

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

Nov 5, 2023 – 11:38 pm GMT

PDB ID : 2VHX

Title : Crystal structure of the ternary complex of L-alanine dehydrogenase from My-

cobacterium tuberculosis with NAD+ and pyruvate

Authors : Agren, D.; Schneider, G.

Deposited on : 2007-11-26

Resolution : 2.00 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 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 : 1.8.4, 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)

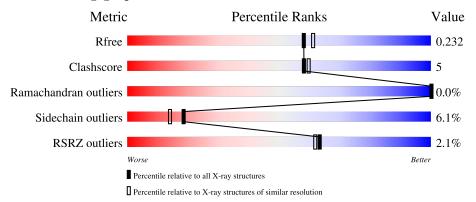
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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			
			2%			
1	A	377	82%	12%	•	-
	_		3%			
1	В	377	86%	10%	٠	
			3%			
1	С	377	84%	11%	٠	<del>.</del>
			_% 			
1	D	377	84%	11%	٠	<b>-</b> □
			2%			
1	Е	377	87%	10%	)	• •

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Mol	Chain	Length	Quality of chain	
			<u>%</u>	
1	F	377	92%	6% ••

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PYR	D	1371	-	X	-	-



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17715 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 ALANINE DEHYDROGENASE.

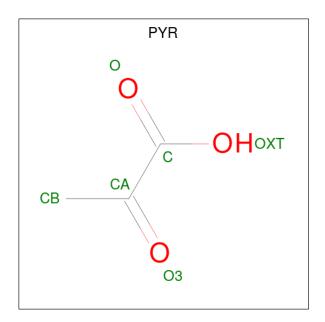
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	368	Total	С	Ν	О	S	0	4	0
1	Λ	300	2727	1716	482	514	15	U	4	
1	В	368	Total	С	N	О	S	0	1	0
1	Ъ	300	2707	1701	477	516	13	U	1	
1	С	365	Total	С	N	О	S	0	0	0
1		300	2682	1686	472	511	13	U	U	
1	D	367	Total	С	N	O	S	0	3	0
1	D	307	2712	1706	478	513	15	U	3	
1	Е	373	Total	С	N	O	S	0	1	0
1	ш	373	2742	1724	485	519	14	U	1	
1	F	373	Total	С	N	О	S	0	1	0
1	I.	313	2742	1724	485	519	14	U	1	

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	В	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

• Molecule 3 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).

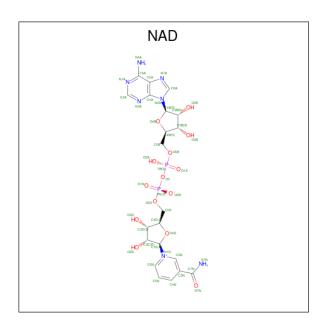




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	В	1	Total C O 6 3 3	0	0
3	С	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	Е	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

 $\bullet$  Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2).$ 





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
4	E	1	Total	С	N	О	Р	0	0
4	E	1	44	21	7	14	2	U	0
4	E	1	Total	С	N	О	Р	0	0
4	Г	1	44	21	7	14	2	U	0

### • Molecule 5 is water.

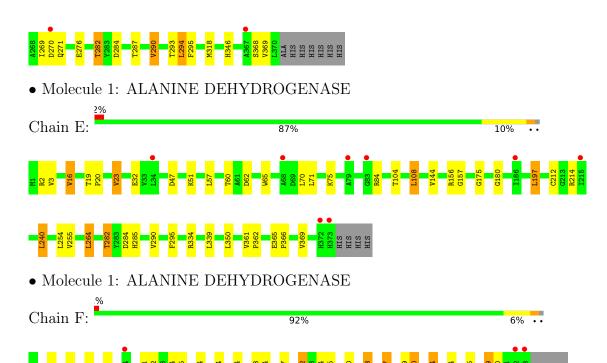
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	184	Total O 184 184	0	0
5	В	228	Total O 228 228	0	0
5	С	185	Total O 185 185	0	0
5	D	232	Total O 232 232	0	0
5	E	195	Total O 195 195	0	0
5	F	252	Total O 252 252	0	0



# 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: ALANINE DEHYDROGENASE Chain A: • Molecule 1: ALANINE DEHYDROGENASE Chain B: • Molecule 1: ALANINE DEHYDROGENASE Chain C: 11% • Molecule 1: ALANINE DEHYDROGENASE Chain D: 84% 11%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	176.25Å 171.77Å 98.25Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	40.00 - 2.00	Depositor
Resolution (A)	61.29 - 2.00	EDS
% Data completeness	90.6 (40.00-2.00)	Depositor
(in resolution range)	90.6 (61.29-2.00)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.75  (at  2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
$R, R_{free}$	0.172 , $0.210$	Depositor
it, it free	0.206 , $0.232$	DCC
$R_{free}$ test set	9182 reflections $(5.04\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, 42.6	EDS
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17715	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.

<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, MG, PYR

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	Bo	nd lengths	В	ond angles
IVIOI	Moi Chain		# Z  > 5	RMSZ	# Z >5
1	A	0.71	0/2787	0.82	3/3793 (0.1%)
1	В	0.78	$2/2755 \ (0.1\%)$	0.81	2/3751 (0.1%)
1	С	0.73	0/2730	0.79	2/3718 (0.1%)
1	D	0.73	0/2769	0.81	7/3769 (0.2%)
1	Е	0.62	0/2797	0.76	4/3811 (0.1%)
1	F	0.74	0/2797	0.77	3/3811 (0.1%)
All	All	0.72	$2/16635 \ (0.0\%)$	0.80	21/22653 (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	D	0	1

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
1	В	323	GLU	CB-CG	-5.67	1.41	1.52
1	В	37	ALA	CA-CB	5.21	1.63	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	D	246	ALA	N-CA-C	-8.71	87.48	111.00
1	В	264	LEU	CA-CB-CG	7.80	133.24	115.30
1	Е	197	LEU	CA-CB-CG	7.31	132.11	115.30
1	Е	334	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	Е	264	LEU	CA-CB-CG	6.91	131.19	115.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	245	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	2727	0	2756	39	0
1	В	2707	0	2716	25	0
1	С	2682	0	2689	28	0
1	D	2712	0	2734	25	0
1	Ε	2742	0	2751	24	0
1	F	2742	0	2751	19	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	0	3	0
3	В	6	0	0	0	0
3	С	6	0	0	0	0
3	D	6	0	0	0	0
3	Ε	6	0	0	3	0
3	F	6	0	0	3	0
4	Ε	44	0	26	3	0
4	F	44	0	26	4	0
5	A	184	0	0	2	0
5	В	228	0	0	3	0
5	С	185	0	0	1	0
5	D	232	0	0	1	0
5	Ε	195	0	0	2	0
5	F	252	0	0	3	0
All	All	17715	0	16449	158	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 5.

The worst 5 of 158 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:F:282:THR:HG22	1:F:285:HIS:H	1.39	0.86	
1:D:267:ILE:HG22	1:D:267:ILE:O	1.75	0.86	
1:A:269:ILE:HG13	1:A:297:CYS:HB3	1.58	0.84	
1:A:75:LYS:NZ	3:A:1373:PYR:CB	2.41	0.82	
1:C:281:THR:HG21	1:C:286:PRO:O	1.80	0.80	

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	Percen	tiles
1	A	368/377 (98%)	360 (98%)	8 (2%)	0	100	100
1	В	365/377 (97%)	358 (98%)	7 (2%)	0	100	100
1	С	361/377 (96%)	357 (99%)	4 (1%)	0	100	100
1	D	366/377 (97%)	358 (98%)	7 (2%)	1 (0%)	41	37
1	Е	372/377 (99%)	366 (98%)	6 (2%)	0	100	100
1	F	372/377 (99%)	367 (99%)	5 (1%)	0	100	100
All	All	2204/2262 (97%)	2166 (98%)	37 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	245	LYS

#### 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 r	number of residues.
---------------------------	---------------------

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/282 (99%)	254 (91%)	25 (9%)	9 6	
1	В	275/282 (98%)	259 (94%)	16 (6%)	20 15	
1	С	273/282 (97%)	251 (92%)	22 (8%)	11 7	
1	D	277/282 (98%)	261 (94%)	16 (6%)	20 15	
1	E	279/282 (99%)	261 (94%)	18 (6%)	17 12	
1	F	279/282 (99%)	270 (97%)	9 (3%)	39 38	
All	All	1662/1692 (98%)	1556 (94%)	106 (6%)	18 13	

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	290	VAL
1	D	264	LEU
1	F	212[A]	CYS
1	С	298	VAL
1	D	101	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	143	GLN
1	Е	148	HIS
1	F	373	HIS
1	Е	206	GLN
1	D	346	HIS

#### 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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	me Chain	Chain Res I	Link	Bond lengths		Bond angles			
MIOI	Type	Chain	nes	tes   Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	$\mid \# Z  > 2$
4	NAD	Е	1375	-	42,48,48	1.71	3 (7%)	50,73,73	1.28	4 (8%)
3	PYR	В	1373	-	5,5,5	2.89	3 (60%)	3,6,6	2.04	1 (33%)
3	PYR	F	1375	-	5,5,5	2.45	2 (40%)	3,6,6	1.90	2 (66%)
3	PYR	Е	1374	-	5,5,5	2.63	3 (60%)	3,6,6	2.15	1 (33%)
3	PYR	С	1371	-	5,5,5	2.98	3 (60%)	3,6,6	0.89	0
3	PYR	A	1373	-	5,5,5	2.66	3 (60%)	3,6,6	2.02	1 (33%)
3	PYR	D	1371	-	5,5,5	2.82	3 (60%)	3,6,6	1.99	2 (66%)
4	NAD	F	1376	-	42,48,48	1.78	3 (7%)	50,73,73	1.61	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	Ε	1375	-	-	5/26/62/62	0/5/5/5
3	PYR	В	1373	-	-	0/4/4/4	-
3	PYR	F	1375	-	-	0/4/4/4	-
3	PYR	Е	1374	-	-	0/4/4/4	-
3	PYR	С	1371	-	-	0/4/4/4	-
3	PYR	A	1373	-	-	0/4/4/4	-
3	PYR	D	1371	-	-	1/4/4/4	-
4	NAD	F	1376	-	-	4/26/62/62	0/5/5/5



The worst	5	of '	23	bond	length	outliers	are	listed	below:
THE WOLDS	$\circ$	01 4	20	DOM	10115 011	Outilities	$\alpha_{\rm L}$	mouca	DCIOW.

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$Ideal(\AA)$
4	Е	1375	NAD	O7N-C7N	8.19	1.39	1.24
4	F	1376	NAD	O7N-C7N	7.48	1.38	1.24
4	F	1376	NAD	C2A-N3A	5.31	1.40	1.32
3	В	1373	PYR	CA-C	-4.85	1.36	1.54
3	Е	1374	PYR	CA-C	-4.73	1.37	1.54

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	F	1376	NAD	C3N-C7N-N7N	5.93	124.86	117.75
4	F	1376	NAD	N3A-C2A-N1A	-5.06	120.77	128.68
4	Е	1375	NAD	N3A-C2A-N1A	-4.87	121.06	128.68
4	F	1376	NAD	O7N-C7N-C3N	-3.54	115.40	119.63
3	В	1373	PYR	OXT-C-CA	3.41	123.30	113.97

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Е	1375	NAD	O4D-C1D-N1N-C2N
4	Е	1375	NAD	O4D-C1D-N1N-C6N
4	Е	1375	NAD	C2D-C1D-N1N-C2N
4	F	1376	NAD	O4D-C1D-N1N-C2N
4	F	1376	NAD	O4D-C1D-N1N-C6N

There are no ring outliers.

5 monomers are involved in 11 short contacts:

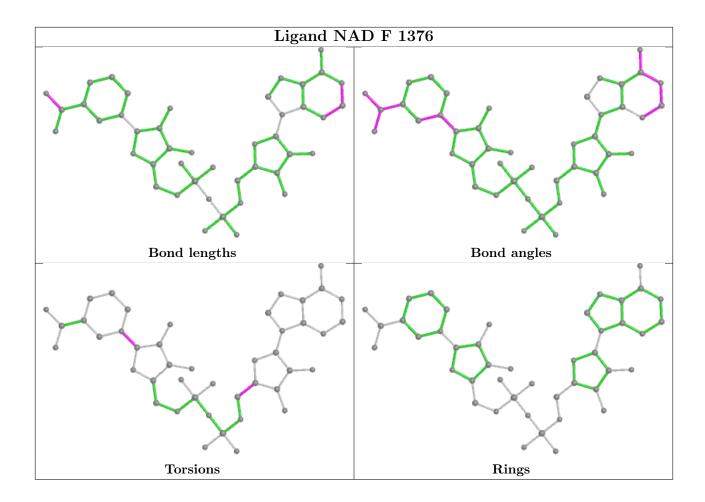
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Ε	1375	NAD	3	0
3	F	1375	PYR	3	0
3	Е	1374	PYR	3	0
3	A	1373	PYR	3	0
4	F	1376	NAD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	368/377 (97%)	0.20	9 (2%) 59 57	3, 17, 29, 42	0
1	В	368/377 (97%)	0.03	10 (2%) 54 53	3, 14, 27, 44	0
1	С	365/377~(96%)	0.16	12 (3%) 46 45	4, 16, 33, 37	0
1	D	367/377 (97%)	0.01	4 (1%) 80 79	3, 14, 28, 46	0
1	E	373/377 (98%)	0.27	8 (2%) 63 62	6, 20, 31, 57	0
1	F	373/377 (98%)	0.10	3 (0%) 86 85	6, 15, 23, 53	0
All	All	2214/2262 (97%)	0.13	46 (2%) 63 62	3, 16, 29, 57	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	360	GLY	4.4
1	Е	372	HIS	3.8
1	A	371	ALA	3.7
1	F	373	HIS	3.6
1	С	283	TYR	3.6

## 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.

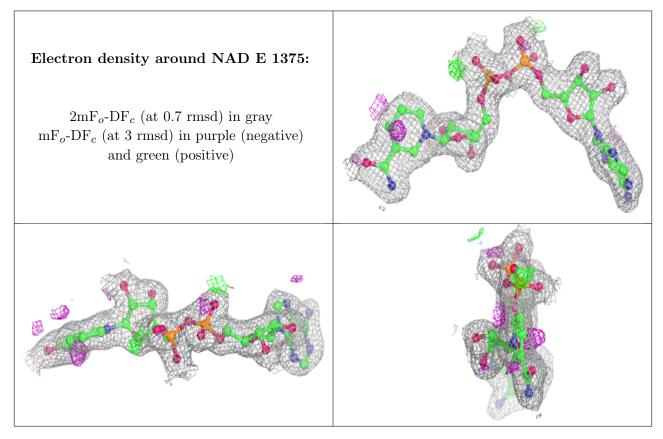


## 6.4 Ligands (i)

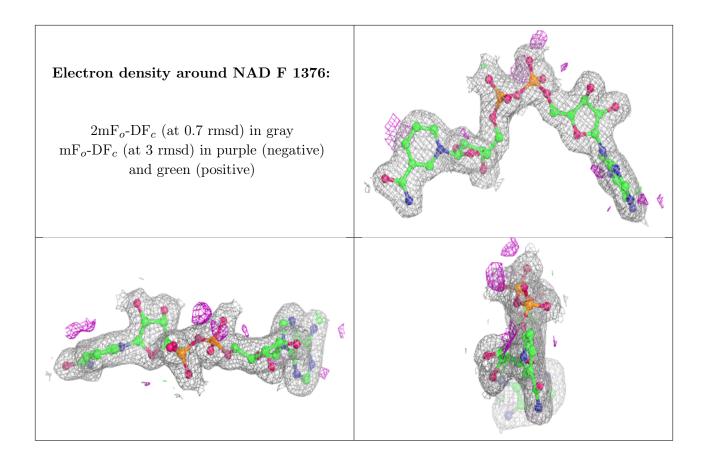
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
2	MG	F	1374	1/1	0.59	0.15	53,53,53,53	0
2	MG	A	1372	1/1	0.73	0.27	32,32,32,32	0
3	PYR	A	1373	6/6	0.82	0.24	34,38,39,39	0
3	PYR	D	1371	6/6	0.84	0.28	39,42,45,47	0
3	PYR	С	1371	6/6	0.87	0.18	37,40,42,43	0
3	PYR	В	1373	6/6	0.87	0.18	32,38,39,39	0
3	PYR	Е	1374	6/6	0.90	0.25	34,37,40,43	0
3	PYR	F	1375	6/6	0.92	0.27	18,23,28,32	0
2	MG	В	1372	1/1	0.94	0.32	28,28,28,28	0
4	NAD	Е	1375	44/44	0.98	0.11	8,13,20,22	0
4	NAD	F	1376	44/44	0.98	0.11	3,7,11,15	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.

