



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:30 pm GMT

PDB ID : 1K4M  
Title : Crystal structure of E.coli nicotinic acid mononucleotide adenylyltransferase complexed to deamido-NAD  
Authors : Zhang, H.; Zhou, T.; Kurnasov, O.; Cheek, S.; Grishin, N.V.; Osterman, A.  
Deposited on : 2001-10-08  
Resolution : 1.90 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

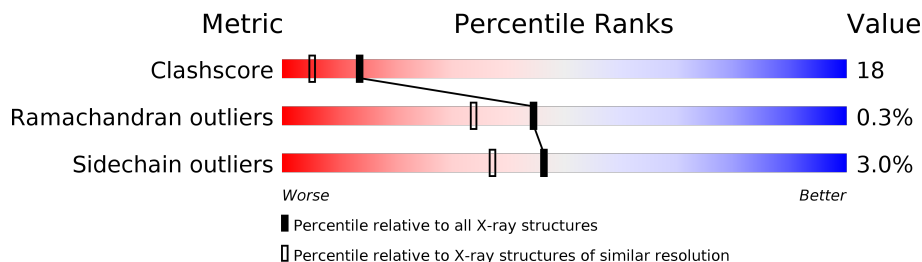
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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	213	
1	B	213	
1	C	213	

## 2 Entry composition [i](#)

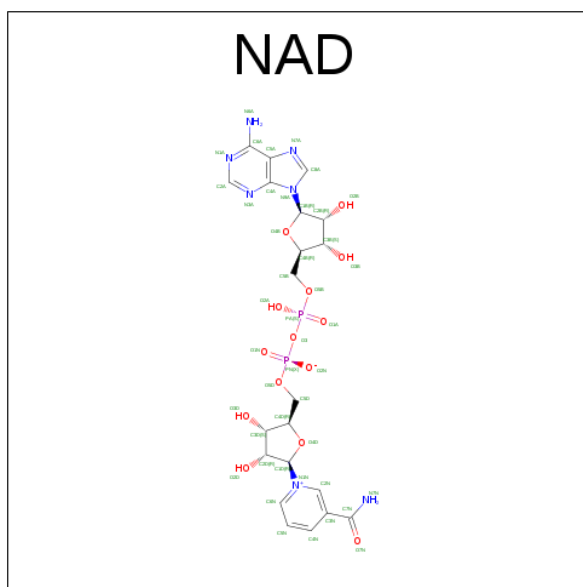
There are 4 unique types of molecules in this entry. The entry contains 5881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NaMN adenylyltransferase.

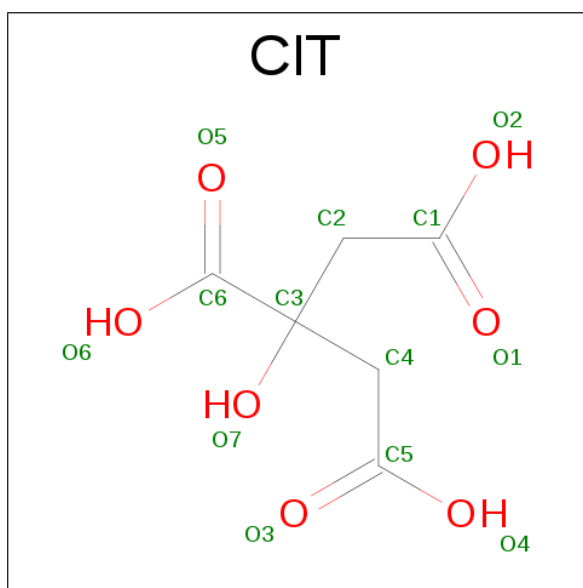
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1733	1111	298	319	5			
1	B	213	Total	C	N	O	S	0	0	0
			1733	1111	298	319	5			
1	C	213	Total	C	N	O	S	0	0	0
			1733	1111	298	319	5			

- 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
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

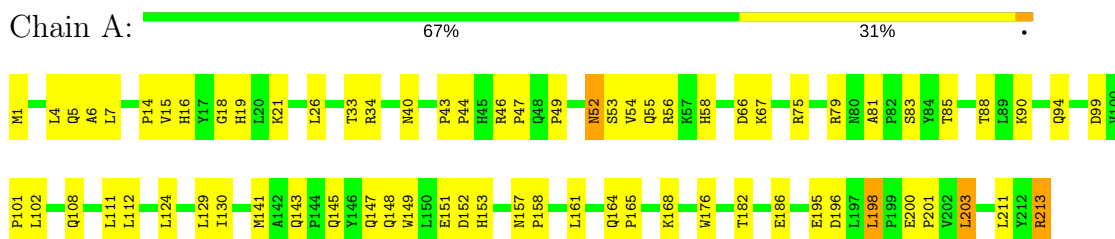
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total	O	0	0
			165	165		
4	B	175	Total	O	0	0
			175	175		
4	C	171	Total	O	0	0
			171	171		

### 3 Residue-property plots

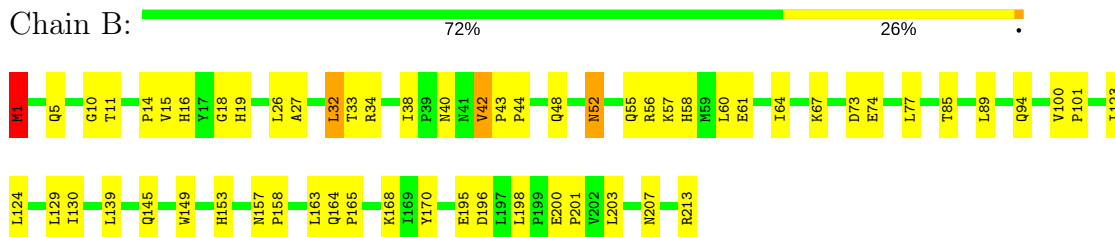
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

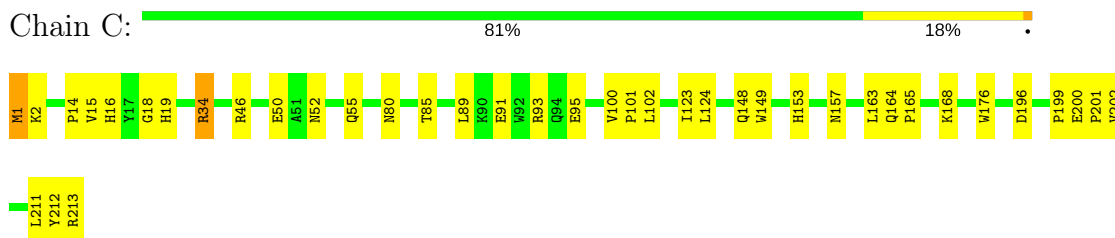
#### • Molecule 1: NaMN adenylyltransferase



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#### • Molecule 1: NaMN adenylyltransferase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.83Å 113.93Å 115.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5881	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	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: NAD, CIT

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	0.52	0/1783	0.70	0/2437
1	B	1.45	2/1783 (0.1%)	1.03	3/2437 (0.1%)
1	C	0.52	0/1783	0.73	0/2437
All	All	0.94	2/5349 (0.0%)	0.83	3/7311 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CG-SD	45.16	2.98	1.81
1	B	1	MET	CB-CG	35.80	2.65	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MET	CG-SD-CE	31.76	151.02	100.20
1	B	1	MET	CB-CG-SD	-16.99	61.44	112.40
1	B	1	MET	CA-CB-CG	-5.82	103.40	113.30

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	A	1733	0	1708	86	0
1	B	1733	0	1708	69	0
1	C	1733	0	1708	43	0
2	A	44	0	26	1	0
2	B	44	0	26	2	0
2	C	44	0	26	1	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
4	A	165	0	0	25	0
4	B	175	0	0	16	0
4	C	171	0	0	10	0
All	All	5881	0	5217	188	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 18.

All (188) 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:34:ARG:CZ	4:B:617:HOH:O	2.05	1.03
1:A:34:ARG:HD2	4:A:684:HOH:O	1.56	1.03
1:A:83:SER:HB2	4:A:737:HOH:O	1.62	0.97
1:A:4:LEU:HD22	4:A:750:HOH:O	1.66	0.95
1:B:157:ASN:HB2	4:B:642:HOH:O	1.66	0.94
1:B:1:MET:HG2	4:B:727:HOH:O	1.70	0.92
1:C:157:ASN:HB2	4:C:708:HOH:O	1.72	0.90
1:A:16:HIS:HD2	1:A:18:GLY:H	1.22	0.87
1:A:52:ASN:C	1:A:52:ASN:HD22	1.77	0.87
1:A:196:ASP:CG	1:B:34:ARG:HG3	1.95	0.86
1:A:34:ARG:HG3	1:C:196:ASP:CG	1.97	0.84
1:B:16:HIS:HD2	1:B:18:GLY:H	1.25	0.83
1:A:157:ASN:HB2	4:A:743:HOH:O	1.79	0.82
1:A:129:LEU:HB2	4:A:741:HOH:O	1.80	0.82
1:A:52:ASN:ND2	1:A:55:GLN:H	1.78	0.82
1:A:52:ASN:HD21	1:A:55:GLN:H	1.29	0.81
1:B:163:LEU:HD12	4:B:765:HOH:O	1.80	0.80
1:B:42:VAL:HG21	1:B:48:GLN:HE22	1.47	0.80
1:B:67:LYS:HE3	4:B:750:HOH:O	1.82	0.80
1:C:52:ASN:H	1:C:55:GLN:HE21	1.31	0.79
1:C:91:GLU:O	1:C:95:GLU:HG3	1.83	0.79
1:C:124:LEU:HD23	4:C:696:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:NH2	4:B:636:HOH:O	2.18	0.76
1:C:213:ARG:HG2	4:C:693:HOH:O	1.87	0.74
1:C:16:HIS:HD2	1:C:18:GLY:H	1.33	0.74
1:C:46:ARG:HD3	4:C:647:HOH:O	1.88	0.73
1:B:1:MET:CB	1:B:1:MET:CG	2.65	0.73
1:A:16:HIS:HD2	1:A:18:GLY:N	1.86	0.73
1:B:16:HIS:HD2	1:B:18:GLY:N	1.86	0.72
1:C:16:HIS:H	1:C:19:HIS:HD2	1.36	0.71
1:A:44:PRO:HD2	4:A:664:HOH:O	1.90	0.71
1:C:34:ARG:HH11	1:C:34:ARG:HB2	1.55	0.71
1:A:54:VAL:HG23	4:A:758:HOH:O	1.89	0.70
1:B:34:ARG:NH2	4:B:617:HOH:O	2.17	0.69
1:A:196:ASP:OD1	1:B:34:ARG:HG3	1.93	0.68
1:B:42:VAL:HG23	4:B:723:HOH:O	1.95	0.67
1:A:198:LEU:HD21	1:A:203:LEU:HG	1.77	0.66
1:A:44:PRO:HG2	4:A:626:HOH:O	1.94	0.66
1:C:34:ARG:HB2	1:C:34:ARG:NH1	2.10	0.66
1:C:80:ASN:HB3	4:C:705:HOH:O	1.96	0.66
1:A:101:PRO:HA	1:A:165:PRO:HA	1.78	0.66
1:C:164:GLN:HG3	4:C:700:HOH:O	1.96	0.66
1:A:55:GLN:NE2	1:A:211:LEU:HD21	2.11	0.65
1:A:148:GLN:NE2	1:A:152:ASP:OD1	2.29	0.65
1:B:1:MET:N	4:B:638:HOH:O	2.29	0.65
1:A:16:HIS:H	1:A:19:HIS:HD2	1.45	0.64
1:A:129:LEU:HD13	4:A:741:HOH:O	1.97	0.64
1:A:58:HIS:HE1	4:A:652:HOH:O	1.80	0.64
1:B:52:ASN:ND2	1:B:55:GLN:H	1.95	0.64
1:C:164:GLN:HE22	1:C:168:LYS:HE2	1.61	0.64
1:C:16:HIS:HD2	1:C:18:GLY:N	1.97	0.63
1:C:34:ARG:HG3	4:C:694:HOH:O	1.98	0.63
1:A:26:LEU:HD21	1:A:130:ILE:HG21	1.81	0.63
1:B:164:GLN:HE22	1:B:168:LYS:HE2	1.63	0.63
1:B:40:ASN:CG	1:B:43:PRO:HG3	2.18	0.62
1:B:195:GLU:O	4:B:646:HOH:O	2.16	0.62
1:A:108:GLN:O	1:A:112:LEU:HD13	2.00	0.61
1:A:52:ASN:ND2	1:A:52:ASN:C	2.49	0.61
1:A:213:ARG:NH2	4:A:740:HOH:O	2.33	0.61
1:B:149:TRP:O	1:B:153:HIS:HD2	1.83	0.61
1:B:42:VAL:HG21	1:B:48:GLN:NE2	2.14	0.60
1:B:1:MET:CB	1:B:1:MET:SD	2.89	0.60
1:A:75:ARG:HD2	1:A:88:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ARG:CZ	4:A:756:HOH:O	2.48	0.60
1:B:195:GLU:O	1:B:196:ASP:HB2	2.01	0.60
1:A:66:ASP:HB3	4:A:742:HOH:O	2.01	0.59
1:A:16:HIS:CD2	1:A:18:GLY:H	2.12	0.59
1:C:200:GLU:HB3	1:C:201:PRO:HD3	1.84	0.59
1:A:143:GLN:NE2	1:A:145:GLN:HE21	2.01	0.59
1:A:149:TRP:O	1:A:153:HIS:HD2	1.85	0.58
1:A:161:LEU:C	4:A:750:HOH:O	2.41	0.58
1:B:198:LEU:HD21	1:B:203:LEU:HG	1.83	0.58
1:B:40:ASN:ND2	1:B:43:PRO:HG3	2.18	0.58
1:A:90:LYS:O	1:A:94:GLN:HG3	2.03	0.58
1:B:94:GLN:HB3	4:B:714:HOH:O	2.03	0.57
1:B:57:LYS:NZ	1:B:74:GLU:OE1	2.37	0.57
1:B:16:HIS:CD2	1:B:18:GLY:H	2.13	0.57
1:B:52:ASN:HD22	1:B:52:ASN:C	2.08	0.56
1:A:1:MET:HG3	1:A:101:PRO:HG3	1.88	0.56
1:A:147:GLN:O	1:A:151:GLU:HG3	2.06	0.55
1:A:83:SER:HB3	4:A:733:HOH:O	2.07	0.55
1:A:46:ARG:HB2	1:A:47:PRO:HD2	1.87	0.55
1:B:89:LEU:HD12	1:B:123:ILE:HG23	1.90	0.54
1:B:1:MET:SD	1:B:1:MET:HB3	2.48	0.54
1:A:16:HIS:H	1:A:19:HIS:CD2	2.24	0.54
1:A:34:ARG:HG3	1:C:196:ASP:OD1	2.08	0.54
1:A:164:GLN:HE22	1:A:168:LYS:HE2	1.71	0.54
1:C:101:PRO:HA	1:C:165:PRO:HA	1.90	0.53
1:A:182:THR:O	1:A:186:GLU:HG3	2.08	0.53
1:A:79:ARG:HG2	1:A:81:ALA:O	2.08	0.53
1:A:111:LEU:HG	1:A:141:MET:HE3	1.90	0.53
1:B:207:ASN:OD1	1:B:213:ARG:NH2	2.34	0.53
1:B:1:MET:CE	1:B:101:PRO:HG3	2.39	0.53
1:C:124:LEU:CD2	4:C:696:HOH:O	2.51	0.52
1:B:16:HIS:H	1:B:19:HIS:HD2	1.57	0.52
1:B:5:GLN:NE2	1:B:100:VAL:HG11	2.24	0.52
1:B:1:MET:CG	1:B:1:MET:SD	2.98	0.52
1:B:48:GLN:HB3	4:B:718:HOH:O	2.10	0.52
1:B:26:LEU:HD21	1:B:130:ILE:HG21	1.92	0.52
1:C:149:TRP:O	1:C:153:HIS:HD2	1.92	0.52
1:A:200:GLU:N	1:A:201:PRO:CD	2.74	0.51
1:A:5:GLN:HB2	1:A:102:LEU:HD12	1.93	0.51
1:B:85:THR:H	2:B:602:NAD:H71N	1.58	0.51
1:C:16:HIS:H	1:C:19:HIS:CD2	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HA	4:A:689:HOH:O	2.11	0.50
1:A:148:GLN:HE21	1:A:152:ASP:CG	2.14	0.50
1:B:139:LEU:N	1:B:139:LEU:HD12	2.27	0.50
1:B:195:GLU:O	1:B:196:ASP:CB	2.60	0.50
1:B:52:ASN:H	1:B:55:GLN:HE21	1.58	0.50
1:A:21:LYS:HE3	1:B:33:THR:HG22	1.94	0.49
1:A:67:LYS:HE2	4:A:680:HOH:O	2.13	0.49
1:A:143:GLN:NE2	1:A:145:GLN:NE2	2.61	0.48
1:A:44:PRO:CG	4:A:626:HOH:O	2.57	0.48
1:A:34:ARG:NH2	4:A:619:HOH:O	2.38	0.48
1:B:5:GLN:HA	4:B:633:HOH:O	2.13	0.48
1:A:1:MET:HE3	1:A:99:ASP:O	2.14	0.48
1:B:27:ALA:HA	1:B:32:LEU:HB2	1.96	0.48
1:C:52:ASN:H	1:C:55:GLN:NE2	2.06	0.48
1:A:52:ASN:H	1:A:55:GLN:HE21	1.62	0.48
1:C:93:ARG:NH2	1:C:102:LEU:HD13	2.29	0.48
1:A:1:MET:CE	1:A:101:PRO:HG3	2.45	0.47
1:B:60:LEU:O	1:B:64:ILE:HG12	2.14	0.47
1:A:34:ARG:NE	4:A:619:HOH:O	2.31	0.47
1:B:52:ASN:H	1:B:55:GLN:NE2	2.12	0.47
1:A:33:THR:O	1:A:34:ARG:HG2	2.15	0.46
1:B:124:LEU:HD21	1:B:129:LEU:HD13	1.97	0.46
1:A:1:MET:N	4:A:640:HOH:O	2.47	0.46
1:C:89:LEU:CD1	1:C:123:ILE:HG23	2.46	0.46
1:B:5:GLN:HE21	1:B:100:VAL:HG11	1.81	0.46
1:A:6:ALA:O	1:A:7:LEU:HD23	2.16	0.46
1:A:124:LEU:CD2	4:A:741:HOH:O	2.64	0.45
1:A:40:ASN:CG	1:A:43:PRO:HG3	2.36	0.45
1:B:15:VAL:HA	1:B:19:HIS:CD2	2.51	0.45
1:B:57:LYS:O	1:B:61:GLU:HG3	2.17	0.45
1:C:163:LEU:HB2	4:C:700:HOH:O	2.15	0.45
1:C:1:MET:HE3	1:C:101:PRO:HD3	1.98	0.45
1:B:16:HIS:H	1:B:19:HIS:CD2	2.35	0.45
1:B:15:VAL:HA	1:B:19:HIS:HD2	1.81	0.45
1:A:34:ARG:HG3	1:C:196:ASP:CB	2.47	0.45
1:C:100:VAL:HG12	1:C:102:LEU:HD12	1.99	0.45
1:C:211:LEU:O	1:C:213:ARG:N	2.46	0.45
1:B:1:MET:HE1	1:B:165:PRO:HA	2.00	0.44
1:B:43:PRO:HA	1:B:44:PRO:HD3	1.82	0.44
1:B:58:HIS:CE1	4:B:657:HOH:O	2.70	0.44
1:C:164:GLN:HE22	1:C:168:LYS:CE	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:HIS:CD2	1:C:18:GLY:H	2.24	0.44
1:A:34:ARG:NE	4:A:756:HOH:O	2.50	0.44
1:A:16:HIS:N	1:A:19:HIS:HD2	2.14	0.44
1:A:1:MET:HE2	1:A:101:PRO:HG3	1.99	0.44
1:A:108:GLN:HE21	1:A:112:LEU:HD11	1.83	0.44
1:B:42:VAL:CG2	1:B:48:GLN:NE2	2.78	0.44
1:B:200:GLU:N	1:B:201:PRO:HD2	2.33	0.44
1:B:16:HIS:CD2	1:B:18:GLY:N	2.76	0.43
1:A:85:THR:H	2:A:601:NAD:H71N	1.67	0.43
1:B:34:ARG:NE	4:B:617:HOH:O	2.35	0.43
1:A:52:ASN:HD21	1:A:55:GLN:N	2.08	0.43
1:A:143:GLN:HE21	1:A:145:GLN:HE21	1.67	0.43
1:A:176:TRP:CH2	1:B:158:PRO:HG2	2.53	0.43
1:A:34:ARG:NE	1:C:196:ASP:OD1	2.52	0.43
1:C:15:VAL:HG13	1:C:15:VAL:O	2.18	0.43
1:C:100:VAL:O	1:C:102:LEU:HD13	2.19	0.43
1:C:149:TRP:O	1:C:153:HIS:CD2	2.70	0.43
1:A:55:GLN:HE22	1:A:211:LEU:HD21	1.82	0.42
1:A:33:THR:C	1:A:34:ARG:HG2	2.39	0.42
1:B:52:ASN:HD22	1:B:55:GLN:H	1.63	0.42
1:A:158:PRO:HG2	1:C:176:TRP:CH2	2.54	0.42
1:A:66:ASP:CB	4:A:742:HOH:O	2.62	0.42
1:A:15:VAL:HA	1:A:19:HIS:CD2	2.54	0.42
1:B:1:MET:HE1	1:B:101:PRO:HG3	2.02	0.42
1:C:1:MET:HE2	1:C:101:PRO:HG3	2.01	0.42
1:A:49:PRO:HG3	1:A:56:ARG:HH21	1.84	0.42
1:C:85:THR:H	2:C:603:NAD:H71N	1.67	0.42
1:C:93:ARG:HH22	1:C:102:LEU:HD13	1.84	0.42
1:A:196:ASP:OD1	1:B:34:ARG:CG	2.66	0.42
1:A:49:PRO:CG	1:A:56:ARG:HH21	2.34	0.41
1:A:211:LEU:O	1:A:213:ARG:HG2	2.20	0.41
1:A:33:THR:O	1:A:34:ARG:HD3	2.20	0.41
1:C:1:MET:CE	1:C:101:PRO:HG3	2.51	0.41
1:B:10:GLY:HA2	2:B:602:NAD:H3D	2.01	0.41
1:A:195:GLU:HG2	4:B:617:HOH:O	2.21	0.41
1:B:11:THR:O	1:B:56:ARG:HD2	2.21	0.41
1:B:158:PRO:HD3	1:B:170:TYR:CE1	2.56	0.41
1:B:40:ASN:ND2	1:B:43:PRO:CG	2.83	0.41
1:B:38:ILE:HG12	1:B:73:ASP:HB3	2.03	0.41
1:C:199:PRO:HB2	1:C:202:VAL:HG23	2.01	0.41
1:A:34:ARG:NH1	4:A:647:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.34	0.40
1:C:2:LYS:HB3	4:C:777:HOH:O	2.20	0.40

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	Percentiles	
1	A	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
1	B	211/213 (99%)	207 (98%)	3 (1%)	1 (0%)	32	20
1	C	211/213 (99%)	208 (99%)	2 (1%)	1 (0%)	32	20
All	All	633/639 (99%)	622 (98%)	9 (1%)	2 (0%)	44	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	212	TYR
1	B	42	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/190 (100%)	184 (97%)	6 (3%)	44	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	190/190 (100%)	184 (97%)	6 (3%)	44	34
1	C	190/190 (100%)	185 (97%)	5 (3%)	51	43
All	All	570/570 (100%)	553 (97%)	17 (3%)	46	37

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	52	ASN
1	A	53	SER
1	A	198	LEU
1	A	203	LEU
1	A	213	ARG
1	B	1	MET
1	B	14	PRO
1	B	32	LEU
1	B	52	ASN
1	B	77	LEU
1	B	145	GLN
1	C	1	MET
1	C	14	PRO
1	C	34	ARG
1	C	50	GLU
1	C	148	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	19	HIS
1	A	52	ASN
1	A	55	GLN
1	A	58	HIS
1	A	143	GLN
1	A	148	GLN
1	A	153	HIS
1	A	164	GLN
1	A	208	GLN
1	B	5	GLN
1	B	16	HIS

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Mol	Chain	Res	Type
1	B	19	HIS
1	B	48	GLN
1	B	52	ASN
1	B	55	GLN
1	B	80	ASN
1	B	94	GLN
1	B	153	HIS
1	B	164	GLN
1	B	208	GLN
1	C	16	HIS
1	C	19	HIS
1	C	55	GLN
1	C	58	HIS
1	C	143	GLN
1	C	145	GLN
1	C	153	HIS
1	C	164	GLN
1	C	189	GLN
1	C	208	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAD	A	601	-	41,48,48	2.02	6 (14%)	43,73,73	1.60	8 (18%)
3	CIT	A	604	-	3,12,12	0.76	0	3,17,17	3.33	2 (66%)
2	NAD	B	602	-	41,48,48	2.01	7 (17%)	43,73,73	1.53	6 (13%)
3	CIT	B	605	-	3,12,12	0.90	0	3,17,17	3.17	2 (66%)
2	NAD	C	603	-	41,48,48	1.83	5 (12%)	43,73,73	1.60	8 (18%)
3	CIT	C	606	-	3,12,12	0.45	0	3,17,17	2.87	2 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	601	-	-	0/22/62/62	0/5/5/5
3	CIT	A	604	-	-	0/6/16/16	0/0/0/0
2	NAD	B	602	-	-	0/22/62/62	0/5/5/5
3	CIT	B	605	-	-	0/6/16/16	0/0/0/0
2	NAD	C	603	-	-	0/22/62/62	0/5/5/5
3	CIT	C	606	-	-	0/6/16/16	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAD	O4B-C1B	-3.18	1.36	1.41
2	A	601	NAD	O4B-C1B	-2.37	1.38	1.41
2	C	603	NAD	C2D-C1D	-2.19	1.50	1.53
2	B	602	NAD	C6N-C5N	-2.10	1.34	1.38
2	B	602	NAD	C2A-N1A	2.36	1.38	1.33
2	A	601	NAD	C2A-N1A	2.42	1.38	1.33
2	C	603	NAD	C6N-N1N	2.77	1.42	1.35
2	B	602	NAD	C6N-N1N	3.48	1.44	1.35
2	A	601	NAD	C6N-N1N	3.73	1.45	1.35
2	A	601	NAD	C2N-C3N	4.68	1.46	1.39
2	C	603	NAD	C2N-C3N	4.68	1.46	1.39
2	B	602	NAD	C2N-C3N	4.94	1.46	1.39
2	B	602	NAD	C4N-C3N	5.65	1.48	1.39
2	A	601	NAD	C4N-C3N	5.75	1.48	1.39
2	C	603	NAD	C4N-C3N	5.87	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	603	NAD	C5N-C4N	6.83	1.52	1.38
2	B	602	NAD	C5N-C4N	7.18	1.52	1.38
2	A	601	NAD	C5N-C4N	7.66	1.53	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	NAD	O7N-C7N-C3N	-4.83	113.97	119.62
2	A	601	NAD	O7N-C7N-C3N	-4.83	113.97	119.62
2	B	602	NAD	O7N-C7N-C3N	-4.77	114.05	119.62
2	C	603	NAD	C5N-C4N-C3N	-4.50	115.06	120.35
2	B	602	NAD	C5N-C4N-C3N	-3.83	115.85	120.35
2	A	601	NAD	C5N-C4N-C3N	-3.68	116.02	120.35
2	A	601	NAD	N3A-C2A-N1A	-2.20	126.94	128.86
2	C	603	NAD	C4D-O4D-C1D	-2.14	107.50	109.77
2	C	603	NAD	N3A-C2A-N1A	-2.10	127.03	128.86
2	B	602	NAD	C4B-O4B-C1B	2.08	111.98	109.77
2	A	601	NAD	C3N-C2N-N1N	2.11	122.55	120.43
2	C	603	NAD	C3N-C2N-N1N	2.21	122.65	120.43
2	A	601	NAD	C5N-C6N-N1N	2.25	123.86	120.40
2	A	601	NAD	C4A-C5A-N7A	2.40	111.72	109.41
2	B	602	NAD	C5N-C6N-N1N	2.43	124.14	120.40
2	B	602	NAD	C4A-C5A-N7A	2.43	111.76	109.41
2	C	603	NAD	C5N-C6N-N1N	2.56	124.34	120.40
3	A	604	CIT	C3-C2-C1	2.74	119.23	114.95
2	A	601	NAD	C4B-O4B-C1B	2.82	112.78	109.77
2	C	603	NAD	C4A-C5A-N7A	3.01	112.32	109.41
3	C	606	CIT	C3-C2-C1	3.17	119.90	114.95
3	B	605	CIT	C3-C2-C1	3.19	119.93	114.95
3	C	606	CIT	C3-C4-C5	3.65	120.65	114.95
2	C	603	NAD	C3N-C7N-N7N	4.12	122.48	117.77
2	B	602	NAD	C3N-C7N-N7N	4.13	122.49	117.77
3	B	605	CIT	C3-C4-C5	4.42	121.85	114.95
2	A	601	NAD	C3N-C7N-N7N	4.98	123.47	117.77
3	A	604	CIT	C3-C4-C5	5.00	122.76	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAD	1	0
2	B	602	NAD	2	0
2	C	603	NAD	1	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.