

wwPDB X-ray Structure Validation Summary Report (i)

Feb 21, 2024 – 12:29 PM EST

PDB ID	:	4NU5
Title	:	Crystal Structure of PTDH R301A
Authors	:	Nair, S.K.; Chekan, J.R.
Deposited on	:	2013-12-03
Resolution	:	2.35 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:

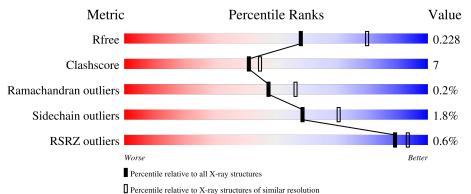
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.35 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	А	329	% 8 9%	11%				
1	В	329	86%	12% ••				



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5434 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 Phosphonate dehydrogenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	328	Total 2501	C 1581		0 454	S 14	0	0	0
1	В	324	Total 2471	C 1559	N 448	O 450	S 14	0	0	0

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Chain	Residue	Modelled	Actual	Comment	Reference
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	13	GLU	ASP	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	26	ILE	MET	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	71	ILE	VAL	conflict	UNP 069054
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	А	130	LYS	GLU	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	132	ARG	GLN	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	137	ARG	GLN	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	150	PHE	ILE	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	175	ALA	GLU	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	215	LEU	GLN	conflict	UNP 069054
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	А	275	GLN	ARG	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	276	GLN	LEU	conflict	UNP 069054
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	А	301	ALA	ARG	engineered mutation	UNP 069054
A319GLUALAconflictUNP 069054A325VALALAconflictUNP 069054B13GLUASPconflictUNP 069054B26ILEMETconflictUNP 069054B71ILEVALconflictUNP 069054B130LYSGLUconflictUNP 069054B130LYSGLUconflictUNP 069054B132ARGGLNconflictUNP 069054B137ARGGLNconflictUNP 069054B150PHEILEconflictUNP 069054B175ALAGLUconflictUNP 069054	А	313	LEU	ILE	conflict	UNP 069054
A325VALALAconflictUNP O69054B13GLUASPconflictUNP O69054B26ILEMETconflictUNP O69054B71ILEVALconflictUNP O69054B130LYSGLUconflictUNP O69054B132ARGGLNconflictUNP O69054B137ARGGLNconflictUNP O69054B150PHEILEconflictUNP O69054B175ALAGLUconflictUNP O69054	А	315	ALA	VAL	conflict	UNP 069054
B13GLUASPconflictUNP 069054B26ILEMETconflictUNP 069054B71ILEVALconflictUNP 069054B130LYSGLUconflictUNP 069054B132ARGGLNconflictUNP 069054B137ARGGLNconflictUNP 069054B137ARGGLNconflictUNP 069054B150PHEILEconflictUNP 069054B175ALAGLUconflictUNP 069054	А	319	GLU	ALA	conflict	UNP 069054
B26ILEMETconflictUNP O69054B71ILEVALconflictUNP O69054B130LYSGLUconflictUNP O69054B132ARGGLNconflictUNP O69054B137ARGGLNconflictUNP O69054B150PHEILEconflictUNP O69054B175ALAGLUconflictUNP O69054	А	325	VAL	ALA	conflict	UNP 069054
B71ILEVALconflictUNP 069054B130LYSGLUconflictUNP 069054B132ARGGLNconflictUNP 069054B137ARGGLNconflictUNP 069054B150PHEILEconflictUNP 069054B175ALAGLUconflictUNP 069054	В	13	GLU	ASP	conflict	UNP 069054
B130LYSGLUconflictUNP O69054B132ARGGLNconflictUNP O69054B137ARGGLNconflictUNP O69054B150PHEILEconflictUNP O69054B175ALAGLUconflictUNP O69054	В	26	ILE	MET	conflict	UNP 069054
B132ARGGLNconflictUNP O69054B137ARGGLNconflictUNP O69054B150PHEILEconflictUNP O69054B175ALAGLUconflictUNP O69054	В	71	ILE	VAL	conflict	UNP 069054
B137ARGGLNconflictUNP O69054B150PHEILEconflictUNP O69054B175ALAGLUconflictUNP O69054	В	130	LYS	GLU	conflict	UNP 069054
B150PHEILEconflictUNP O69054B175ALAGLUconflictUNP O69054	В	132	ARG	GLN	conflict	UNP 069054
B 175 ALA GLU conflict UNP O69054	В	137	ARG	GLN	conflict	UNP 069054
	В	150	PHE	ILE	conflict	UNP 069054
B215LEUGLNconflictUNP O69054		175	ALA	GLU	conflict	UNP 069054
	В	215	LEU	GLN	conflict	UNP 069054

There are 32 discrepancies between the modelled and reference sequences:

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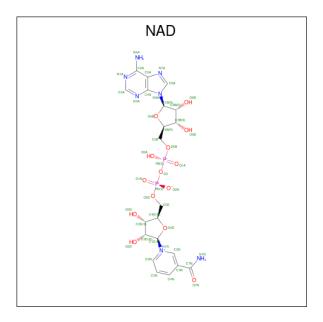


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Chain	Residue	Modelled	Actual Comment		Reference
В	275	GLN	ARG	conflict	UNP O69054
В	276	GLN	LEU	conflict	UNP 069054
В	301	ALA	ARG	engineered mutation	UNP O69054
В	313	LEU	ILE	conflict	UNP 069054
В	315	ALA	VAL	conflict	UNP 069054
В	319	GLU	ALA	conflict	UNP O69054
В	325	VAL	ALA	conflict	UNP 069054

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• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
9	Λ	1	Total	С	Ν	Ο	Р	0	0	
	A	1	44	21	7	14	2	0	0	
0	P	1	Total	С	Ν	Ο	Р	0	0	
	D		44	21	7	14	2	0	U	

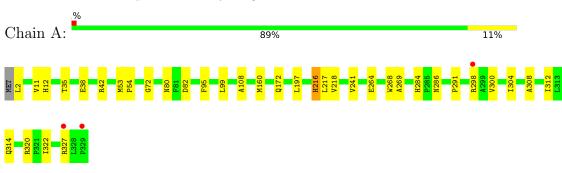
• Molecule 3 is water.

[Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	А	188	Total O 188 188	0	0
	3	В	186	Total O 186 186	0	0



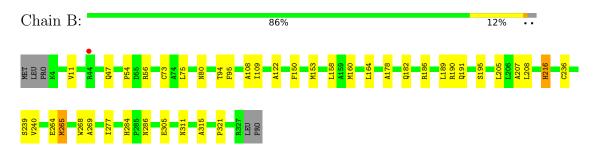
3 Residue-property plots (i)

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: Phosphonate dehydrogenase

• Molecule 1: Phosphonate dehydrogenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	116.49Å 80.46 Å 81.97 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 - 2.35	Depositor
Resolution (A)	47.48 - 2.35	EDS
% Data completeness	$93.0\ (25.00-2.35)$	Depositor
(in resolution range)	92.8(47.48-2.35)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	$3.98 (at 2.34 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.230	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.183 , 0.228	DCC
R_{free} test set	1534 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.8	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 41.6	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5434	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.50	0/2548	0.64	0/3468	
1	В	0.48	0/2516	0.62	0/3422	
All	All	0.49	0/5064	0.63	0/6890	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2501	0	2519	32	0
1	В	2471	0	2483	40	0
2	А	44	0	26	0	0
2	В	44	0	26	1	0
3	А	188	0	0	3	0
3	В	186	0	0	9	0
All	All	5434	0	5054	72	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 7.

The worst 5 of 72 close contacts within the same asymmetric unit are listed below, sorted by their



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:CYS:HB2	3:B:1083:HOH:O	1.31	1.25
1:B:265:MET:HE2	1:B:277:ILE:HG13	1.50	0.92
1:A:108:ALA:HB3	1:A:160:MET:HE3	1.53	0.91
1:A:108:ALA:CB	1:A:160:MET:CE	2.57	0.82
1:B:236:CYS:SG	3:B:1083:HOH:O	2.35	0.81

clash magnitude.

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	Perce	entiles
1	А	326/329~(99%)	315~(97%)	10 (3%)	1 (0%)	41	47
1	В	322/329~(98%)	312 (97%)	10 (3%)	0	100	100
All	All	648/658~(98%)	627~(97%)	20 (3%)	1 (0%)	47	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	82	ASP

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	256/257~(100%)	253~(99%)	3(1%)	71 82		
1	В	252/257~(98%)	246~(98%)	6(2%)	49 59		
All	All	508/514~(99%)	499~(98%)	9~(2%)	59 70		

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	216	HIS
1	В	265	MET
1	В	47	GLN
1	В	56	ARG
1	В	95	PHE

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such side chains are listed below:

Mol	Chain	Res	Type
1	В	80	ASN
1	В	118	HIS
1	В	284	HIS
1	В	216	HIS
1	А	165	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)

2 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	Turne	Chain	Res Link		Bond lengths			Bond angles		
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAD	А	800	-	42,48,48	0.65	0	50,73,73	1.25	4 (8%)
2	NAD	В	800	-	42,48,48	0.82	0	50,73,73	1.25	5 (10%)

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	А	800	-	-	2/26/62/62	0/5/5/5
2	NAD	В	800	-	-	4/26/62/62	0/5/5/5

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	А	800	NAD	N3A-C2A-N1A	-5.02	120.83	128.68
2	В	800	NAD	N3A-C2A-N1A	-4.91	121.01	128.68
2	В	800	NAD	C3N-C7N-N7N	2.99	121.33	117.75
2	А	800	NAD	C3D-C2D-C1D	2.74	105.10	100.98
2	В	800	NAD	C3D-C2D-C1D	2.53	104.79	100.98

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

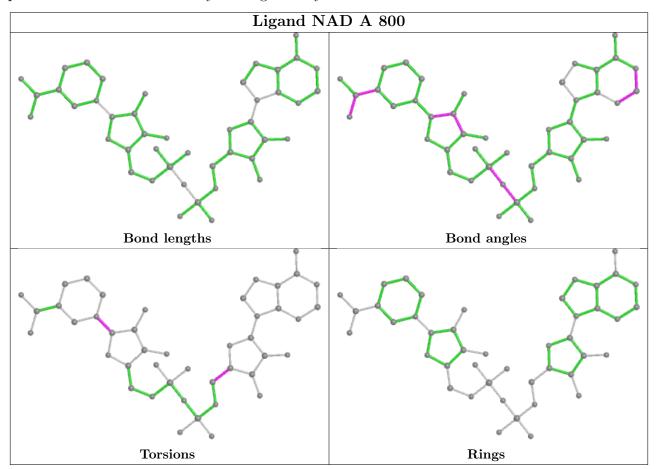
Mol	Chain	Res	Type	Atoms
2	А	800	NAD	O4D-C1D-N1N-C6N
2	В	800	NAD	O4D-C1D-N1N-C2N
2	В	800	NAD	O4D-C1D-N1N-C6N
2	В	800	NAD	O4B-C4B-C5B-O5B
2	В	800	NAD	C2D-C1D-N1N-C2N

There are no ring outliers.

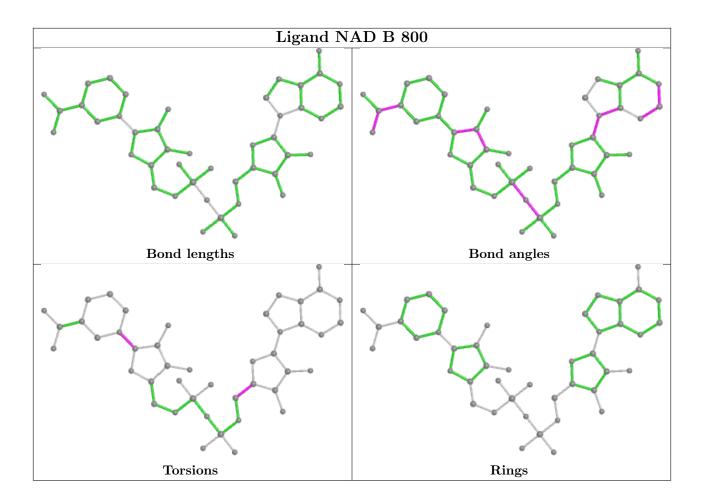


Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	800	NAD	1	0

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>2		$OWAB(Å^2)$	Q < 0.9	
1	А	328/329~(99%)	-0.34	3~(0%)	84	90	24, 35, 48, 59	0
1	В	324/329~(98%)	-0.40	1 (0%)	94	97	24, 35, 47, 58	0
All	All	652/658~(99%)	-0.37	4 (0%)	89	93	24, 35, 48, 59	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	329	PRO	2.6
1	А	327	ARG	2.3
1	А	298	ARG	2.3
1	В	44	ARG	2.1

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	$B-factors(Å^2)$	Q < 0.9
2	NAD	А	800	44/44	0.97	0.09	24,31,41,43	0

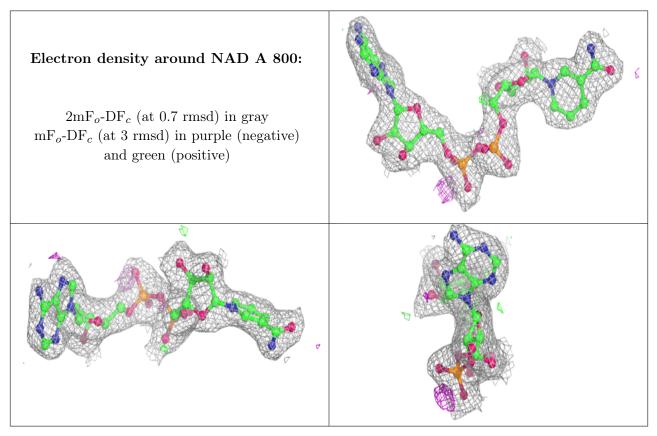
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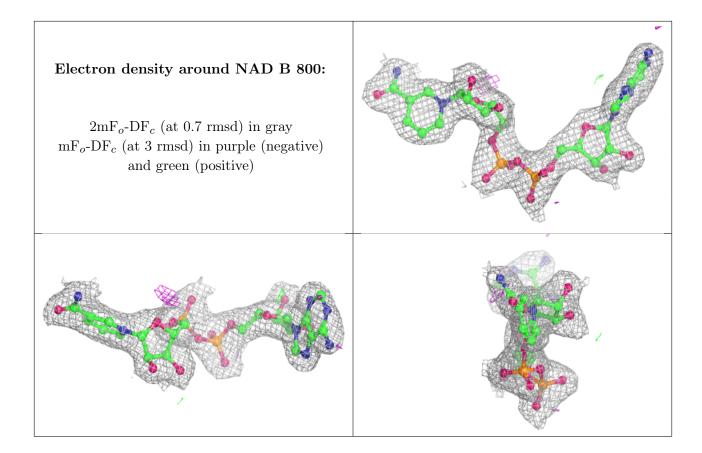
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	NAD	В	800	44/44	0.98	0.11	23,31,40,42	0

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.

