



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 AM GMT

PDB ID : 2NSY  
Title : CRYSTAL STRUCTURE OF NH<sub>3</sub>-DEPENDENT NAD<sup>+</sup> SYNTHETASE  
FROM BACILLUS SUBTILIS IN COMPLEX WITH NAD-ADENYLATE  
Authors : Rizzi, M.; Bolognesi, M.; Coda, A.  
Deposited on : 1998-07-14  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

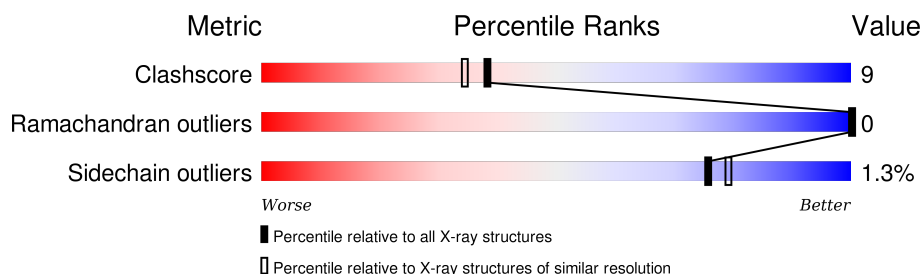
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	271	 80% 17% •
1	B	271	 81% 16% •

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
6	GOL	A	308	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4940 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.

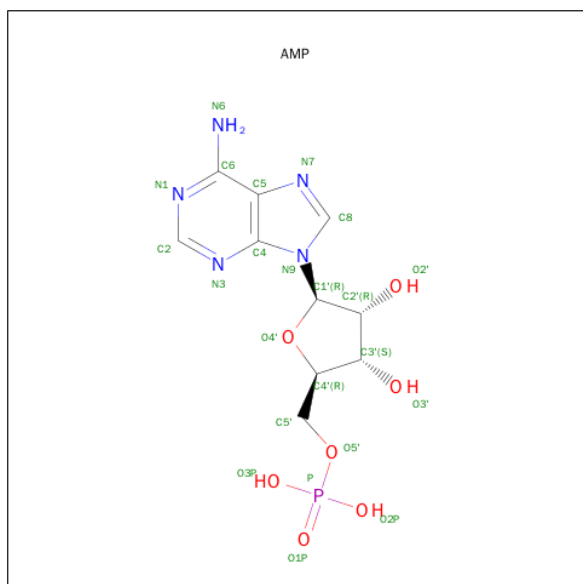
- Molecule 1 is a protein called PROTEIN (NAD SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	4	0
			2143	1343	364	431	5			
1	B	271	Total	C	N	O	S	0	3	0
			2138	1340	364	429	5			

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

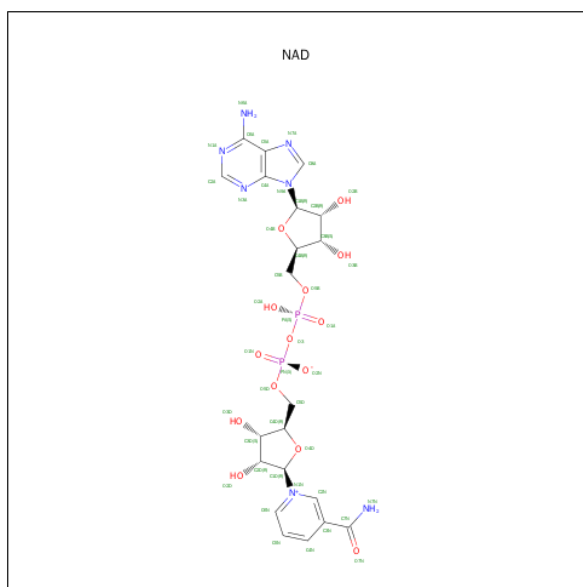
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



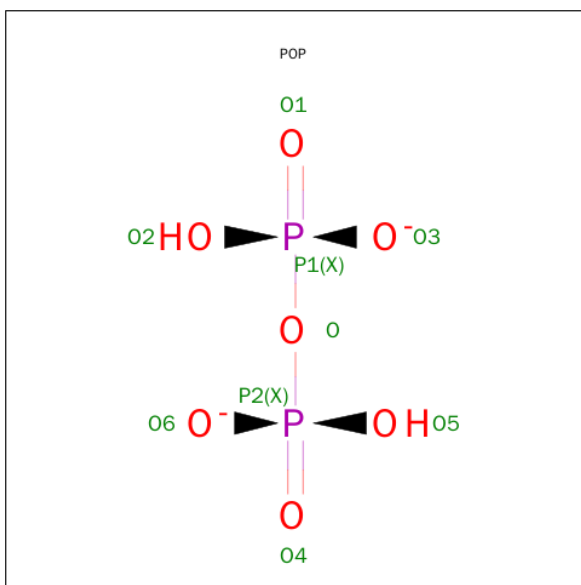
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			43	21	6	14	2		
4	B	1	Total	C	N	O	P	0	0
			43	21	6	14	2		

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $H_2O_7P_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

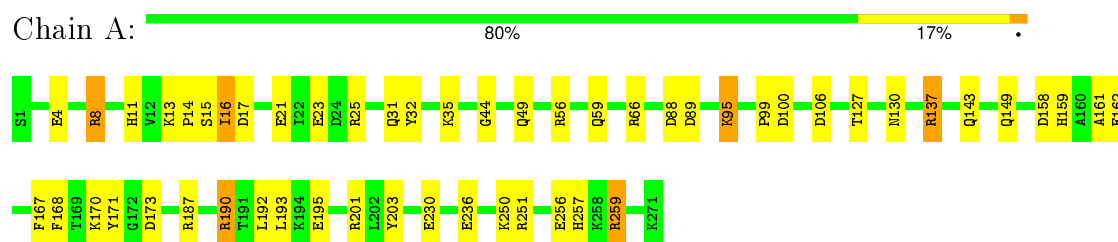
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	265	Total 265	O 265	0	0
7	B	228	Total 228	O 228	0	0

### 3 Residue-property plots

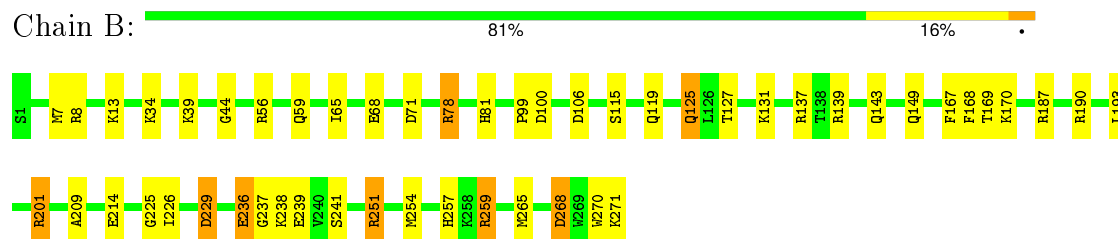
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (NAD SYNTHETASE)



- Molecule 1: PROTEIN (NAD SYNTHETASE)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.48 Å   85.62 Å   60.12 Å 90.00°   110.76°   90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	92.0 (15.00-2.00)	Depositor
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.155 , 0.180	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP



## 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: GOL, MG, POP, NAD, AMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.99	2/2198 (0.1%)	2.19	37/2956 (1.3%)
1	B	0.90	1/2189 (0.0%)	1.52	27/2944 (0.9%)
All	All	0.95	3/4387 (0.1%)	1.88	64/5900 (1.1%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	6
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	ARG	CD-NE	15.68	1.73	1.46
1	A	162	GLU	CD-OE1	6.11	1.32	1.25
1	B	236	GLU	CD-OE1	5.59	1.31	1.25

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ARG	NE-CZ-NH1	-58.85	90.88	120.30
1	A	8	ARG	NH1-CZ-NH2	43.45	167.19	119.40
1	A	8	ARG	NE-CZ-NH2	-39.26	100.67	120.30
1	A	8	ARG	CD-NE-CZ	-21.97	92.84	123.60
1	B	190	ARG	NE-CZ-NH1	17.09	128.85	120.30
1	B	259	ARG	NE-CZ-NH2	-16.89	111.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	B	265	MET	CG-SD-CE	-13.46	78.66	100.20
1	B	56	ARG	NE-CZ-NH2	-11.09	114.76	120.30
1	A	187	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	137	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	A	106	ASP	CB-CG-OD1	9.73	127.06	118.30
1	A	187	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	A	56	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	B	201	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	139	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	256[A]	GLU	OE1-CD-OE2	-9.08	112.40	123.30
1	A	256[B]	GLU	OE1-CD-OE2	-9.08	112.40	123.30
1	A	259	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	B	229	ASP	CB-CG-OD1	8.46	125.92	118.30
1	B	190	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	78	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	251	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	187	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	B	56	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	A	89	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	B	137	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	236	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	B	139	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	229	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	A	251	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	11	HIS	O-C-N	-7.00	111.51	122.70
1	A	173	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	B	137	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	78	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	B	187	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	230	GLU	OE1-CD-OE2	-6.79	115.15	123.30
1	B	106	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	16	ILE	CA-C-O	6.69	134.15	120.10
1	B	236	GLU	OE1-CD-OE2	-6.69	115.28	123.30
1	A	195	GLU	OE1-CD-OE2	6.48	131.08	123.30
1	B	187	ARG	NH1-CZ-NH2	6.48	126.53	119.40
1	A	190	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	56	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	270	TRP	O-C-N	6.06	132.40	122.70
1	B	268	ASP	O-C-N	-5.98	113.13	122.70
1	A	16	ILE	CA-C-N	-5.95	104.11	117.20
1	A	15[A]	SER	O-C-N	5.90	132.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15[B]	SER	O-C-N	5.90	132.15	122.70
1	B	8	ARG	CD-NE-CZ	5.86	131.80	123.60
1	A	14	PRO	O-C-N	5.86	132.07	122.70
1	A	158	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	171	TYR	CB-CG-CD2	5.33	124.20	121.00
1	A	32	TYR	CZ-CE2-CD2	-5.33	115.01	119.80
1	A	14	PRO	CA-C-N	-5.28	105.58	117.20
1	A	66	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	259	ARG	NH1-CZ-NH2	5.26	125.18	119.40
1	A	201	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	190	ARG	CD-NE-CZ	5.18	130.86	123.60
1	B	268	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	89	ASP	OD1-CG-OD2	5.09	132.97	123.30
1	B	168	PHE	CB-CG-CD1	5.08	124.36	120.80
1	A	17	ASP	CA-CB-CG	5.07	124.56	113.40
1	A	25	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	A	259	ARG	Sidechain
1	B	201	ARG	Sidechain
1	B	241	SER	Mainchain
1	B	251	ARG	Sidechain
1	B	259	ARG	Sidechain
1	B	268	ASP	Mainchain
1	B	78	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2143	0	2114	34	2
1	B	2138	0	2112	42	2
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	23	0	12	0	0
3	B	23	0	12	0	0
4	A	43	0	24	1	0
4	B	43	0	24	13	0
5	A	9	0	0	0	0
5	B	9	0	0	0	0
6	A	6	0	8	5	0
6	B	6	0	8	0	0
7	A	265	0	0	15	3
7	B	228	0	0	7	3
All	All	4940	0	4314	80	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (80) 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)
4:B:303:NAD:O5B	4:B:303:NAD:PA	0.98	1.38
4:B:303:NAD:O5B	4:B:303:NAD:C5B	1.79	1.31
1:B:34:LYS:HE3	7:B:843:HOH:O	1.38	1.21
1:B:34:LYS:NZ	1:B:65:ILE:HG12	1.72	1.04
1:B:34:LYS:CE	7:B:843:HOH:O	1.96	1.00
6:A:308:GOL:H11	7:A:801:HOH:O	1.59	1.00
1:B:34:LYS:HZ1	1:B:65:ILE:HG12	1.22	0.99
4:B:303:NAD:PA	4:B:303:NAD:C5B	2.60	0.89
1:A:88:ASP:HB2	7:A:546:HOH:O	1.78	0.83
1:B:39:LYS:CE	1:B:71:ASP:OD2	2.30	0.80
1:B:209:ALA:HB2	4:B:303:NAD:C7N	2.14	0.78
4:B:303:NAD:O5B	4:B:303:NAD:O2A	1.99	0.78
1:A:23:GLU:HG3	7:A:729:HOH:O	1.86	0.74
1:A:149:GLN:HE22	1:B:127:THR:H	1.36	0.73
1:A:130:ASN:HD22	1:B:149:GLN:HE21	1.40	0.69
6:A:308:GOL:C1	7:A:801:HOH:O	2.25	0.68
1:B:119:GLN:HE22	1:B:125:GLN:NE2	1.91	0.68
4:B:303:NAD:O1A	4:B:303:NAD:O5B	2.03	0.67
1:A:127:THR:H	1:B:149:GLN:HE22	1.44	0.66
1:B:39:LYS:HE3	1:B:71:ASP:OD2	1.93	0.65
4:B:303:NAD:C7N	7:B:586:HOH:O	2.45	0.65
1:A:13:LYS:HD2	1:A:16:ILE:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:LYS:NZ	1:B:257:HIS:HD2	1.95	0.64
1:A:35:LYS:NZ	1:B:271:LYS:OXT	2.32	0.63
1:B:119:GLN:NE2	1:B:125:GLN:HE21	1.96	0.63
1:A:170:LYS:NZ	1:A:257:HIS:HD2	1.96	0.63
1:B:119:GLN:HE22	1:B:125:GLN:HE21	1.46	0.62
1:A:4:GLU:CD	7:A:803:HOH:O	2.38	0.62
1:A:23:GLU:HG3	7:A:731:HOH:O	2.00	0.61
1:A:16:ILE:HA	7:A:497:HOH:O	2.02	0.59
1:B:34:LYS:HZ3	1:B:65:ILE:HG12	1.64	0.59
6:A:308:GOL:H32	7:A:800:HOH:O	2.03	0.58
1:B:34:LYS:CD	7:B:843:HOH:O	2.42	0.58
6:A:308:GOL:C3	7:A:800:HOH:O	2.52	0.58
1:B:39:LYS:NZ	1:B:71:ASP:OD2	2.37	0.57
1:B:209:ALA:CB	4:B:303:NAD:C7N	2.82	0.57
1:B:34:LYS:NZ	1:B:65:ILE:CG1	2.60	0.56
1:A:4:GLU:HG2	1:A:8:ARG:CZ	2.35	0.56
1:B:170:LYS:HZ2	1:B:257:HIS:HD2	1.51	0.56
1:A:21[B]:GLU:CD	7:A:693:HOH:O	2.44	0.56
4:B:303:NAD:O5B	4:B:303:NAD:O3	2.10	0.56
1:A:31:GLN:NE2	7:A:732:HOH:O	2.38	0.56
1:B:226:ILE:HD12	1:B:251:ARG:NH1	2.21	0.55
1:A:257:HIS:HE1	7:A:528:HOH:O	1.91	0.53
1:A:44:GLY:H	1:A:143:GLN:NE2	2.07	0.53
1:B:169:THR:OG1	4:B:303:NAD:H6N	2.09	0.52
1:B:34:LYS:HZ1	1:B:65:ILE:CG1	2.09	0.52
1:B:236:GLU:OE1	1:B:238:LYS:NZ	2.41	0.51
1:A:130:ASN:HD22	1:B:149:GLN:NE2	2.08	0.51
1:A:23:GLU:CG	7:A:731:HOH:O	2.58	0.50
1:B:44:GLY:H	1:B:143:GLN:NE2	2.10	0.49
1:B:209:ALA:HB2	4:B:303:NAD:O7N	2.13	0.49
1:A:149:GLN:NE2	1:B:127:THR:H	2.09	0.49
1:A:16:ILE:HB	7:A:497:HOH:O	2.14	0.48
1:B:13:LYS:NZ	7:B:539:HOH:O	2.25	0.48
1:A:95:LYS:HB2	1:A:95:LYS:HE2	1.41	0.47
1:B:115[B]:SER:OG	1:B:131:LYS:HE2	2.14	0.47
1:B:59:GLN:NE2	1:B:99:PRO:HA	2.31	0.45
1:A:168:PHE:CZ	6:A:308:GOL:H2	2.53	0.44
1:A:13:LYS:CD	1:A:16:ILE:HG22	2.46	0.44
1:A:59:GLN:NE2	1:A:99:PRO:HA	2.33	0.44
1:A:59:GLN:HE22	1:A:100:ASP:H	1.66	0.44
1:A:127:THR:H	1:B:149:GLN:NE2	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:HIS:HE1	7:B:388:HOH:O	2.00	0.43
1:A:170:LYS:HZ2	1:A:257:HIS:HD2	1.64	0.43
1:B:170:LYS:HZ2	1:B:257:HIS:CD2	2.33	0.43
1:B:7:MET:HE1	1:B:237:GLY:CA	2.48	0.43
1:A:190:ARG:HG3	1:A:203:TYR:HB2	2.01	0.43
1:B:254:MET:HE2	1:B:254:MET:HB2	1.77	0.43
1:B:257:HIS:HE1	7:B:439:HOH:O	2.01	0.43
1:A:49:GLN:HG3	1:A:193:LEU:CD1	2.48	0.43
1:A:16:ILE:CA	7:A:497:HOH:O	2.62	0.42
1:B:209:ALA:HB2	4:B:303:NAD:C3N	2.48	0.42
1:A:159:HIS:HD2	1:A:161:ALA:H	1.68	0.42
1:B:59:GLN:HE22	1:B:100:ASP:H	1.67	0.41
1:A:170:LYS:HZ1	1:A:257:HIS:HD2	1.68	0.41
1:A:167:PHE:CE2	4:A:301:NAD:H2N	2.56	0.40
1:B:167:PHE:CE2	4:B:303:NAD:H2N	2.56	0.40
1:B:225:GLY:C	1:B:226:ILE:HG13	2.42	0.40

All (5) 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)
1:A:4:GLU:OE2	7:B:622:HOH:O[2_656]	1.53	0.67
7:A:627:HOH:O	7:B:532:HOH:O[1_655]	1.60	0.60
1:B:68:GLU:OE2	7:A:674:HOH:O[1_554]	2.05	0.15
7:A:420:HOH:O	7:B:781:HOH:O[2_656]	2.09	0.11
1:A:250:LYS:NZ	1:B:214:GLU:OE1[1_655]	2.15	0.05

## 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	273/271 (101%)	273 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	272/271 (100%)	272 (100%)	0	0	100	100
All	All	545/542 (101%)	545 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	230/226 (102%)	228 (99%)	2 (1%)	84	88
1	B	229/226 (101%)	225 (98%)	4 (2%)	68	71
All	All	459/452 (102%)	453 (99%)	6 (1%)	76	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LYS
1	A	192	LEU
1	B	125	GLN
1	B	193	LEU
1	B	229	ASP
1	B	239	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	59	GLN
1	A	117	GLN
1	A	119	GLN
1	A	143	GLN
1	A	149	GLN
1	A	159	HIS

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Mol	Chain	Res	Type
1	A	257	HIS
1	B	59	GLN
1	B	81	HIS
1	B	117	GLN
1	B	125	GLN
1	B	143	GLN
1	B	149	GLN
1	B	257	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMP	A	300	2,4	20,25,25	1.05	0	22,38,38	1.48	4 (18%)
4	NAD	A	301	3	37,47,48	1.46	4 (10%)	45,71,73	1.94	6 (13%)
6	GOL	A	308	-	5,5,5	0.73	0	5,5,5	1.39	1 (20%)
5	POP	A	863	2	8,8,8	7.09	2 (25%)	13,13,13	1.48	2 (15%)
3	AMP	B	302	2,4	20,25,25	1.35	3 (15%)	22,38,38	1.97	9 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAD	B	303	3	37,47,48	2.97	6 (16%)	45,71,73	2.61	11 (24%)
6	GOL	B	309	-	5,5,5	1.32	1 (20%)	5,5,5	1.72	1 (20%)
5	POP	B	862	2	8,8,8	1.42	1 (12%)	13,13,13	1.30	1 (7%)

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
3	AMP	A	300	2,4	-	0/6/26/26	0/3/3/3
4	NAD	A	301	3	-	0/20/60/62	0/5/5/5
6	GOL	A	308	-	-	0/4/4/4	0/0/0/0
5	POP	A	863	2	-	0/6/6/6	0/0/0/0
3	AMP	B	302	2,4	-	0/6/26/26	0/3/3/3
4	NAD	B	303	3	-	0/20/60/62	0/5/5/5
6	GOL	B	309	-	-	0/4/4/4	0/0/0/0
5	POP	B	862	2	-	0/6/6/6	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	863	POP	P2-O	-13.32	1.30	1.61
4	B	303	NAD	PA-O5B	-13.25	0.98	1.59
3	B	302	AMP	C5-C4	-2.35	1.35	1.40
4	B	303	NAD	O4D-C1D	-2.26	1.38	1.41
5	B	862	POP	P1-O3	-2.17	1.43	1.50
4	A	301	NAD	C4N-C3N	2.01	1.43	1.39
4	B	303	NAD	C6N-C5N	2.08	1.43	1.38
4	A	301	NAD	C2A-N1A	2.08	1.37	1.33
3	B	302	AMP	P-O3P	2.09	1.62	1.54
6	B	309	GOL	O2-C2	2.55	1.51	1.43
4	A	301	NAD	O7N-C7N	2.94	1.30	1.21
4	B	303	NAD	O7N-C7N	3.35	1.32	1.21
3	B	302	AMP	O4'-C1'	3.77	1.46	1.41
4	A	301	NAD	O4B-C1B	5.80	1.48	1.41
4	B	303	NAD	O4B-C1B	6.12	1.48	1.41
4	B	303	NAD	O5B-C5B	8.44	1.79	1.44
5	A	863	POP	P1-O	14.86	1.94	1.61

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	NAD	C5N-C4N-C3N	-4.70	114.66	120.64
4	B	303	NAD	C2N-C3N-C7N	-4.29	113.89	119.78
4	A	301	NAD	C5N-C4N-C3N	-4.10	115.42	120.64
4	B	303	NAD	O3D-C3D-C4D	-3.93	99.28	111.05
4	B	303	NAD	C6N-C5N-C4N	-3.91	113.53	119.44
4	A	301	NAD	C4A-C5A-N7A	-3.69	106.08	109.48
4	B	303	NAD	O5D-C5D-C4D	-3.63	95.72	109.12
5	B	862	POP	P2-O-P1	-3.45	123.05	132.73
4	B	303	NAD	C4A-C5A-N7A	-3.41	106.34	109.48
3	B	302	AMP	C2'-C1'-N9	-3.14	109.50	114.29
5	A	863	POP	O-P2-O4	-3.08	98.09	107.70
5	A	863	POP	P2-O-P1	-3.00	124.31	132.73
6	B	309	GOL	O2-C2-C3	-2.90	95.37	108.65
3	A	300	AMP	O3P-P-O5'	-2.86	98.32	106.56
4	A	301	NAD	C6N-C5N-C4N	-2.78	115.24	119.44
3	A	300	AMP	C2'-C1'-N9	-2.68	110.20	114.29
3	B	302	AMP	O3P-P-O5'	-2.61	99.05	106.56
3	B	302	AMP	C1'-N9-C4	-2.57	123.06	126.94
4	A	301	NAD	C1B-N9A-C4A	-2.52	123.14	126.94
6	A	308	GOL	O3-C3-C2	-2.48	98.14	110.18
3	B	302	AMP	C2-N1-C6	-2.33	114.61	118.77
3	B	302	AMP	O4'-C1'-N9	-2.11	103.68	108.10
4	B	303	NAD	N3A-C2A-N1A	2.01	130.43	128.89
4	B	303	NAD	O3-PA-O5B	2.13	108.58	102.94
3	B	302	AMP	C4'-O4'-C1'	2.57	112.55	109.72
3	A	300	AMP	C4-C5-N7	2.98	112.22	109.48
3	B	302	AMP	N3-C2-N1	3.24	131.38	128.89
3	A	300	AMP	O2P-P-O1P	3.44	121.65	110.58
3	B	302	AMP	O5'-P-O1P	3.57	116.23	107.14
3	B	302	AMP	O2P-P-O1P	3.87	123.05	110.58
4	B	303	NAD	O4D-C1D-N1N	4.20	112.75	108.13
4	A	301	NAD	C5N-C6N-N1N	4.55	128.35	120.47
4	B	303	NAD	C5N-C6N-N1N	5.71	130.36	120.47
4	A	301	NAD	C2N-C3N-C4N	7.81	124.46	117.51
4	B	303	NAD	C2N-C3N-C4N	11.17	127.45	117.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	NAD	1	0
6	A	308	GOL	5	0
4	B	303	NAD	13	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.