

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

#### Aug 29, 2020 – 10:05 PM BST

PDB ID	:	6NOR
$\operatorname{Title}$	:	Crystal structure of GenD2 from gentamicin A biosynthesis in complex with
		NAD
Authors	:	Araujo, N.C.; Bury, P.S.; Huang, F.; Leadlay, P.F.; Dias, M.V.B.
Deposited on	:	2019-01-16
$\operatorname{Resolution}$	:	2.40  Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

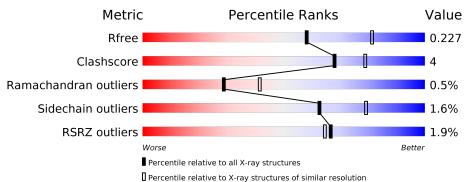
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\operatorname{EDS}$	:	2.13
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 >=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	361	% • 88%	8% •••
1	В	361	% <b>8</b> 5%	8% • 6%
1	С	361	% <b>8</b> 6%	8% • 6%
1	D	361	83%	11% • 6%
1	Е	361	86%	7% • 6%
1	F	361	88%	5% • 6%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16105 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1 A	349	Total	С	Ν	Ο	S	0	0	0
		549	2618	1639	480	490	9	0	0	0
1	В	341	Total	С	Ν	Ο	S	0	1	0
	D	041	2572	1610	471	482	9	0		0
1	С	340	Total	С	Ν	Ο	S	0	0	0
	U	540	2553	1599	464	481	9	0	0	U
1	D	341	Total	С	Ν	Ο	S	0	0	0
	D	041	2560	1603	468	480	9	0		
1	Е	338	Total	С	Ν	Ο	S	0	0	0
	000	2547	1594	465	479	9	0	0	0	
1	1 F	F 340	Total	С	Ν	Ο	S	0	0	0
		040	2555	1600	467	479	9		0	U

• Molecule 1 is a protein called Putative NAD dependent dehydrogenase.

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q70KD1
А	-18	GLY	-	expression tag	UNP Q70KD1
A	-17	SER	-	expression tag	UNP Q70KD1
А	-16	SER	-	expression tag	UNP Q70KD1
А	-15	HIS	-	expression tag	UNP Q70KD1
А	-14	HIS	-	expression tag	UNP Q70KD1
А	-13	HIS	-	expression tag	UNP Q70KD1
A	-12	HIS	-	expression tag	UNP Q70KD1
A	-11	HIS	-	expression tag	UNP Q70KD1
A	-10	HIS	-	expression tag	UNP Q70KD1
А	-9	SER	-	expression tag	UNP Q70KD1
А	-8	SER	-	expression tag	UNP Q70KD1
A	-7	GLY	-	expression tag	UNP Q70KD1
А	-6	LEU	-	expression tag	UNP Q70KD1
А	-5	VAL	-	expression tag	UNP Q70KD1
А	-4	PRO	-	expression tag	UNP Q70KD1
А	-3	ARG	-	expression tag	UNP Q70KD1



6N	OR

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	GLY	-	expression tag	UNP Q70KD1
А	-1	SER	-	expression tag	UNP Q70KD1
А	0	HIS	_	expression tag	UNP Q70KD1
В	-19	MET	-	initiating methionine	UNP Q70KD1
В	-18	GLY	-	expression tag	UNP Q70KD1
В	-17	SER	_	expression tag	UNP Q70KD1
В	-16	SER	_	expression tag	UNP Q70KD1
В	-15	HIS	-	expression tag	UNP Q70KD1
В	-14	HIS	-	expression tag	UNP Q70KD1
В	-13	HIS	-	expression tag	UNP Q70KD1
В	-12	HIS	-	expression tag	UNP Q70KD1
В	-11	HIS	-	expression tag	UNP Q70KD1
В	-10	HIS	-	expression tag	UNP Q70KD1
В	-9	SER	-	expression tag	UNP Q70KD1
В	-8	SER	-	expression tag	UNP Q70KD1
В	-7	GLY	-	expression tag	UNP Q70KD1
В	-6	LEU	_	expression tag	UNP Q70KD1
В	-5	VAL	_	expression tag	UNP Q70KD1
В	-4	PRO	_	expression tag	UNP Q70KD1
В	-3	ARG	-	expression tag	UNP Q70KD1
В	-2	GLY	-	expression tag	UNP Q70KD1
В	-1	SER	-	expression tag	UNP Q70KD1
В	0	HIS	-	expression tag	UNP Q70KD1
С	-19	MET	-	initiating methionine	UNP Q70KD1
С	-18	GLY	-	expression tag	UNP Q70KD1
С	-17	SER	-	expression tag	UNP Q70KD1
С	-16	SER	-	expression tag	UNP Q70KD1
С	-15	HIS	-	expression tag	UNP Q70KD1
С	-14	HIS	-	expression tag	UNP Q70KD1
С	-13	HIS	-	expression tag	UNP Q70KD1
С	-12	HIS	-	expression tag	UNP Q70KD1
С	-11	HIS	-	expression tag	UNP Q70KD1
С	-10	HIS	-	expression tag	UNP Q70KD1
С	-9	SER	-	expression tag	UNP Q70KD1
С	-8	SER	-	expression tag	UNP Q70KD1
С	-7	GLY	_	expression tag	UNP Q70KD1
С	-6	LEU	-	expression tag	UNP Q70KD1
С	-5	VAL	-	expression tag	UNP Q70KD1
С	-4	PRO	-	expression tag	UNP Q70KD1
С	-3	ARG	-	expression tag	UNP Q70KD1
С	-2	GLY	-	expression tag	UNP Q70KD1
С	-1	SER	-	expression tag	UNP Q70KD1



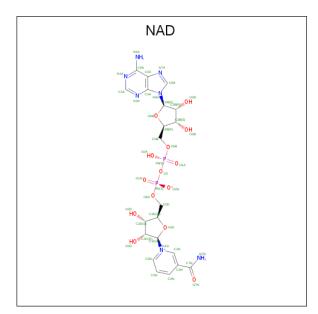
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Chain	Residue	Modelled	Actual	Comment	Reference					
С	0	HIS	-	expression tag	UNP Q70KD1					
D	-19	MET	-	initiating methionine	UNP Q70KD1					
D	-18	GLY	-	expression tag	UNP Q70KD1					
D	-17	SER	-	expression tag	UNP Q70KD1					
D	-16	SER	-	expression tag	UNP Q70KD1					
D	-15	HIS	-	expression tag	UNP Q70KD1					
D	-14	HIS	-	expression tag	UNP Q70KD1					
D	-13	HIS	-	expression tag	UNP Q70KD1					
D	-12	HIS	-	expression tag	UNP Q70KD1					
D	-11	HIS	-	expression tag	UNP Q70KD1					
D	-10	HIS	-	expression tag	UNP Q70KD1					
D	-9	SER	-	expression tag	UNP Q70KD1					
D	-8	SER	-	expression tag	UNP Q70KD1					
D	-7	GLY	-	expression tag	UNP Q70KD1					
D	-6	LEU	-	expression tag	UNP Q70KD1					
D	-5	VAL	-	expression tag	UNP Q70KD1					
D	-4	PRO	-	expression tag	UNP Q70KD1					
D	-3	ARG	-	expression tag	UNP Q70KD1					
D	-2	GLY	-	expression tag	UNP Q70KD1					
D	-1	SER	-	expression tag	UNP Q70KD1					
D	0	HIS	-	expression tag	UNP Q70KD1					
Ε	-19	MET	-	initiating methionine	UNP Q70KD1					
Е	-18	GLY	-	expression tag	UNP Q70KD1					
Е	-17	SER	-	expression tag	UNP Q70KD1					
Ε	-16	SER	-	expression tag	UNP Q70KD1					
Ε	-15	HIS	-	expression tag	UNP Q70KD1					
Ε	-14	HIS	-	expression tag	UNP Q70KD1					
Ε	-13	HIS	-	expression tag	UNP Q70KD1					
Ε	-12	HIS	-	expression tag	UNP Q70KD1					
Ε	-11	HIS	-	expression tag	UNP Q70KD1					
Ε	-10	HIS	-	expression tag	UNP Q70KD1					
Е	-9	SER	-	expression tag	UNP Q70KD1					
Е	-8	SER	-	expression tag	UNP Q70KD1					
Е	-7	GLY	-	expression tag	UNP Q70KD1					
Ε	-6	LEU	-	expression tag	UNP Q70KD1					
Е	-5	VAL	-	expression tag	UNP Q70KD1					
Ε	-4	PRO	-	expression tag	UNP Q70KD1					
Ε	-3	ARG	-	expression tag	UNP Q70KD1					
Е	-2	GLY	-	expression tag	UNP Q70KD1					
Ε	-1	SER	-	expression tag	UNP Q70KD1					
Е	0	HIS	-	expression tag	UNP Q70KD1					
F	-19	MET	-	initiating methionine	UNP Q70KD1					



Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
F	-18	GLY	-	expression tag	UNP Q70KD1
F	-17	SER	-	expression tag	UNP Q70KD1
F	-16	SER	-	expression tag	UNP Q70KD1
F	-15	HIS	-	expression tag	UNP Q70KD1
F	-14	HIS	-	expression tag	UNP Q70KD1
F	-13	HIS	-	expression tag	UNP Q70KD1
F	-12	HIS	-	expression tag	UNP Q70KD1
F	-11	HIS	_	expression tag	UNP Q70KD1
F	-10	HIS	-	expression tag	UNP Q70KD1
F	-9	SER	-	expression tag	UNP Q70KD1
F	-8	$\operatorname{SER}$	-	expression tag	UNP Q70KD1
F	-7	GLY	_	expression tag	UNP Q70KD1
F	-6	LEU	_	expression tag	UNP Q70KD1
F	-5	VAL	-	expression tag	UNP Q70KD1
F	-4	PRO	_	expression tag	UNP Q70KD1
F	-3	ARG	-	expression tag	UNP Q70KD1
F	-2	GLY	-	expression tag	UNP Q70KD1
F	-1	SER	_	expression tag	UNP Q70KD1
F	0	HIS	-	expression tag	UNP Q70KD1

• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Δ	1	Total	С	Ν	Ο	Р	0	0
		1	44	21	7	14	2	0	0



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	В	1	Total	С	Ν	Ο	Р	0	0	
	D	T	44	21	7	14	2	0	0	
2	С	1	Total	С	Ν	Ο	Р	0	0	
	U	T	44	21	7	14	2	0	U	
2	Л	1	Total	С	Ν	Ο	Р	0	0	
	D	T	44	21	7	14	2	0	0	
2	Е	1	Total	С	Ν	Ο	Р	0	0	
	Ľ	T	44	21	7	14	2	0	0	
2	F	1	Total	С	Ν	Ο	Р	0	0	
	Ľ		44	21	7	14	2	U	0	

• Molecule 3 is water.

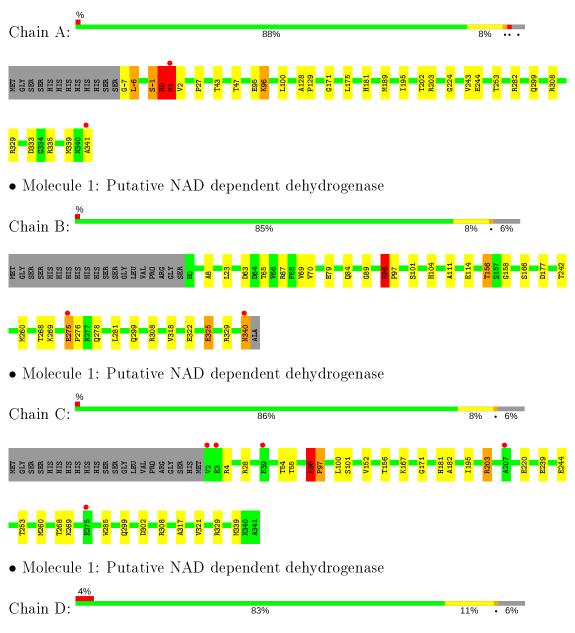
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	91	Total O 91 91	0	0
3	В	66	Total O 66 66	0	0
3	С	67	Total O 67 67	0	0
3	D	50	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 50 & 50 \end{array}$	0	0
3	Е	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	0	0
3	F	100	Total O 100 100	0	0



## 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: Putative NAD dependent dehydrogenase







# 198 198 190 190 190 190 190 190 114 114 114 114 114 114 114 115 1160 1161 1161 1161 1161 1161 1161 1161 1161 1161 1161 1161 1161 1161 1161 1161 1162 1163 1163 1163 1163 1163 1163 1163 1163 1163 1163 1163 1163 1163 1163 1164 1163 1164

• Molecule 1: Putative NAD dependent dehydrogenase

Chain E:	3%		8	6%						7%	• 6%			
MET GLY SER HIS HIS HIS	HIS HIS SER SER SER GLY VAL	PRU GLY SER HIS MET VAL	2    3    3    3	D36 R37	E39 R40 V41	T43 V53	D58	A62 F68	K96	156	6158	A168	D177	H181

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• Molecule 1: Putative NAD dependent dehydrogenase

Chain F:	88%	5% • 6%	
MET SER SER SER HIS HIS HIS HIS SER PIC CLY VAL VAL VAL VAL VAL SER SER SER SER SER RET	156 157 157 158 158 158 158 159 159 159 159 159 159 159 159 159 159	F154 S166 L175 L175 A197 A197 T202 R203 R203 R203 R203 R275 B275	Y293





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	124.00Å $124.00$ Å $272.57$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	49.95 - 2.40	Depositor
Resolution (A)	49.96 - 2.40	EDS
% Data completeness	99.9(49.95-2.40)	Depositor
(in resolution range)	$99.9 \ (49.96 - 2.40)$	EDS
R <sub>merge</sub>	0.18	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.31 (at 2.39 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
D D .	0.175 , $0.223$	Depositor
$R, R_{free}$	0.184 , $0.227$	DCC
$R_{free}$ test set	2007 reflections $(2.10%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36 , $34.2$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16105	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



 $<sup>^1 {\</sup>rm Intensities}$  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

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		
	Cham	RMSZ   #  Z  > 5		RMSZ	# Z  > 5	
1	А	0.48	0/2674	0.61	2/3650~(0.1%)	
1	В	0.44	0/2629	0.59	2/3588~(0.1%)	
1	С	0.45	0/2607	0.57	1/3560~(0.0%)	
1	D	0.42	0/2614	0.58	1/3569~(0.0%)	
1	Е	0.42	0/2601	0.53	0/3550	
1	F	0.47	0/2609	0.59	1/3562~(0.0%)	
All	All	0.44	0/15734	0.58	7/21479~(0.0%)	

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

Mol	Chain	#Chirality outliers	<b>#Planarity outliers</b>
1	А	0	1
1	В	0	2
1	С	0	1
1	D	0	1
1	Е	0	1
1	F	0	3
All	All	0	9

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	F	96	LYS	C-N-CD	-10.37	97.80	120.60
1	С	96	LYS	C-N-CD	-8.16	102.64	120.60
1	В	96	LYS	C-N-CD	-7.52	104.05	120.60
1	В	96	LYS	CD-CE-NZ	-7.50	94.44	111.70



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	0	HIS	N-CA-CB	6.67	122.60	110.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1	MET	Peptide
1	В	275	GLU	Peptide
1	В	96	LYS	Peptide
1	С	96	LYS	Peptide
1	D	96	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	А	2618	0	2555	24	0
1	В	2572	0	2511	22	0
1	С	2553	0	2485	18	0
1	D	2560	0	2494	29	0
1	Е	2547	0	2482	19	0
1	F	2555	0	2492	10	0
2	А	44	0	25	1	0
2	В	44	0	25	0	0
2	С	44	0	25	1	0
2	D	44	0	25	1	0
2	Е	44	0	25	1	0
2	F	44	0	25	2	0
3	А	91	0	0	1	1
3	В	66	0	0	3	0
3	С	67	0	0	2	1
3	D	50	0	0	5	0
3	Е	62	0	0	0	1
3	F	100	0	0	1	1
All	All	16105	0	15169	118	2

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 4.

The worst 5 of 118 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:B:96:LYS:NZ	1:B:177:ASP:O	1.96	0.97
1:E:156:THR:HG23	1:E:158:GLY:H	1.30	0.96
1:B:340:ASN:ND2	1:D:56:THR:HG21	1.91	0.85
1:A:203:ARG:HH21	1:C:220:GLU:HG3	1.41	0.82
1:E:340:ASN:HD22	1:E:340:ASN:H	1.25	0.81

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
3:E:545:HOH:O	3:F:545:HOH:O[4_655]	1.92	0.28
3:A:552:HOH:O	3:C:561:HOH:O[5_554]	2.09	0.11

#### 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	Perce	ntiles
1	А	347/361~(96%)	336~(97%)	9(3%)	2(1%)	25	36
1	В	340/361~(94%)	328~(96%)	10 (3%)	2(1%)	25	36
1	С	338/361~(94%)	330~(98%)	7 (2%)	1 (0%)	41	55
1	D	339/361~(94%)	322~(95%)	14 (4%)	3 (1%)	17	25
1	Ε	336/361~(93%)	329~(98%)	6 (2%)	1 (0%)	41	55
1	F	338/361~(94%)	326~(96%)	10 (3%)	2 (1%)	25	36
All	All	2038/2166~(94%)	$1971 \ (97\%)$	56 (3%)	11 (0%)	29	41

5 of 11 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	А	0	HIS
1	А	1	MET
1	В	97	PRO
1	С	97	PRO
1	D	97	PRO

#### 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	А	260/274~(95%)	257~(99%)	3(1%)	71 85
1	В	256/274~(93%)	250 (98%)	6 (2%)	50 70
1	С	254/274~(93%)	249 (98%)	5 (2%)	55 74
1	D	254/274~(93%)	251 (99%)	3 (1%)	71 85
1	Е	254/274~(93%)	251 (99%)	3 (1%)	71 85
1	F	254/274~(93%)	250 (98%)	4 (2%)	62 79
All	All	1532/1644~(93%)	1508~(98%)	24 (2%)	62 79

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	96	LYS
1	С	203	ARG
1	F	154	PHE
1	С	101	SER
1	С	167	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ε	340	ASN



#### 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)

6 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	Tuno	Chain	Res	Link	B	ond leng	gths	B	ond ang	les
	Type	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	F	401	-	42,48,48	4.99	16 (38%)	50,73,73	1.60	<mark>8 (16%)</mark>
2	NAD	D	401	-	42,48,48	<mark>5.26</mark>	15 (35%)	50,73,73	1.55	8 (16%)
2	NAD	В	401	-	42,48,48	5.21	15 (35%)	50,73,73	1.57	7 (14%)
2	NAD	С	401	-	42,48,48	<b>5.15</b>	16 (38%)	50,73,73	1.48	<mark>6 (12%)</mark>
2	NAD	А	401	-	42,48,48	5.20	16 (38%)	50,73,73	1.57	<u>6 (12%)</u>
2	NAD	Е	401	-	42,48,48	<mark>5.28</mark>	15 (35%)	50,73,73	1.46	<mark>6 (12%)</mark>

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	F	401	-	-	5/26/62/62	0/5/5/5
2	NAD	D	401	-	-	4/26/62/62	0/5/5/5



Mol	Type	Chain	Res	$\mathbf{Link}$	Chirals	Torsions	Rings
2	NAD	В	401	-	-	5/26/62/62	0/5/5/5
2	NAD	С	401	-	-	5/26/62/62	0/5/5/5
2	NAD	А	401	-	-	5/26/62/62	0/5/5/5
2	NAD	Е	401	-	-	5/26/62/62	0/5/5/5

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	401	NAD	C2B-C1B	-17.25	1.27	1.53
2	Е	401	NAD	C2B-C1B	-17.23	1.27	1.53
2	В	401	NAD	C2B-C1B	-16.99	1.28	1.53
2	С	401	NAD	C2B-C1B	-16.84	1.28	1.53
2	D	401	NAD	C2B-C1B	-16.79	1.28	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	401	NAD	N3A-C2A-N1A	-5.88	119.48	128.68
2	F	401	NAD	N3A-C2A-N1A	-5.82	119.59	128.68
2	Е	401	NAD	N3A-C2A-N1A	-5.61	119.91	128.68
2	В	401	NAD	C5A-C6A-N6A	5.61	128.87	120.35
2	D	401	NAD	N3A-C2A-N1A	-5.46	120.15	128.68

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

5 monomers are involved in 6 short contacts:

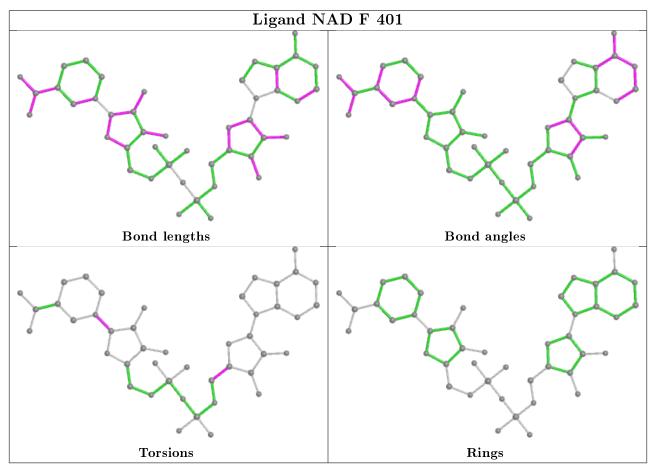
Mol	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
2	F	401	NAD	2	0
2	D	401	NAD	1	0
2	С	401	NAD	1	0



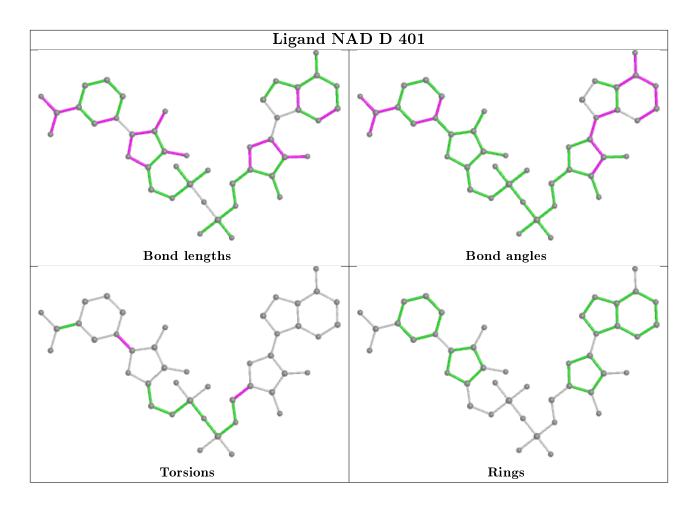
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	401	NAD	1	0
2	Е	401	NAD	1	0

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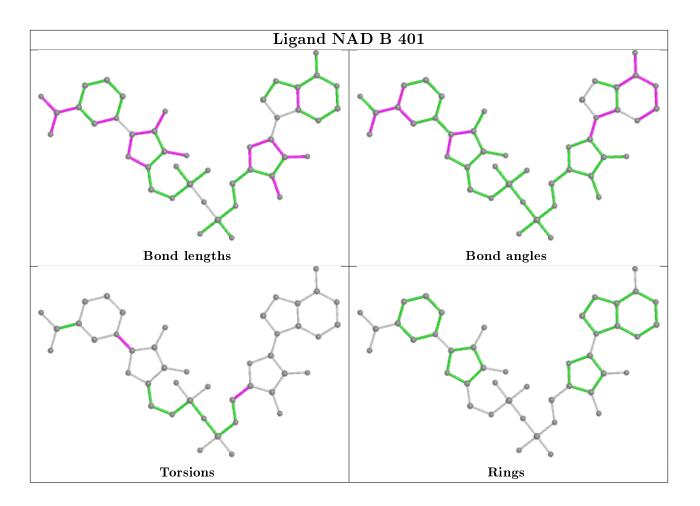
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



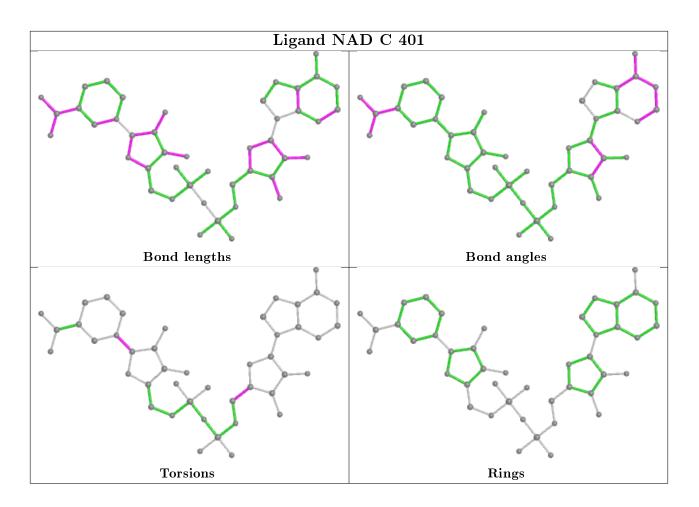




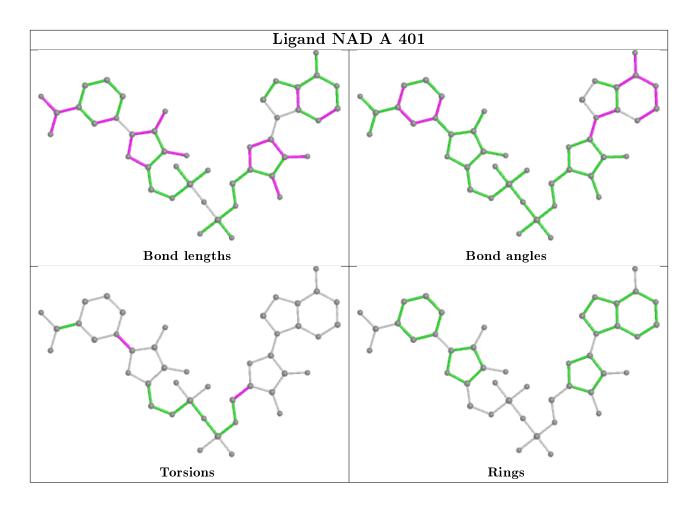




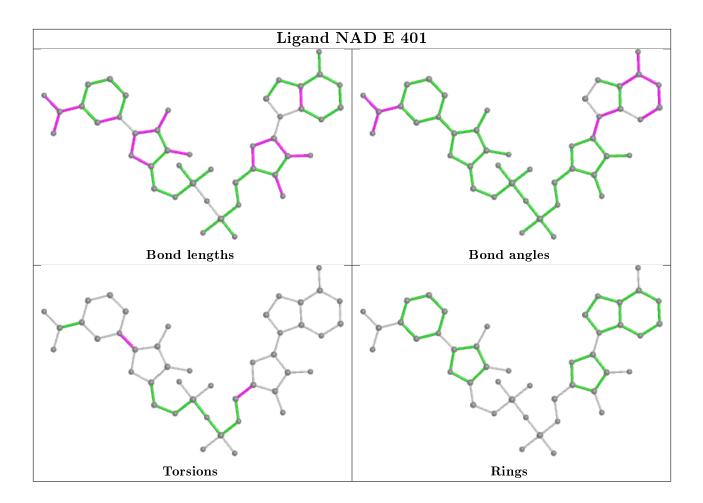












#### 5.7 Other polymers (i)

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	<RSRZ $>$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	А	349/361~(96%)	-0.32	2 (0%) 89 88	17, 23, 54, 119	1 (0%)
1	В	341/361~(94%)	-0.25	2 (0%) 89 88	19, 30, 60, 92	0
1	С	340/361~(94%)	-0.22	5 (1%) 73 72	19, 29, 57, 88	0
1	D	341/361~(94%)	0.13	16 (4%) 31 30	21, 37, 69, 108	0
1	Е	338/361~(93%)	-0.00	12 (3%) 42 42	21, 35, 62, 91	0
1	F	340/361~(94%)	-0.47	1 (0%) 94 93	18, 24, 47, 105	0
All	All	2049/2166~(94%)	-0.19	38 (1%) 66 64	17, 30, 61, 119	1 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	1	MET	7.5
1	А	341	ALA	5.8
1	D	207	ALA	5.7
1	Е	207	ALA	4.5
1	D	2	VAL	4.0

## 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.

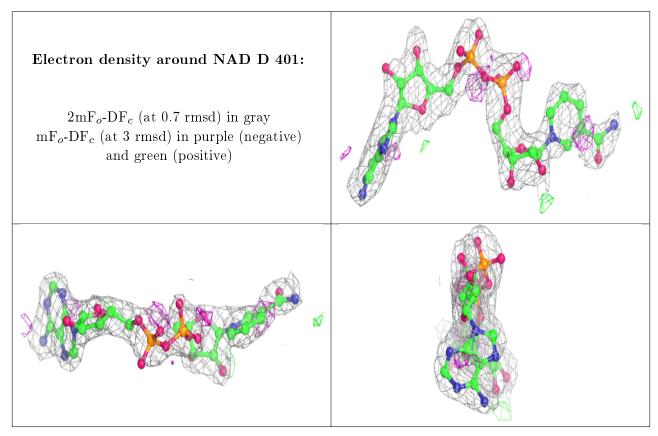


### 6.4 Ligands (i)

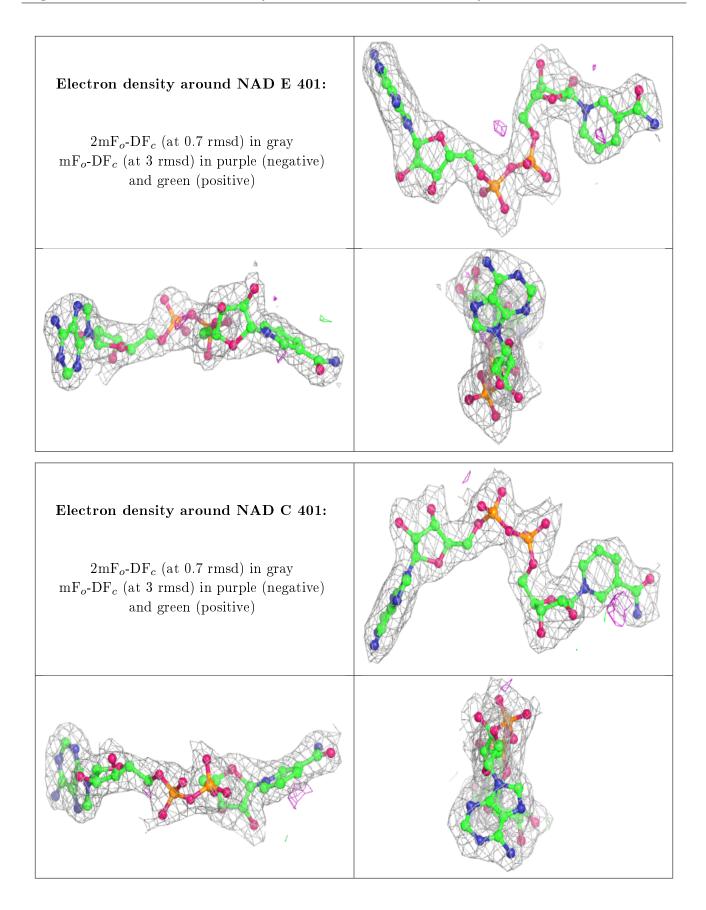
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	$Q{<}0.9$
2	NAD	D	401	44/44	0.91	0.21	$49,\!57,\!73,\!99$	0
2	NAD	Е	401	44/44	0.96	0.15	$30,\!44,\!57,\!61$	0
2	NAD	С	401	44/44	0.97	0.14	24,32,42,47	0
2	NAD	F	401	44/44	0.98	0.11	18,21,29,33	0
2	NAD	А	401	44/44	0.98	0.11	17,20,26,34	0
2	NAD	В	401	44/44	0.98	0.12	$20,\!30,\!37,\!45$	0

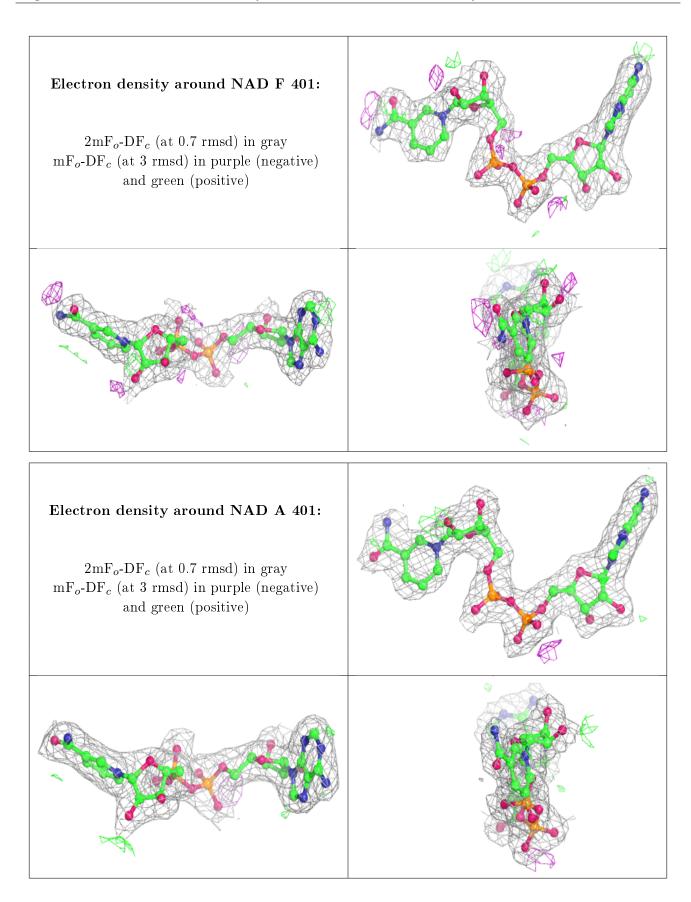
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



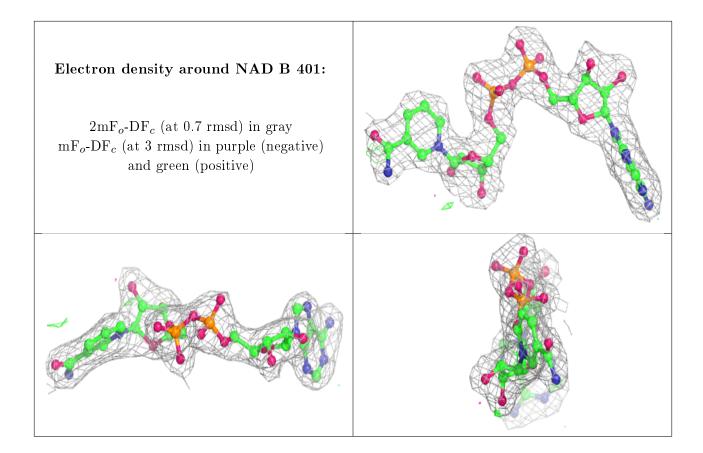












#### 6.5 Other polymers (i)

There are no such residues in this entry.

