

# Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 08:02 AM JST

PDB ID : 7FCM

Title : Crystal structure of Moraxella catarrhalis enoyl-ACP-reductase (FabI) in com-

plex with NAD and Triclosan

Authors: Katiki, M.; Neetu, N.; Pratap, S.; Kumar, P.

Deposited on : 2021-07-15

Resolution : 2.22 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 (i) symbol.

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

The following versions of software and data (see references (1)) 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 : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

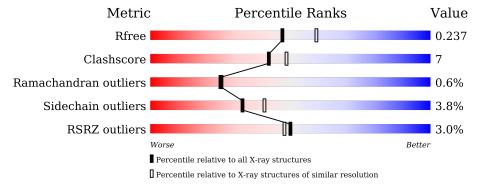
Validation Pipeline (wwPDB-VP) : 2.36

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.22 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	287	78%	15%	7%
1	В	287	79%	13%	• 6%



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4321 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	268	Total	C	N	0	S	0	0	0
			2004	1265	344	387	8			
1	R	269	Total	$\mathbf{C}$	N	Ο	S	0	0	0
1	Б	209	2009	1268	345	388	8	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP D5VCE0
A	-11	HIS	-	expression tag	UNP D5VCE0
A	-10	HIS	-	expression tag	UNP D5VCE0
A	-9	HIS	-	expression tag	UNP D5VCE0
A	-8	HIS	-	expression tag	UNP D5VCE0
A	-7	HIS	-	expression tag	UNP D5VCE0
A	-6	GLU	-	expression tag	UNP D5VCE0
A	-5	ASN	-	expression tag	UNP D5VCE0
A	-4	LEU	-	expression tag	UNP D5VCE0
A	-3	TYR	-	expression tag	UNP D5VCE0
A	-2	PHE	-	expression tag	UNP D5VCE0
A	-1	GLN	-	expression tag	UNP D5VCE0
A	0	SER	-	expression tag	UNP D5VCE0
A	222	GLN	GLY	variant	UNP D5VCE0
В	-12	HIS	-	expression tag	UNP D5VCE0
В	-11	HIS	-	expression tag	UNP D5VCE0
В	-10	HIS	-	expression tag	UNP D5VCE0
В	-9	HIS	-	expression tag	UNP D5VCE0
В	-8	HIS	-	expression tag	UNP D5VCE0
В	-7	HIS	-	expression tag	UNP D5VCE0
В	-6	GLU	-	expression tag	UNP D5VCE0
В	-5	ASN	-	expression tag	UNP D5VCE0
В	-4	LEU	-	expression tag	UNP D5VCE0
В	-3	TYR	-	expression tag	UNP D5VCE0
В	-2	PHE	-	expression tag	UNP D5VCE0

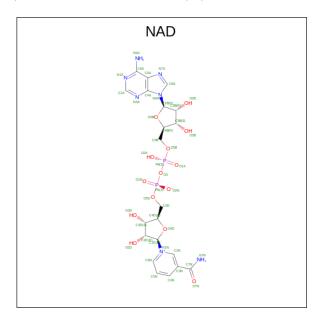
Continued on next page...



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
В	-1	GLN	-	expression tag	UNP D5VCE0
В	0	SER	-	expression tag	UNP D5VCE0
В	222	GLN	GLY	variant	UNP D5VCE0

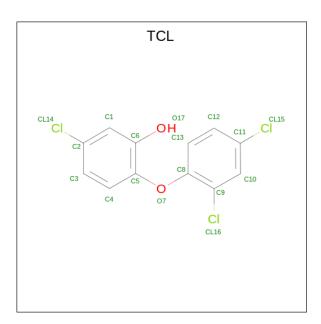
• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
9	Λ	1	Total	С	N	О	Р	0	0
	А	1	44	21	7	14	2	U	0
9	D	1	Total	С	N	О	Р	0	0
	Б	1	44	21	7	14	2	U	0

• Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula:  $C_{12}H_7Cl_3O_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	٨	1	Total	С	Cl	О	0	0
3	А	1	17	12	3	3 2	0	U
9	D	1	Total	С	Cl	О	0	0
3	Б	1	17	12	3	2		U

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

• Molecule 5 is water.

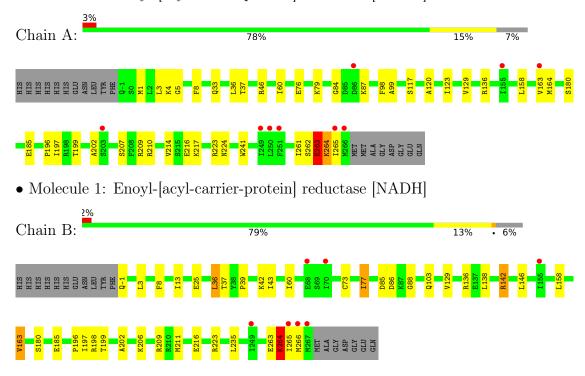
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	91	Total O 91 91	0	0
5	В	94	Total O 94 94	0	0



### 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: Enoyl-[acyl-carrier-protein] reductase [NADH]





### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	75.52Å 78.56Å 89.23Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	46.48 - 2.22	Depositor
Resolution (A)	46.48 - 2.22	EDS
% Data completeness	98.7 (46.48-2.22)	Depositor
(in resolution range)	98.7 (46.48-2.22)	EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.63 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D	0.174 , 0.237	Depositor
$R, R_{free}$	0.174 , $0.237$	DCC
$R_{free}$ test set	1334 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39, 54.8	EDS
L-test for twinning <sup>2</sup>	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.002 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4321	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 41.72 % 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 2.2645e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, TCL, CA

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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.42	0/2034	0.79	4/2750 (0.1%)
1	В	0.43	0/2039	0.79	3/2757 (0.1%)
All	All	0.43	0/4073	0.79	7/5507 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	В	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	A	129	VAL	CA-CB-CG2	5.75	119.52	110.90
1	A	264	LYS	CB-CA-C	-5.63	99.14	110.40
1	A	46	ARG	CB-CG-CD	5.34	125.49	111.60
1	В	129	VAL	CA-CB-CG2	5.34	118.92	110.90
1	В	142	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	В	129	VAL	CA-CB-CG1	5.12	118.58	110.90
1	A	129	VAL	CA-CB-CG1	5.05	118.47	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	263	GLU	Peptide
1	В	264	LYS	Peptide

#### 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	2004	0	2021	31	0
1	В	2009	0	2023	27	0
2	A	44	0	26	3	0
2	В	44	0	26	3	0
3	A	17	0	7	0	0
3	В	17	0	7	0	0
4	A	1	0	0	0	0
5	A	91	0	0	2	1
5	В	94	0	0	5	0
All	All	4321	0	4110	57	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (57) 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:A:197:ILE:H	2:A:301:NAD:H72N	1.21	0.88
1:A:76:GLU:OE1	1:A:79:LYS:NZ	2.09	0.85
1:A:207:SER:OG	1:A:210:ARG:NH1	2.09	0.84
1:B:-1:GLN:HG2	5:B:487:HOH:O	1.80	0.80
1:A:33:GLN:OE1	5:A:401:HOH:O	1.99	0.80
1:B:197:ILE:H	2:B:301:NAD:H72N	1.33	0.76
1:A:99:ALA:HB2	1:A:164:MET:CE	2.16	0.75
1:A:99:ALA:HB2	1:A:164:MET:HE3	1.71	0.72
1:A:214:VAL:HG13	1:A:264:LYS:HE2	1.71	0.72
1:B:103:GLN:HB3	1:B:163:VAL:HG21	1.78	0.66
1:A:214:VAL:HG13	1:A:264:LYS:CE	2.25	0.66
1:A:120:ALA:HB1	1:A:164:MET:CE	2.26	0.65
1:A:217:LYS:HB2	1:A:264:LYS:HZ2	1.62	0.64

Continued on next page...



Continued from previous page...

Continued from pred		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	overlap (Å)
1:B:211:MET:HG2	5:B:477:HOH:O	2.01	0.61
1:A:136:ARG:NH2	1:A:185:GLU:OE1	2.31	0.60
1:B:136:ARG:NH2	1:B:185:GLU:OE1	2.30	0.60
1:A:216:GLU:HG3	1:A:223:ARG:HA	1.85	0.58
1:B:86:ASP:O	1:B:142:ARG:NH1	2.37	0.57
1:B:103:GLN:HB3	1:B:163:VAL:CG2	2.36	0.56
1:A:84:GLY:O	1:A:87:LYS:HD3	2.06	0.55
1:A:196:PRO:HA	2:A:301:NAD:N7N	2.22	0.55
1:A:209:ARG:HG3	1:A:209:ARG:HH11	1.72	0.55
1:B:264:LYS:NZ	1:B:264:LYS:HB2	2.21	0.55
1:B:73:CYS:O	1:B:77:ILE:HG23	2.08	0.54
1:A:99:ALA:HB2	1:A:164:MET:HE2	1.90	0.53
1:A:1:MET:HB3	1:A:4:LYS:HD3	1.91	0.53
1:B:199:THR:H	1:B:202:ALA:HB3	1.74	0.53
1:A:263:GLU:N	1:A:263:GLU:OE1	2.43	0.52
1:B:60:ILE:HD12	1:B:77:ILE:HG22	1.91	0.52
1:B:263:GLU:N	1:B:263:GLU:OE1	2.39	0.52
1:A:199:THR:H	1:A:202:ALA:HB3	1.75	0.52
1:A:209:ARG:HG3	1:A:209:ARG:NH1	2.27	0.50
1:A:196:PRO:HA	2:A:301:NAD:H71N	1.77	0.49
1:B:77:ILE:HD11	1:B:138:LEU:HD13	1.94	0.48
1:B:39:PRO:HB3	2:B:301:NAD:C2A	2.43	0.47
1:A:98:PHE:HB3	1:A:123:ILE:HG21	1.95	0.47
1:A:5:GLY:HA2	1:A:33:GLN:HE22	1.81	0.46
1:B:264:LYS:O	1:B:264:LYS:HG3	2.13	0.45
1:B:196:PRO:HA	2:B:301:NAD:N7N	2.31	0.45
1:B:39:PRO:HG2	1:B:43:ILE:HD12	1.99	0.44
1:B:209:ARG:HG3	5:B:406:HOH:O	2.18	0.44
1:A:37:THR:HA	1:A:60:ILE:O	2.19	0.43
1:B:3:LEU:HD13	1:B:8:PHE:CE2	2.53	0.43
1:A:3:LEU:HD13	1:A:8:PHE:CE2	2.55	0.42
1:B:163:VAL:H	1:B:163:VAL:HG23	1.50	0.42
1:A:60:ILE:HD13	1:A:76:GLU:HB3	2.00	0.42
1:A:241:TRP:CH2	1:B:235:LEU:HD21	2.54	0.42
1:A:217:LYS:CB	1:A:264:LYS:HZ2	2.31	0.42
1:B:37:THR:HA	1:B:60:ILE:O	2.19	0.42
1:A:224:ASN:HB3	5:A:402:HOH:O	2.19	0.42
1:B:216:GLU:HG3	1:B:223:ARG:HA	2.01	0.41
1:B:25:GLU:HG2	5:B:474:HOH:O	2.20	0.41
1:B:198:ARG:NH2	5:B:406:HOH:O	2.53	0.41
1:A:117:SER:HA	1:A:163:VAL:HG21	2.02	0.41

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:B:88:GLY:C	1:B:142:ARG:HD3	2.40	0.41
1:B:13:ILE:HD12	1:B:36:LEU:HG	2.02	0.41
1:A:261:ILE:HG22	1:A:262:SER:O	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
5:A:446:HOH:O	5:A:473:HOH:O[3_545]	2.13	0.07

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	$266/287 \ (93\%)$	255 (96%)	10 (4%)	1 (0%)	34 37
1	В	$267/287 \ (93\%)$	256 (96%)	9 (3%)	2 (1%)	22 21
All	All	533/574 (93%)	511 (96%)	19 (4%)	3 (1%)	25 25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	264	LYS
1	В	265	ILE
1	A	263	GLU

#### 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	$209/225 \ (93\%)$	204 (98%)	5 (2%)	49 60
1	В	$209/225 \ (93\%)$	198 (95%)	11 (5%)	22 26
All	All	418/450 (93%)	402 (96%)	16 (4%)	33 41

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	158	LEU
1	A	180	SER
1	A	263	GLU
1	A	265	ILE
1	В	36	LEU
1	В	42	LYS
1	В	77	ILE
1	В	85	ASP
1	В	146	LEU
1	В	158	LEU
1	В	163	VAL
1	В	180	SER
1	В	206	LYS
1	В	264	LYS
1	В	266	MET

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

Mol	Chain	$\operatorname{Res}$	Type
1	A	6	GLN
1	A	33	GLN
1	A	224	ASN
1	В	6	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)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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		rpe Chain Res		Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	A	301	-	42,48,48	0.96	1 (2%)	50,73,73	1.06	4 (8%)
3	TCL	A	302	-	18,18,18	0.37	0	25,25,25	0.55	0
3	TCL	В	302	-	18,18,18	0.62	0	25,25,25	0.91	0
2	NAD	В	301	-	42,48,48	0.94	1 (2%)	50,73,73	1.07	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	301	-	-	4/26/62/62	0/5/5/5
3	TCL	A	302	-	-	0/4/4/4	0/2/2/2
3	TCL	В	302	-	-	0/4/4/4	0/2/2/2
2	NAD	В	301	-	-	6/26/62/62	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
2	В	301	NAD	C2N-N1N	4.59	1.40	1.35
2	A	301	NAD	C2N-N1N	4.30	1.40	1.35



All	(6)	) bond	angle	outliers	are	listed	below:
-----	-----	--------	-------	----------	-----	--------	--------

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	301	NAD	O4D-C1D-C2D	-3.95	101.16	106.93
2	В	301	NAD	C6N-N1N-C2N	-3.70	118.60	121.97
2	A	301	NAD	O4B-C1B-C2B	-2.72	102.94	106.93
2	A	301	NAD	C6N-N1N-C2N	-2.28	119.90	121.97
2	В	301	NAD	O4D-C1D-C2D	-2.16	103.77	106.93
2	A	301	NAD	C5A-C6A-N6A	2.15	123.62	120.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O2N
2	В	301	NAD	C5D-O5D-PN-O1N
2	В	301	NAD	C5D-O5D-PN-O2N
2	В	301	NAD	O4D-C1D-N1N-C2N
2	В	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C5D-O5D-PN-O3
2	В	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	O4B-C4B-C5B-O5B
2	В	301	NAD	O4B-C4B-C5B-O5B

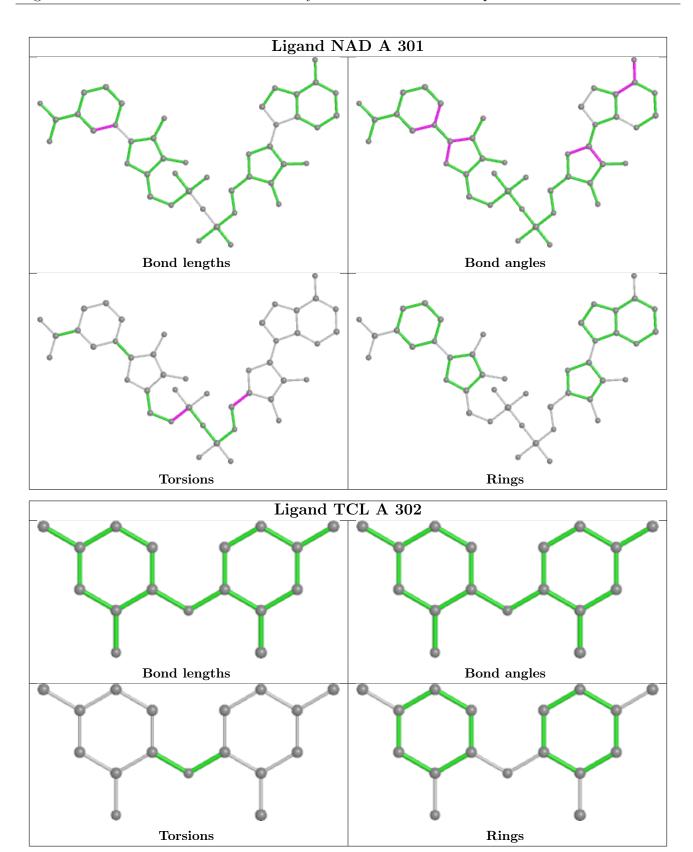
There are no ring outliers.

2 monomers are involved in 6 short contacts:

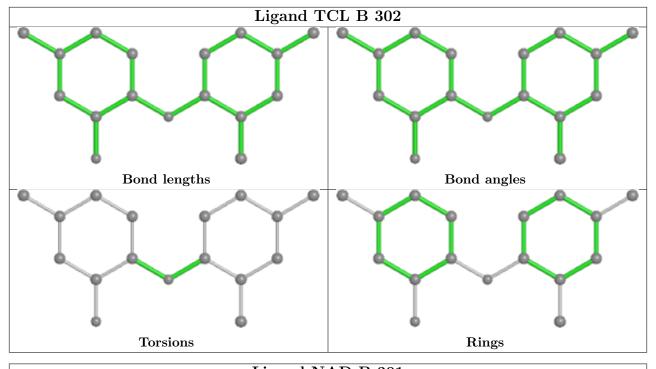
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	3	0
2	В	301	NAD	3	0

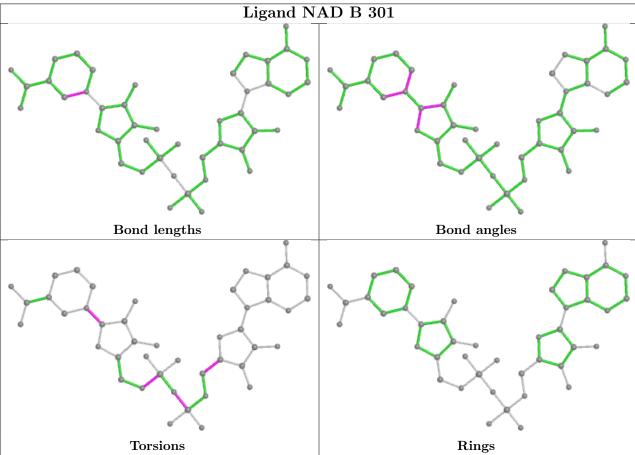
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	268/287 (93%)	-0.12	9 (3%) 45 43	23, 37, 63, 83	0
1	В	$269/287 \ (93\%)$	-0.03	7 (2%) 56 54	23, 36, 63, 91	0
All	All	537/574 (93%)	-0.08	16 (2%) 50 48	23, 36, 63, 91	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	267	MET	3.9
1	В	266	MET	3.7
1	A	249	ILE	3.7
1	A	203	SER	3.7
1	В	155	ILE	3.1
1	В	265	ILE	3.0
1	A	266	MET	2.9
1	A	155	ILE	2.7
1	A	251	PHE	2.6
1	A	250	LEU	2.4
1	В	70	ILE	2.3
1	A	163	VAL	2.3
1	A	86	ASP	2.2
1	В	68	GLU	2.1
1	A	265	ILE	2.0
1	В	249	ILE	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)

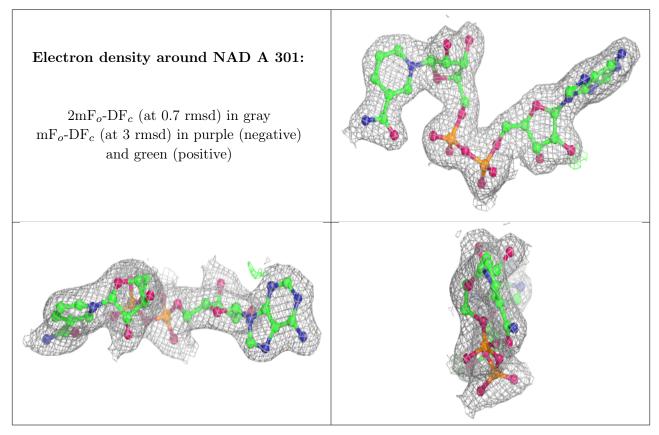
There are no monosaccharides in this entry.

### 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	NAD	A	301	44/44	0.96	0.10	26,32,36,37	0
2	NAD	В	301	44/44	0.96	0.09	26,31,38,40	0
3	TCL	A	302	17/17	0.98	0.07	31,36,44,46	0
3	TCL	В	302	17/17	0.98	0.08	30,34,41,42	0
4	CA	A	303	1/1	0.99	0.16	40,40,40,40	0

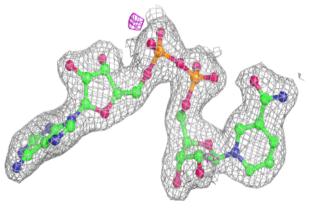
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

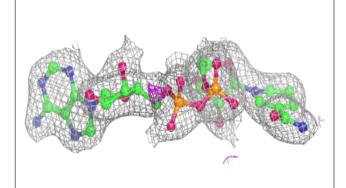


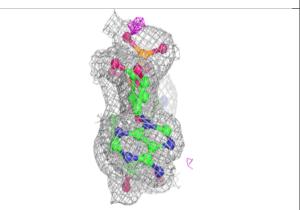


#### Electron density around NAD B 301:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 0.7 rmsd) in gray  $\mathrm{mF}_o\text{-}\mathrm{DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)

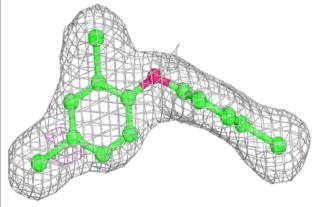


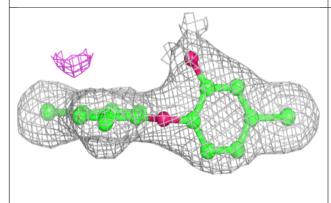


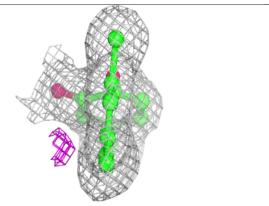


#### Electron density around TCL A 302:

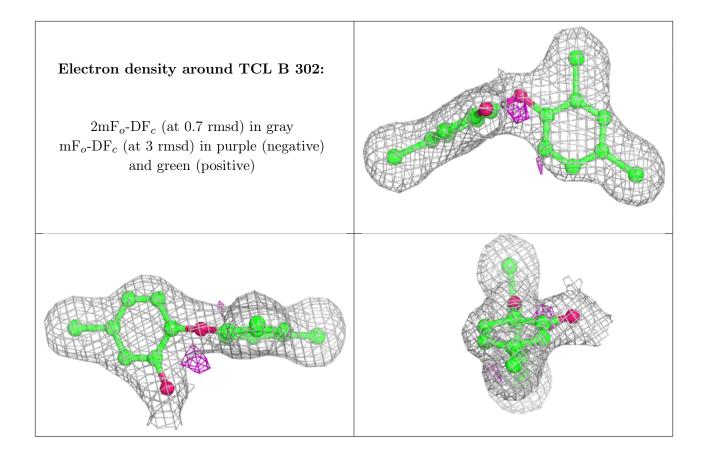
 $2 \text{mF}_o\text{-DF}_c$  (at 0.7 rmsd) in gray  $\text{mF}_o\text{-DF}_c$  (at 3 rmsd) in purple (negative) and green (positive)











## 6.5 Other polymers (i)

There are no such residues in this entry.

