13 (30%)	50,73,73	2.56	8 (16%)
2	NAD	I	1001	-	42,48,48	3.67	11 (26%)	50,73,73	2.33	7 (14%)
2	NAD	E	1001	-	42,48,48	4.12	11 (26%)	50,73,73	2.30	10 (20%)
2	NAD	K	1001	-	42,48,48	4.06	12 (28%)	50,73,73	2.21	7 (14%)
2	NAD	P	1001	-	42,48,48	3.77	13 (30%)	50,73,73	2.56	9 (18%)
2	NAD	M	1001	-	42,48,48	3.98	11 (26%)	50,73,73	2.41	11 (22%)
2	NAD	H	1001	-	42,48,48	3.82	13 (30%)	50,73,73	2.66	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	1001	-	-	14/26/62/62	0/5/5/5
2	NAD	G	1001	-	-	14/26/62/62	0/5/5/5
2	NAD	I	1001	-	-	10/26/62/62	0/5/5/5
2	NAD	E	1001	-	-	11/26/62/62	0/5/5/5
2	NAD	K	1001	-	-	11/26/62/62	0/5/5/5
2	NAD	P	1001	-	-	11/26/62/62	0/5/5/5
2	NAD	M	1001	-	-	11/26/62/62	0/5/5/5
2	NAD	H	1001	-	-	12/26/62/62	0/5/5/5

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1001	NAD	C2A-N3A	13.24	1.52	1.32
2	E	1001	NAD	C2A-N1A	13.04	1.57	1.33
2	E	1001	NAD	C2A-N3A	12.99	1.52	1.32
2	K	1001	NAD	C2A-N3A	12.98	1.52	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1001	NAD	C2A-N3A	12.82	1.52	1.32

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001	NAD	N3A-C2A-N1A	-13.85	109.87	128.67
2	I	1001	NAD	N3A-C2A-N1A	-12.78	111.32	128.67
2	P	1001	NAD	N3A-C2A-N1A	-11.74	112.73	128.67
2	H	1001	NAD	N3A-C2A-N1A	-11.66	112.84	128.67
2	A	1001	NAD	N3A-C2A-N1A	-11.62	112.90	128.67

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NAD	C5D-O5D-PN-O3
2	A	1001	NAD	C5D-O5D-PN-O2N
2	A	1001	NAD	O4D-C1D-N1N-C2N
2	A	1001	NAD	O4D-C1D-N1N-C6N
2	A	1001	NAD	C2D-C1D-N1N-C2N

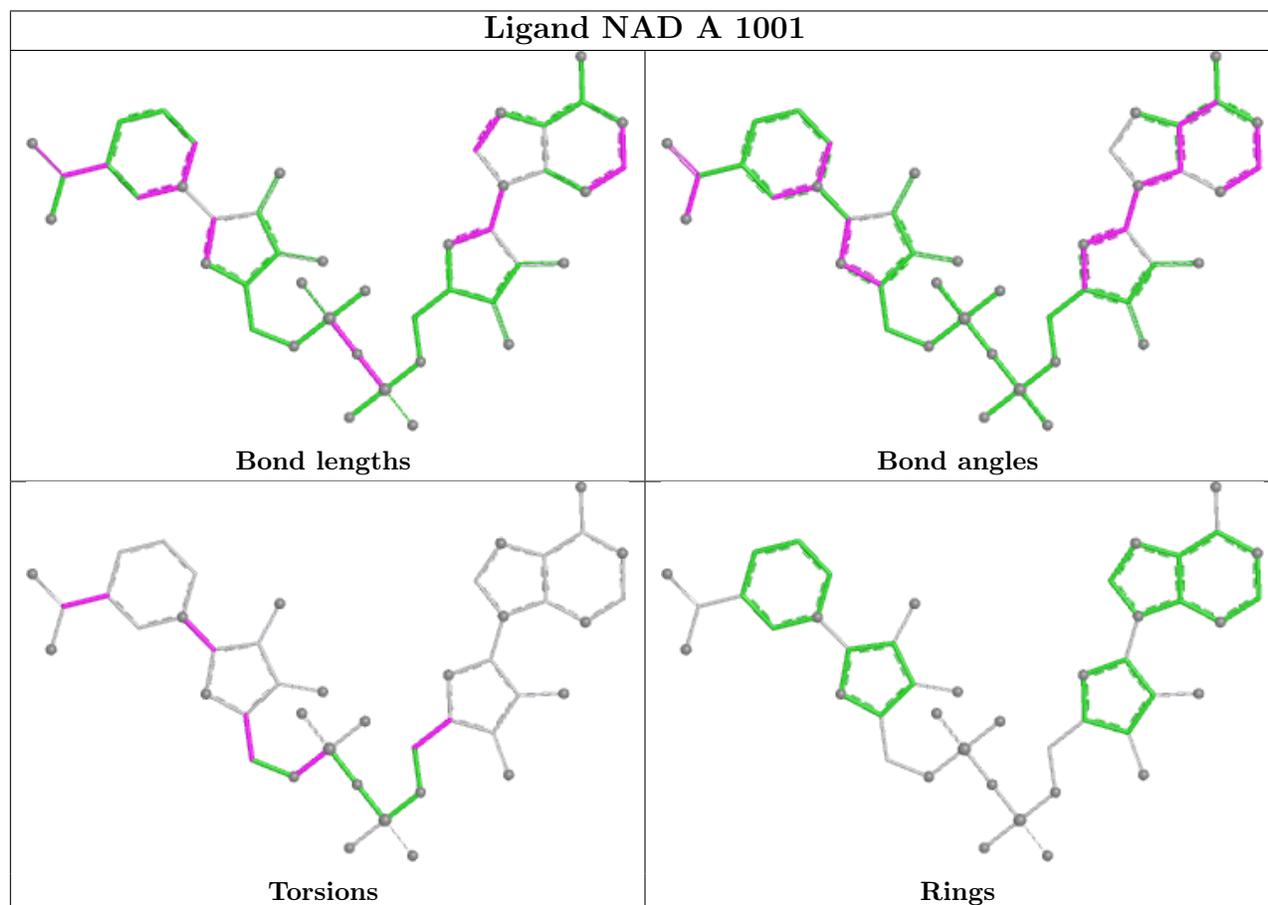
There are no ring outliers.

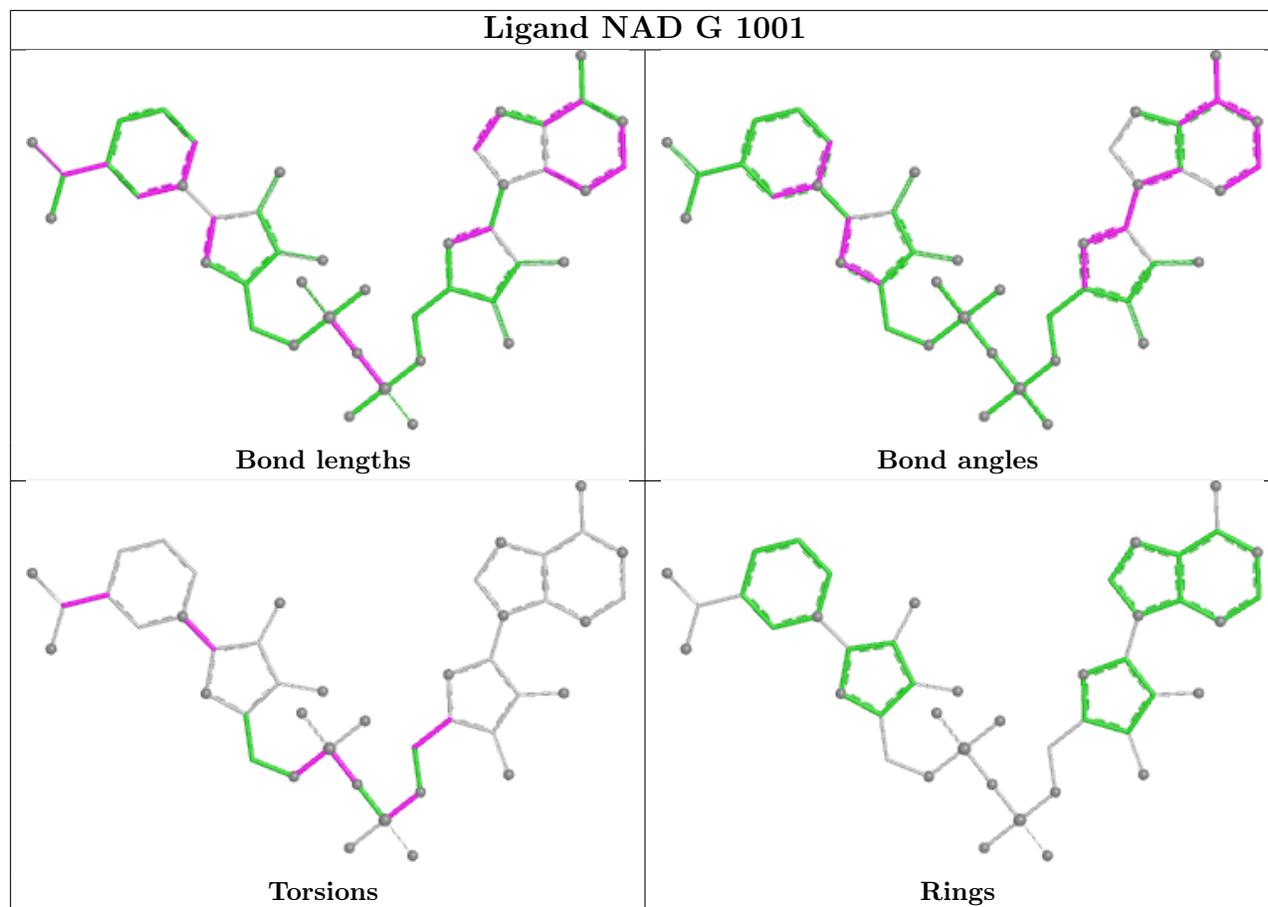
8 monomers are involved in 21 short contacts:

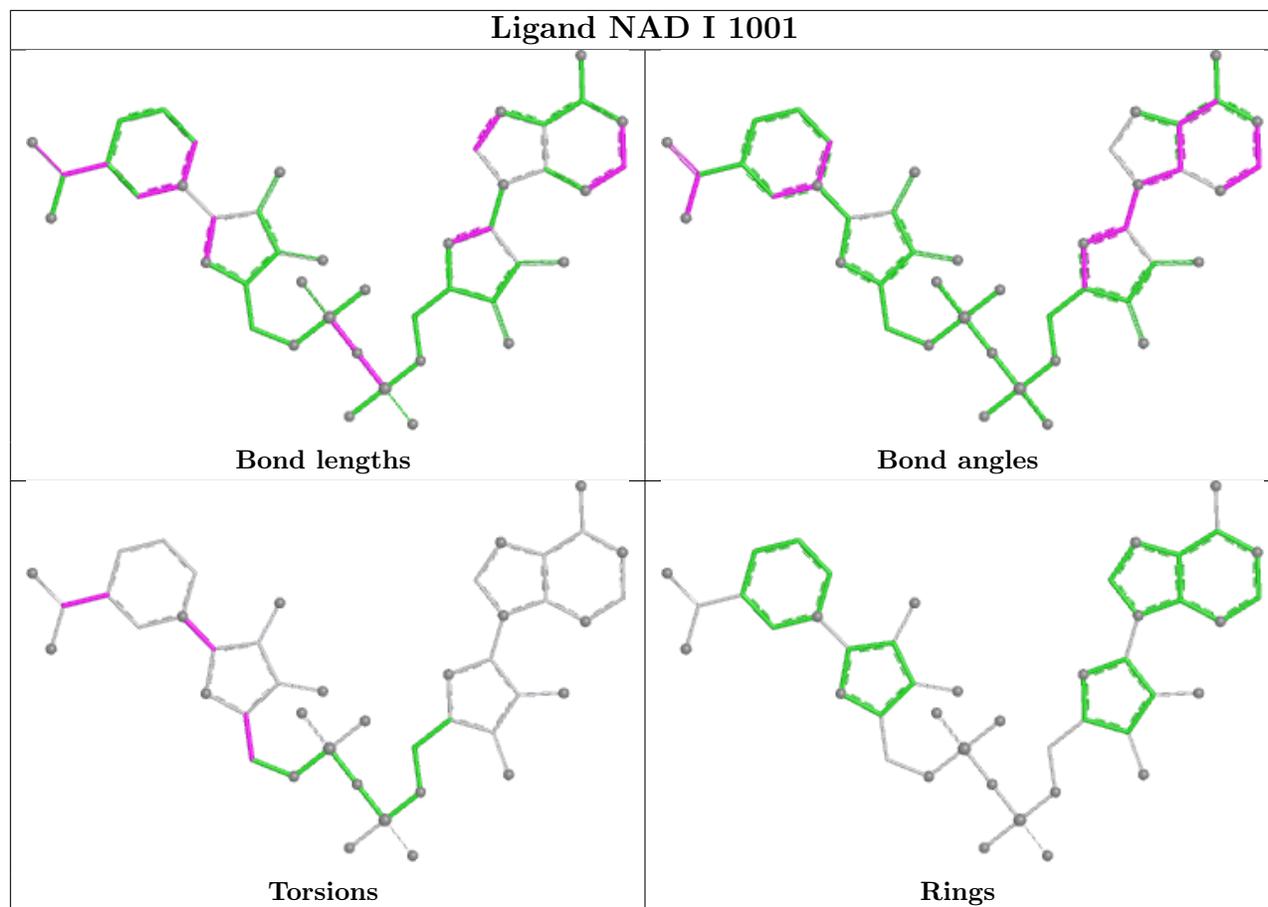
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAD	2	0
2	G	1001	NAD	4	0
2	I	1001	NAD	1	0
2	E	1001	NAD	3	0
2	K	1001	NAD	2	0
2	P	1001	NAD	3	0
2	M	1001	NAD	4	0
2	H	1001	NAD	2	0

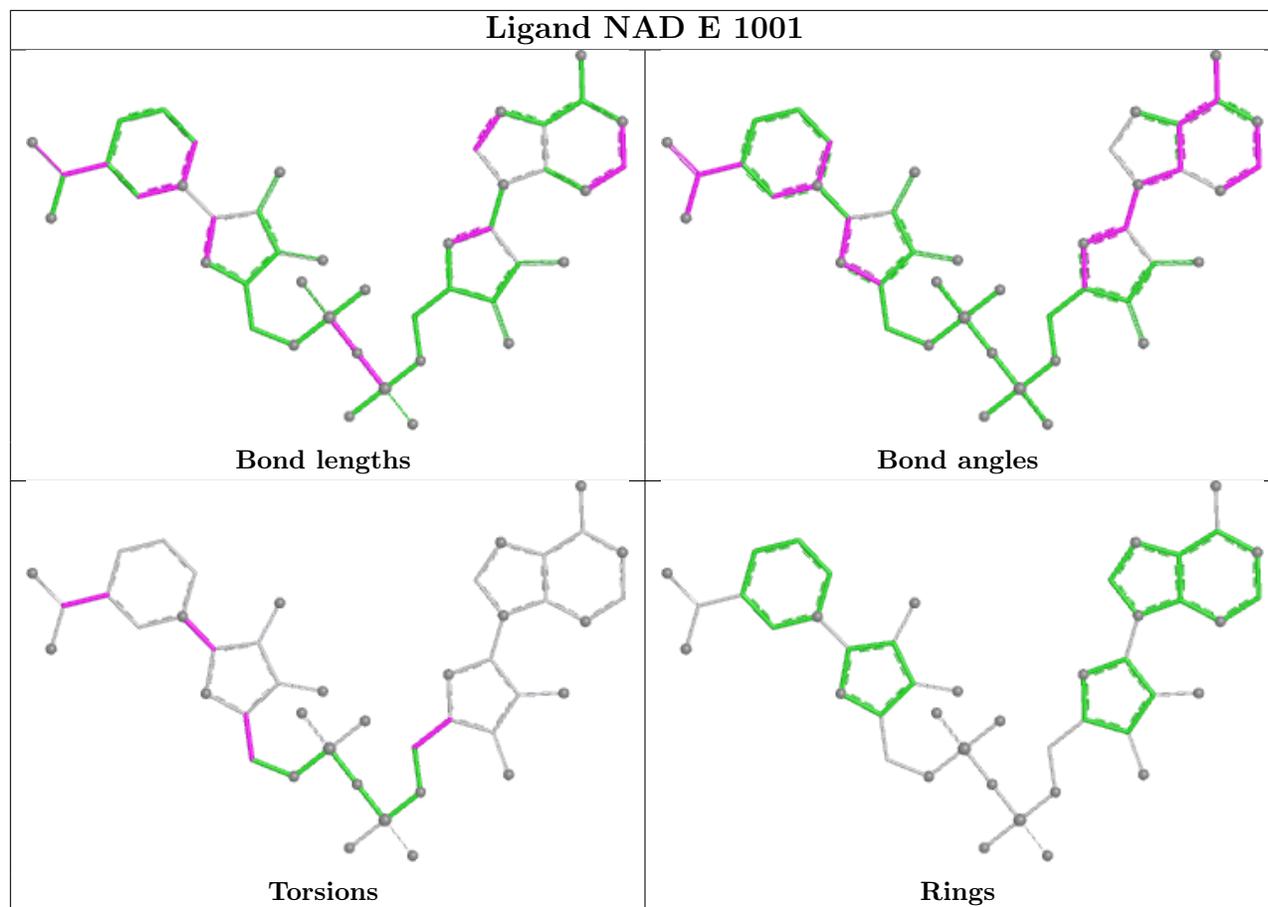
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

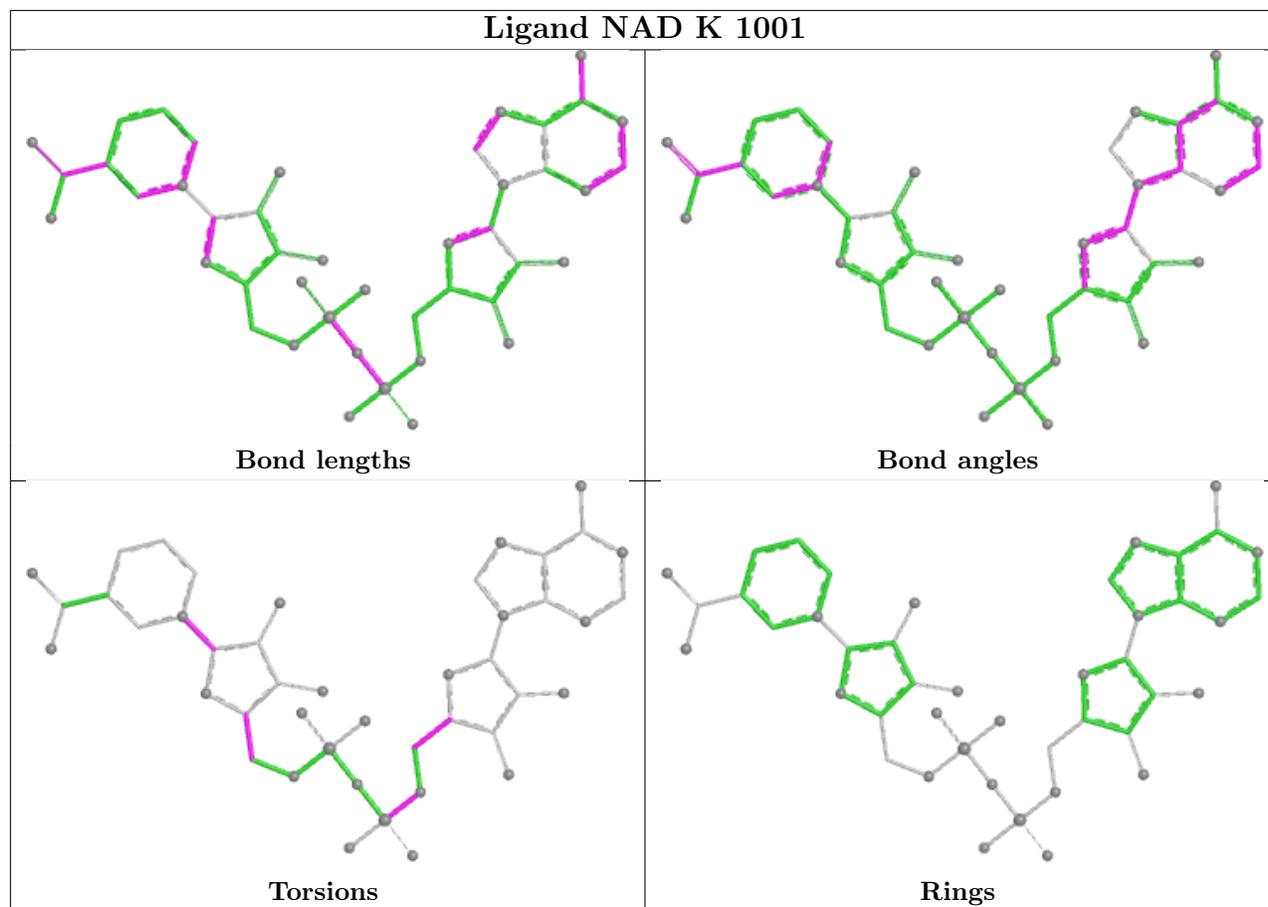
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

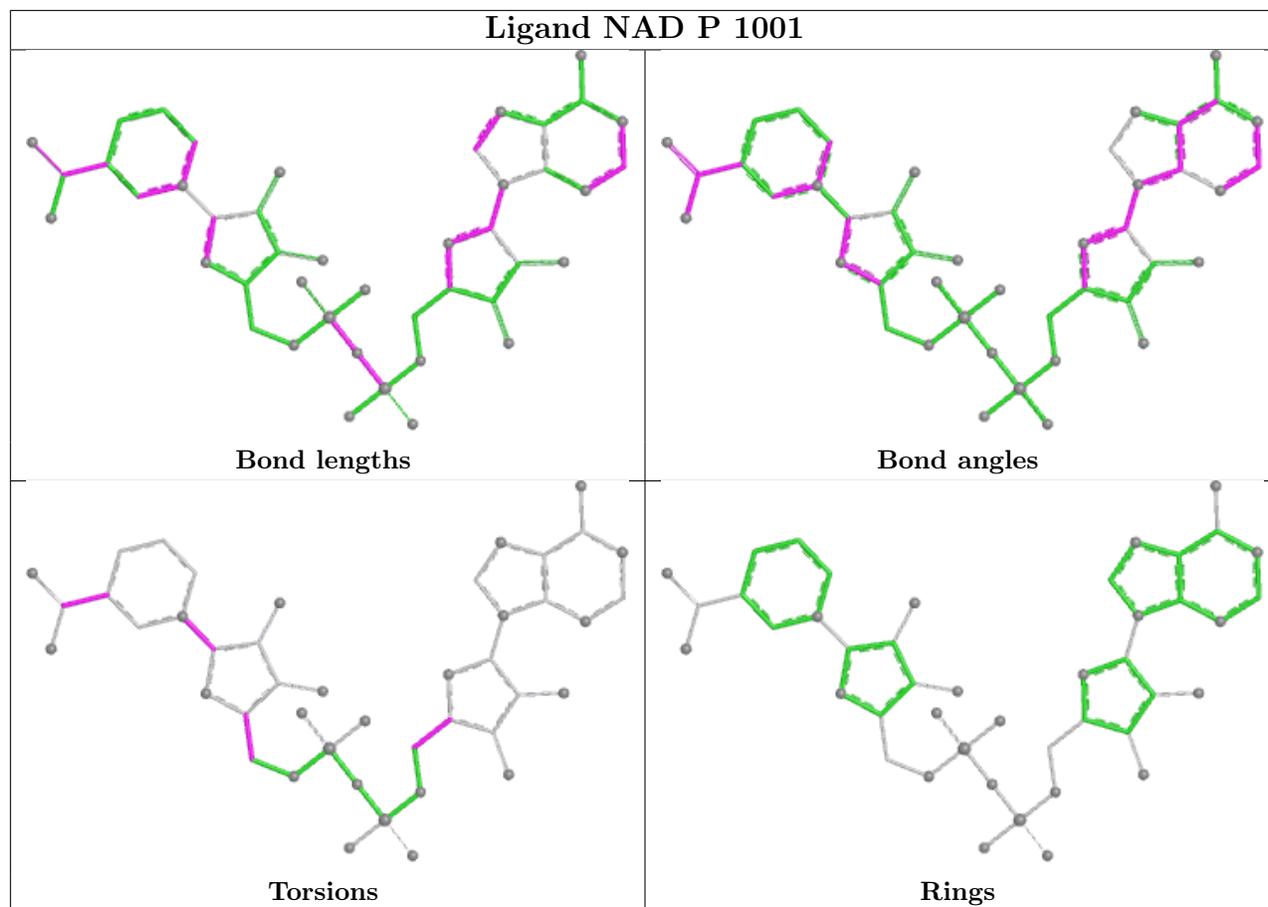


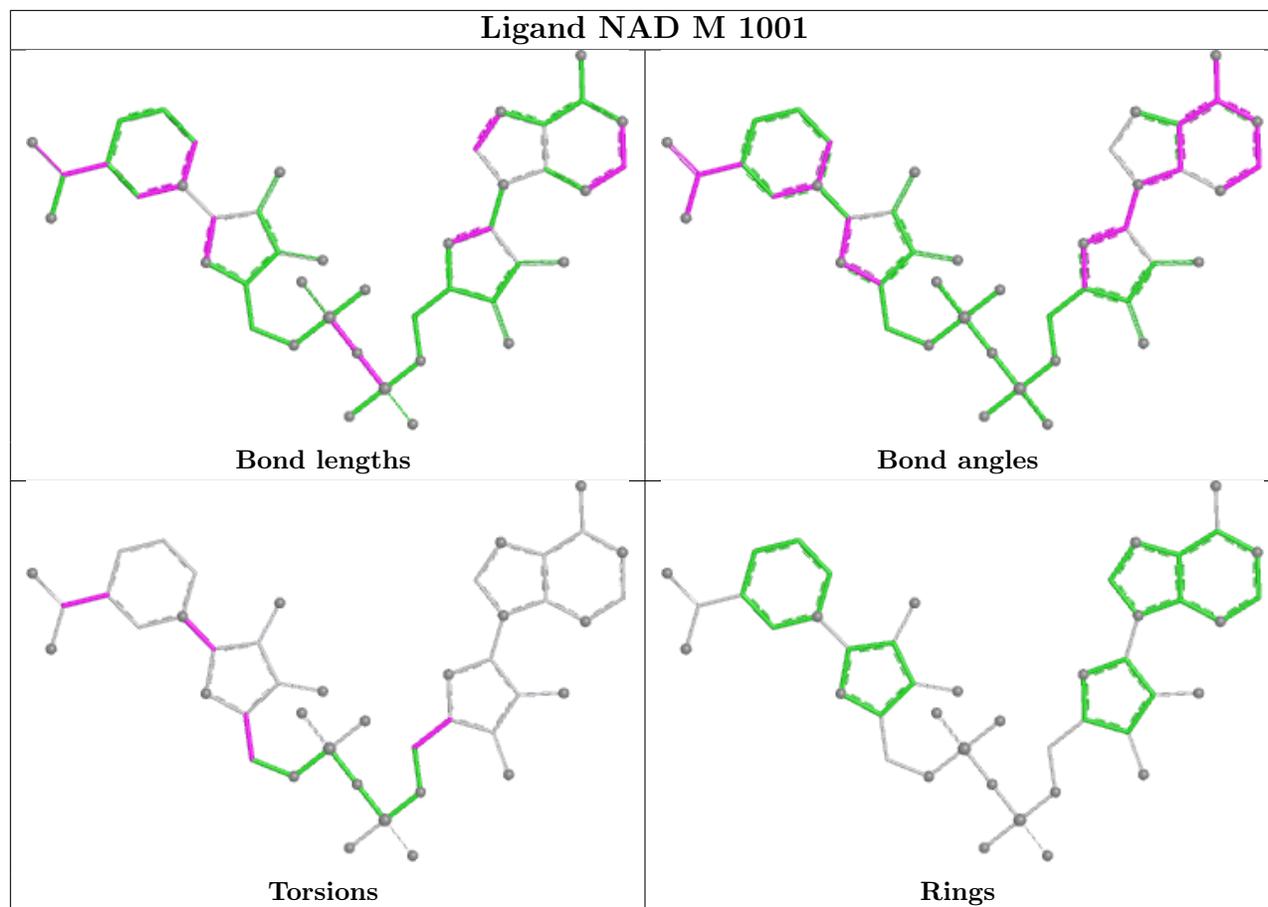


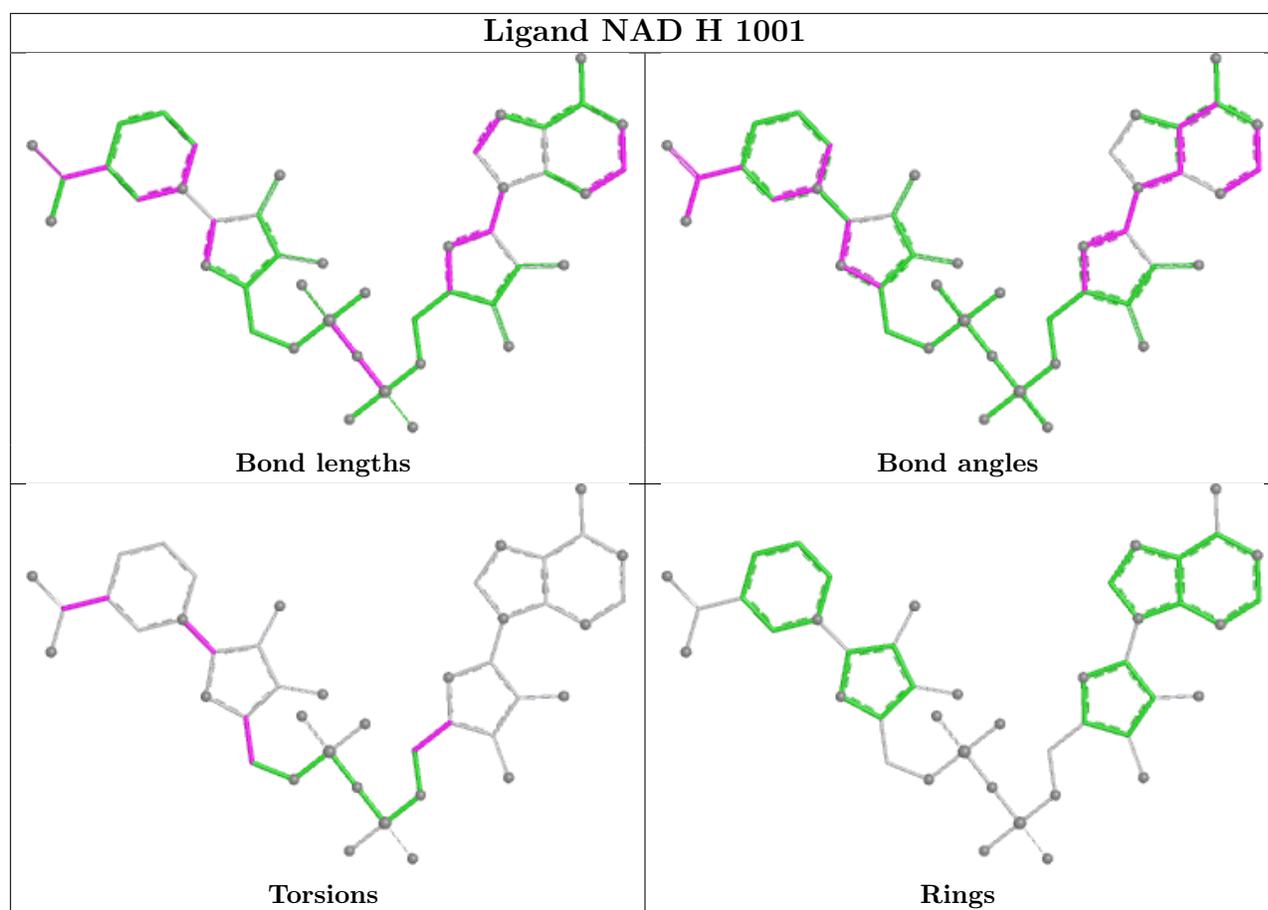












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	393/405 (97%)	-0.49	0 100 100	38, 62, 77, 109	0
1	B	391/405 (96%)	-0.49	1 (0%) 94 83	42, 61, 83, 97	0
1	C	393/405 (97%)	-0.46	0 100 100	41, 64, 86, 100	0
1	D	395/405 (97%)	-0.48	0 100 100	44, 64, 85, 109	0
1	E	391/405 (96%)	-0.45	0 100 100	41, 65, 85, 104	0
1	F	392/405 (96%)	-0.46	0 100 100	40, 68, 87, 103	0
1	G	392/405 (96%)	-0.49	0 100 100	46, 68, 89, 103	0
1	H	393/405 (97%)	-0.29	0 100 100	43, 76, 98, 116	0
1	I	393/405 (97%)	-0.37	1 (0%) 94 83	49, 75, 100, 138	0
1	J	391/405 (96%)	-0.45	0 100 100	38, 62, 93, 107	0
1	K	391/405 (96%)	-0.44	0 100 100	38, 61, 90, 111	0
1	L	395/405 (97%)	-0.45	0 100 100	45, 66, 89, 123	0
1	M	391/405 (96%)	-0.44	0 100 100	38, 63, 84, 98	0
1	N	392/405 (96%)	-0.38	1 (0%) 94 83	48, 72, 92, 115	0
1	O	391/405 (96%)	-0.42	0 100 100	43, 70, 100, 123	0
1	P	392/405 (96%)	-0.43	0 100 100	40, 65, 86, 112	0
All	All	6276/6480 (96%)	-0.44	3 (0%) 100 100	38, 66, 91, 138	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	354	GLU	2.5
1	I	2	ILE	2.2
1	B	330	GLU	2.2

## 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](#)

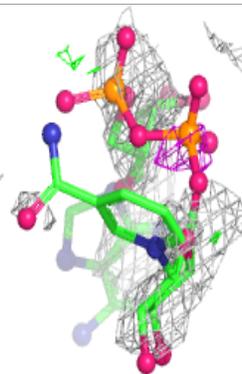
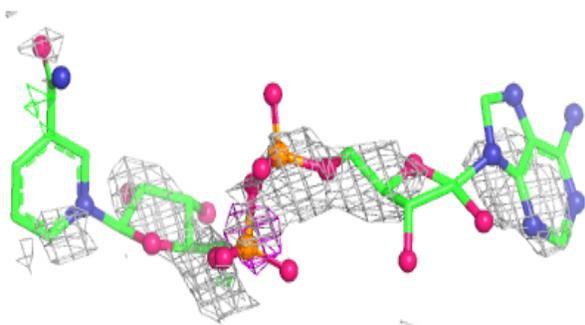
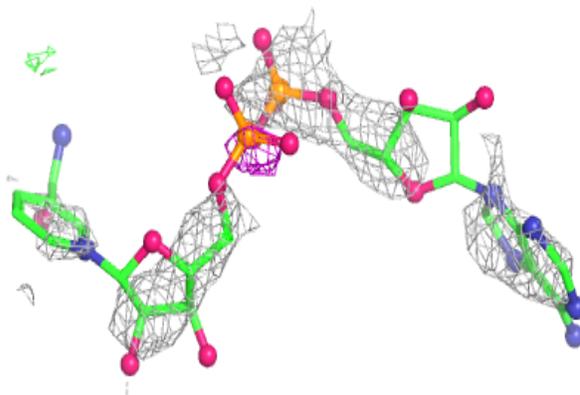
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	M	1001	44/44	0.69	0.43	113,116,133,136	44
2	NAD	K	1001	44/44	0.71	0.41	72,95,105,111	44
2	NAD	E	1001	44/44	0.73	0.40	83,97,115,117	44
2	NAD	I	1001	44/44	0.81	0.32	83,92,103,105	44
2	NAD	G	1001	44/44	0.84	0.29	80,89,100,101	44
2	NAD	A	1001	44/44	0.86	0.29	65,85,96,99	44
2	NAD	P	1001	44/44	0.86	0.26	77,83,93,96	44
2	NAD	H	1001	44/44	0.87	0.24	76,88,95,97	44

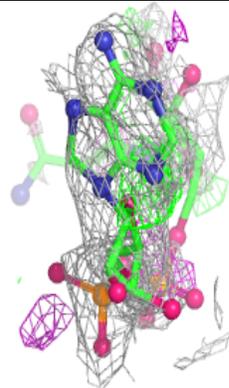
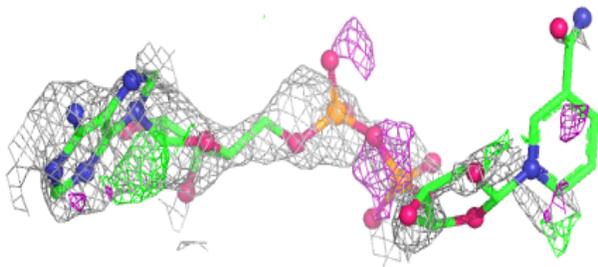
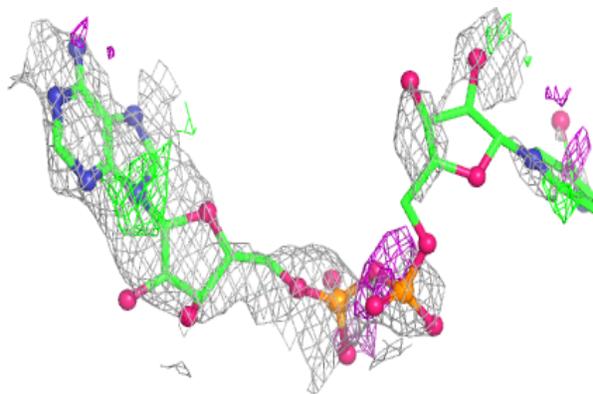
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD M 1001:**

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

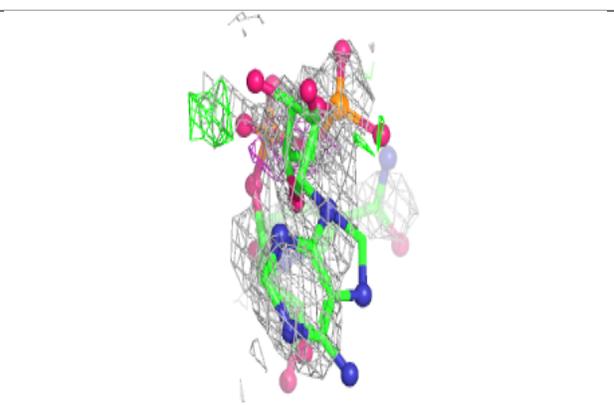
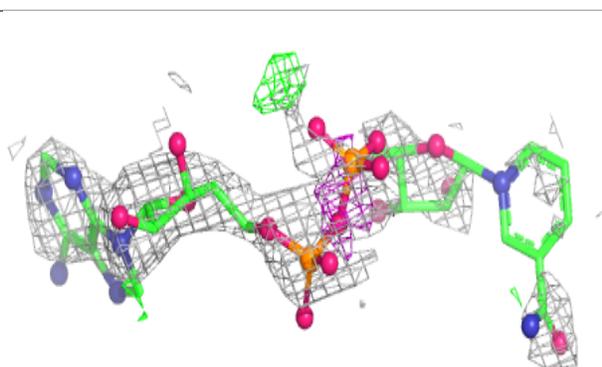
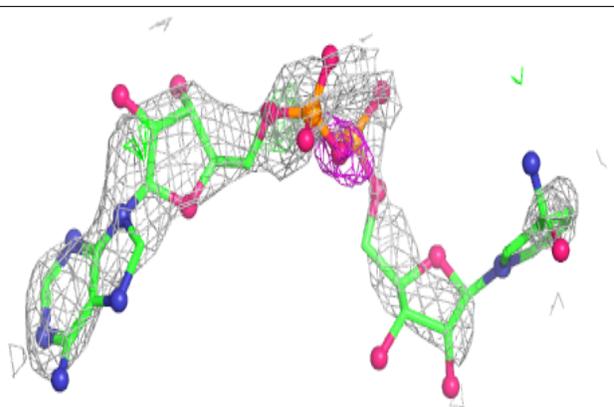
**Electron density around NAD K 1001:**

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

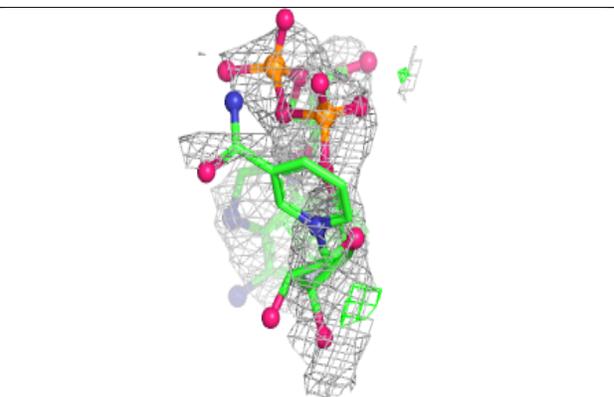
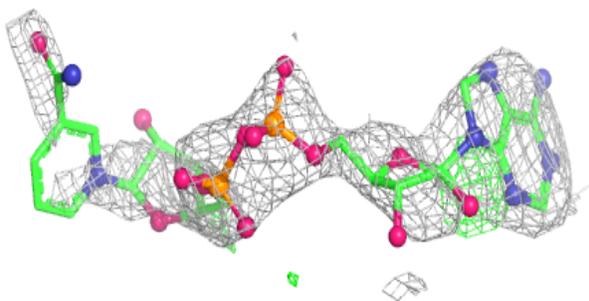
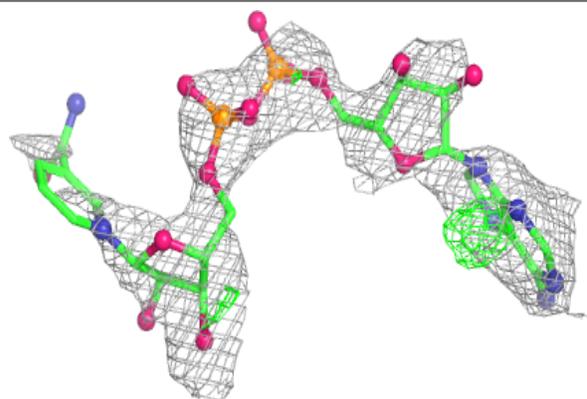


**Electron density around NAD E 1001:**

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

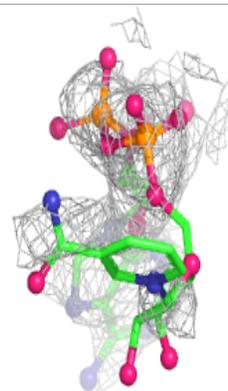
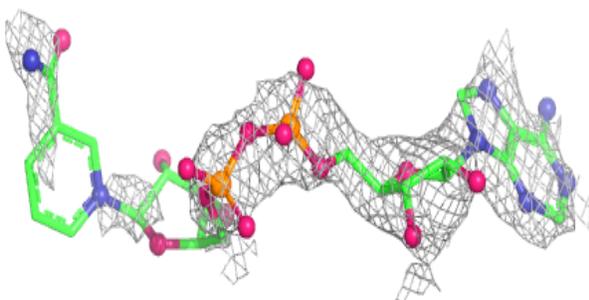
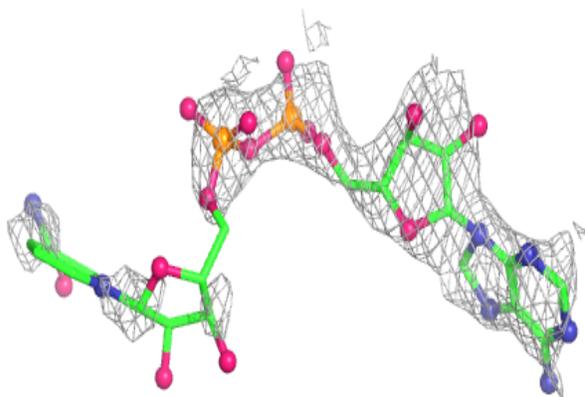
**Electron density around NAD I 1001:**

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

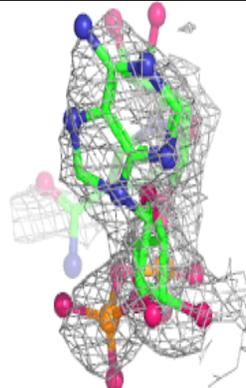
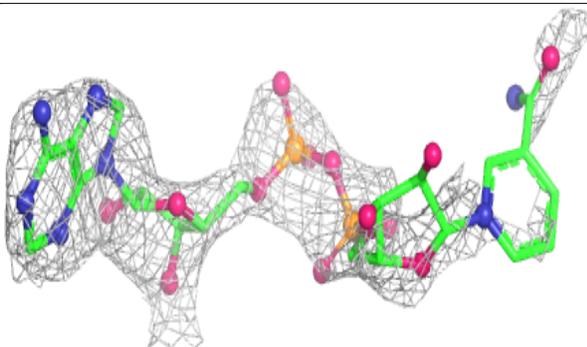
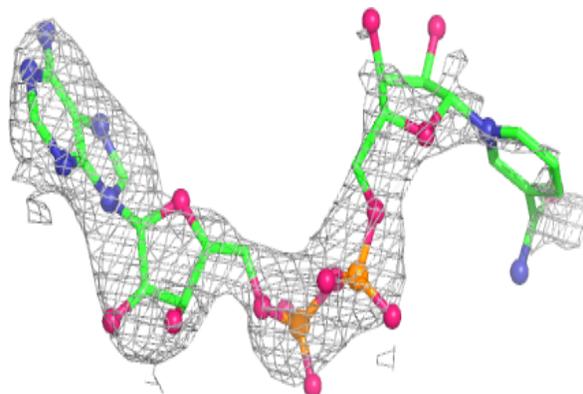


**Electron density around NAD G 1001:**

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

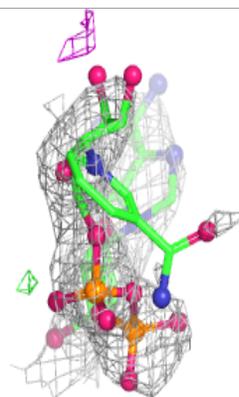
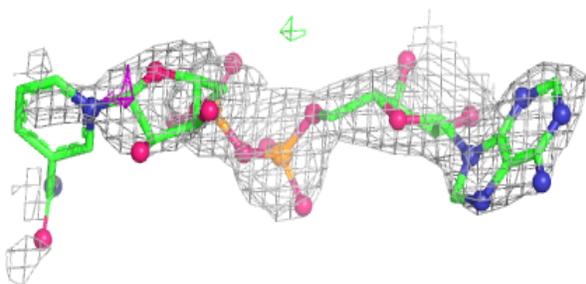
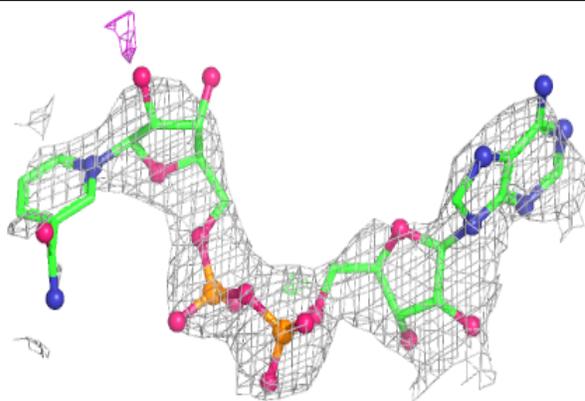
**Electron density around NAD A 1001:**

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

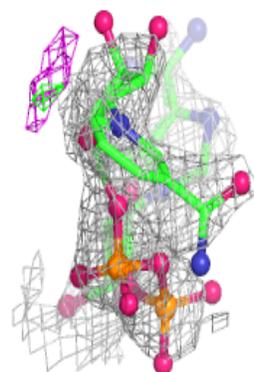
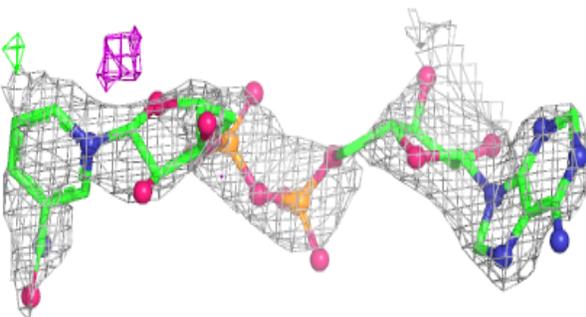
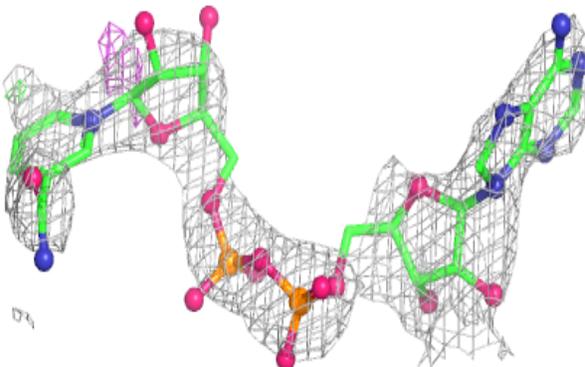


**Electron density around NAD P 1001:**

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

**Electron density around NAD H 1001:**

$2mF_o-DF_c$  (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.