



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 12:04 pm GMT

PDB ID : 6C8Q
Title : Crystal structure of NAD synthetase (NadE) from *Enterococcus faecalis* in complex with NAD⁺
Authors : Stogios, P.J.; Skarina, T.; McChesney, C.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-01-25
Resolution : 2.58 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

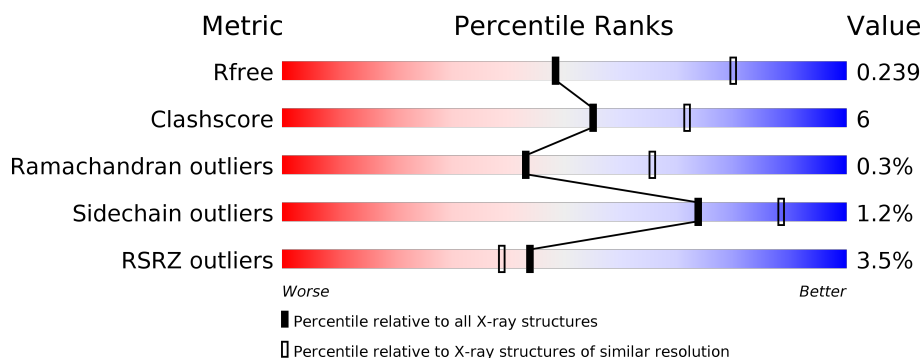
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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))
R_{free}	111664	3182 (2.60-2.56)
Clashscore	122126	3541 (2.60-2.56)
Ramachandran outliers	120053	3489 (2.60-2.56)
Sidechain outliers	120020	3489 (2.60-2.56)
RSRZ outliers	108989	3120 (2.60-2.56)

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. 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.

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 88%, yellow 88%, yellow 99%, grey 99%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 0% 88% 9% • </div> </div>
1	B	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 91%, yellow 91%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 91% 6% • </div> </div>
1	C	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 86%, yellow 86%, yellow 95%, grey 95%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 86% 9% • • </div> </div>
1	D	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 83%, yellow 83%, yellow 96%, grey 96%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 83% 13% • </div> </div>
1	E	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, green 3%, green 83%, yellow 83%, yellow 96%, grey 96%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 83% 13% • </div> </div>
1	F	275	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 8%, green 8%, green 68%, yellow 68%, yellow 95%, grey 95%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 8% 68% 27% • • </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	275	 3% 84% 12% •
1	H	275	 3% 86% 11% •

2 Entry composition

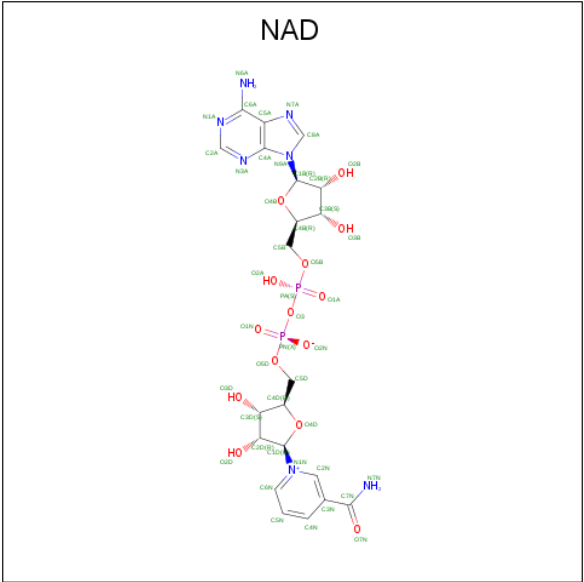
There are 3 unique types of molecules in this entry. The entry contains 17889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NH(3)-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	1	0
			2099	1336	351	406	6			
1	B	266	Total	C	N	O	S	0	1	0
			2082	1328	349	398	7			
1	C	265	Total	C	N	O	S	0	2	0
			2075	1322	348	398	7			
1	D	264	Total	C	N	O	S	0	1	0
			2063	1313	346	398	6			
1	E	263	Total	C	N	O	S	0	1	0
			2055	1307	344	397	7			
1	F	264	Total	C	N	O	S	0	2	0
			2072	1321	348	396	7			
1	G	265	Total	C	N	O	S	0	1	0
			2074	1323	348	397	6			
1	H	267	Total	C	N	O	S	0	2	0
			2094	1337	350	401	6			

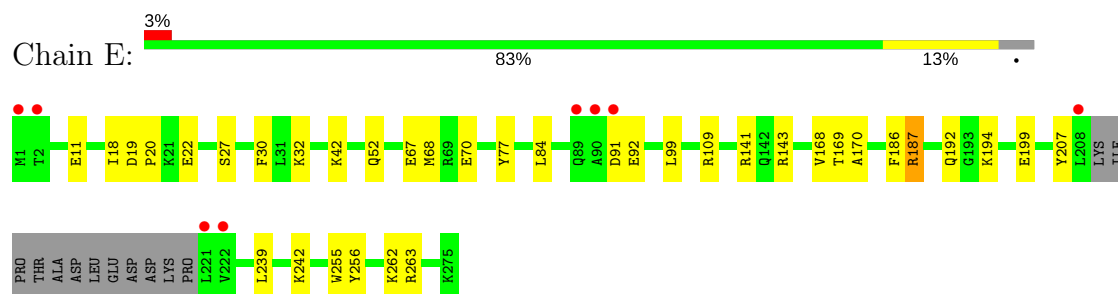
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



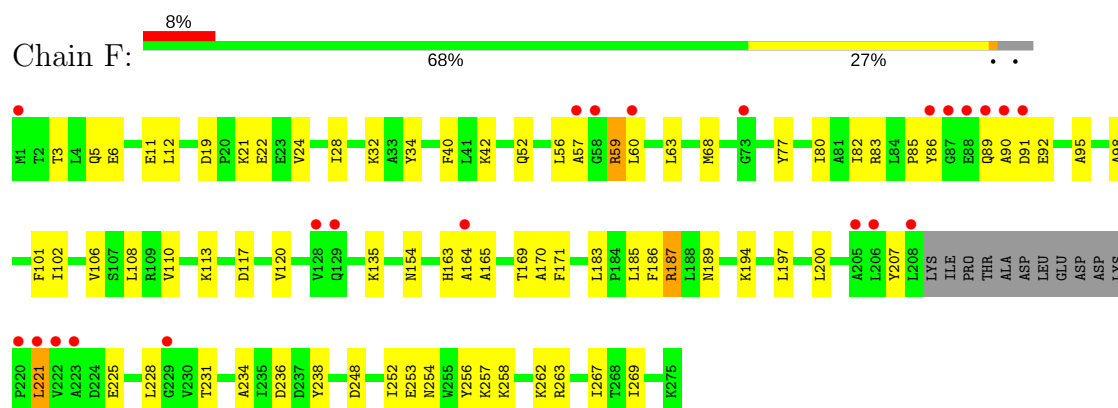
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	128	Total 130	O 130	0	2
3	F	42	Total 43	O 43	0	1
3	G	120	Total 121	O 121	0	1
3	H	127	Total 127	O 127	0	0

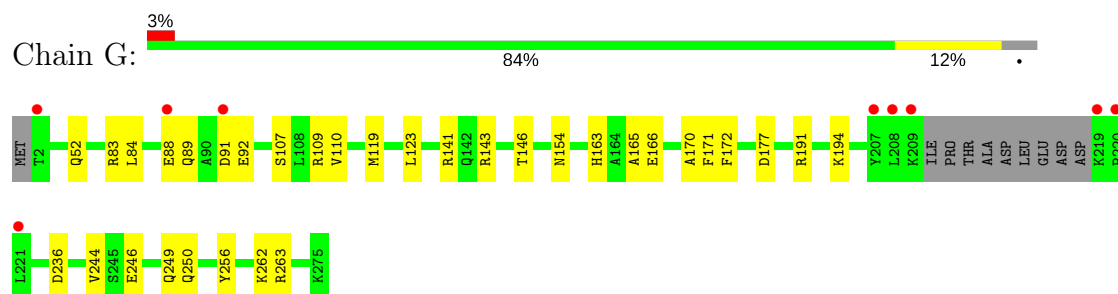
• Molecule 1: NH(3)-dependent NAD(+) synthetase



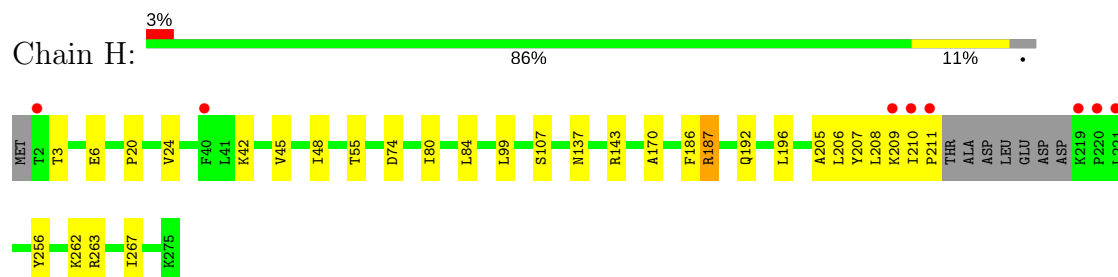
• Molecule 1: NH(3)-dependent NAD(+) synthetase



• Molecule 1: NH(3)-dependent NAD(+) synthetase



• Molecule 1: NH(3)-dependent NAD(+) synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.44Å 85.17Å 175.81Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	24.78 – 2.58 24.78 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.78-2.58) 89.9 (24.78-2.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.26 (at 2.57Å)	Xtriage
Refinement program	PHENIX (dev_2733: ???)	Depositor
R, R_{free}	0.188 , 0.239 0.187 , 0.239	Depositor DCC
R_{free} test set	2020 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17889	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2139	0.41	0/2887
1	B	0.25	0/2122	0.40	0/2863
1	C	0.24	0/2117	0.40	0/2858
1	D	0.24	0/2102	0.42	0/2838
1	E	0.25	0/2093	0.41	0/2825
1	F	0.27	0/2115	0.47	0/2854
1	G	0.29	0/2114	0.42	0/2853
1	H	0.25	0/2138	0.40	0/2887
All	All	0.25	0/16940	0.42	0/22865

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	A	2099	0	2094	17	0
1	B	2082	0	2092	13	0
1	C	2075	0	2087	18	0
1	D	2063	0	2064	24	0
1	E	2055	0	2056	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2072	0	2080	62	0
1	G	2074	0	2080	22	0
1	H	2094	0	2102	18	0
2	A	44	0	24	3	0
2	B	44	0	24	2	0
2	C	44	0	24	1	0
2	D	35	0	17	2	0
2	E	36	0	18	2	0
2	F	44	0	24	1	0
2	G	44	0	24	3	0
2	H	44	0	24	2	0
3	A	174	0	0	1	0
3	B	136	0	0	2	0
3	C	128	0	0	1	0
3	D	81	0	0	1	0
3	E	130	0	0	1	0
3	F	43	0	0	0	0
3	G	121	0	0	1	0
3	H	127	0	0	0	0
All	All	17889	0	16834	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 6.

The worst 5 of 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)
2:B:301:NAD:C1D	2:B:301:NAD:O4D	1.63	1.23
2:B:301:NAD:O4B	2:B:301:NAD:C1B	1.63	1.23
2:G:301:NAD:O4B	2:G:301:NAD:C1B	1.64	1.22
2:F:301:NAD:O4B	2:F:301:NAD:C1B	1.63	1.21
2:E:301:NAD:O4B	2:E:301:NAD:C1B	1.63	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	265/275 (96%)	263 (99%)	1 (0%)	1 (0%)	36	59
1	B	263/275 (96%)	257 (98%)	5 (2%)	1 (0%)	36	59
1	C	263/275 (96%)	255 (97%)	7 (3%)	1 (0%)	36	59
1	D	261/275 (95%)	252 (97%)	8 (3%)	1 (0%)	36	59
1	E	260/275 (94%)	255 (98%)	4 (2%)	1 (0%)	36	59
1	F	262/275 (95%)	251 (96%)	10 (4%)	1 (0%)	36	59
1	G	262/275 (95%)	255 (97%)	7 (3%)	0	100	100
1	H	265/275 (96%)	256 (97%)	8 (3%)	1 (0%)	36	59
All	All	2101/2200 (96%)	2044 (97%)	50 (2%)	7 (0%)	43	65

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	ARG
1	H	187	ARG
1	A	187	ARG
1	B	187	ARG
1	D	187	ARG

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	219/224 (98%)	218 (100%)	1 (0%)	90	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	217/224 (97%)	216 (100%)	1 (0%)	90	96
1	C	217/224 (97%)	212 (98%)	5 (2%)	53	76
1	D	215/224 (96%)	213 (99%)	2 (1%)	81	92
1	E	214/224 (96%)	212 (99%)	2 (1%)	81	92
1	F	216/224 (96%)	212 (98%)	4 (2%)	60	80
1	G	216/224 (96%)	211 (98%)	5 (2%)	53	76
1	H	219/224 (98%)	218 (100%)	1 (0%)	90	96
All	All	1733/1792 (97%)	1712 (99%)	21 (1%)	74	88

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	27	SER
1	F	21	LYS
1	G	91	ASP
1	D	46	LEU
1	G	92	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	142	GLN
1	G	250	GLN
1	H	142	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

8 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	301	-	40,48,48	4.36	13 (32%)	44,73,73	2.14	6 (13%)
2	NAD	B	301	-	40,48,48	4.41	13 (32%)	44,73,73	2.12	6 (13%)
2	NAD	C	301	-	40,48,48	4.40	13 (32%)	44,73,73	2.10	6 (13%)
2	NAD	D	301	-	33,38,48	4.49	12 (36%)	34,58,73	2.40	5 (14%)
2	NAD	E	301	-	33,39,48	4.13	12 (36%)	36,60,73	2.31	5 (13%)
2	NAD	F	301	-	40,48,48	4.37	13 (32%)	44,73,73	2.21	6 (13%)
2	NAD	G	301	-	40,48,48	4.37	13 (32%)	44,73,73	2.18	6 (13%)
2	NAD	H	301	-	40,48,48	4.37	13 (32%)	44,73,73	2.14	5 (11%)

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	301	-	-	0/22/62/62	0/5/5/5
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
2	NAD	C	301	-	-	0/22/62/62	0/5/5/5
2	NAD	D	301	-	-	0/18/51/62	0/4/4/5
2	NAD	E	301	-	-	0/18/54/62	0/4/4/5
2	NAD	F	301	-	-	0/22/62/62	0/5/5/5
2	NAD	G	301	-	-	0/22/62/62	0/5/5/5
2	NAD	H	301	-	-	0/22/62/62	0/5/5/5

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAD	C1D-C2D	-11.58	1.32	1.51
2	D	301	NAD	O4D-C4D	-7.31	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAD	C2D-C1D	-7.12	1.31	1.53
2	E	301	NAD	O4B-C4B	-7.07	1.29	1.45
2	G	301	NAD	O4B-C4B	-6.91	1.29	1.45

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	NAD	N3A-C2A-N1A	-10.86	119.57	128.86
2	A	301	NAD	N3A-C2A-N1A	-10.82	119.60	128.86
2	F	301	NAD	N3A-C2A-N1A	-10.80	119.62	128.86
2	C	301	NAD	N3A-C2A-N1A	-10.66	119.74	128.86
2	D	301	NAD	N3A-C2A-N1A	-10.64	119.76	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	3	0
2	B	301	NAD	2	0
2	C	301	NAD	1	0
2	D	301	NAD	2	0
2	E	301	NAD	2	0
2	F	301	NAD	1	0
2	G	301	NAD	3	0
2	H	301	NAD	2	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 ⓘ

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, 95th 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	A	268/275 (97%)	-0.45	4 (1%) 73 71	30, 43, 68, 166	0
1	B	266/275 (96%)	-0.34	5 (1%) 66 63	31, 47, 86, 133	0
1	C	265/275 (96%)	-0.33	7 (2%) 56 51	37, 51, 85, 166	0
1	D	264/275 (96%)	0.17	11 (4%) 36 31	46, 74, 116, 186	0
1	E	263/275 (95%)	-0.17	8 (3%) 50 46	34, 54, 88, 162	0
1	F	264/275 (96%)	0.53	22 (8%) 11 9	51, 92, 139, 212	0
1	G	265/275 (96%)	-0.15	9 (3%) 45 40	36, 54, 93, 157	0
1	H	267/275 (97%)	-0.15	8 (2%) 50 46	37, 56, 84, 188	0
All	All	2122/2200 (96%)	-0.11	74 (3%) 44 39	30, 56, 112, 212	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	210	ILE	7.7
1	E	208	LEU	7.0
1	H	211	PRO	6.8
1	E	221	LEU	6.3
1	E	222	VAL	6.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 95th 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	F	301	44/44	0.82	0.29	99,108,136,137	0
2	NAD	E	301	36/44	0.91	0.16	76,89,95,100	0
2	NAD	G	301	44/44	0.94	0.16	56,68,103,107	0
2	NAD	C	301	44/44	0.95	0.13	44,53,77,78	0
2	NAD	D	301	35/44	0.95	0.13	59,67,81,84	0
2	NAD	H	301	44/44	0.95	0.16	41,54,105,112	0
2	NAD	B	301	44/44	0.96	0.14	45,52,89,91	0
2	NAD	A	301	44/44	0.96	0.13	31,44,79,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.