



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 9, 2017 – 11:09 am GMT

PDB ID : 5KMR
Title : The structure of type II NADH dehydrogenase from *Caldalkalibacillus thermarum* complexed with NAD⁺ at 3.0 angstrom resolution.
Authors : Cook, G.M.; Aragao, D.; Nakatani, Y.
Deposited on : 2016-06-27
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	recalc28906
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28906

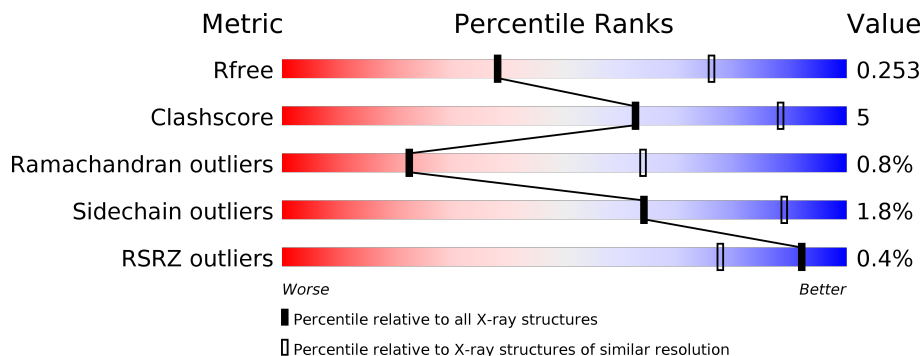
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 ≥ 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	405	<div> <div>80%</div> <div>16%</div> <div>••</div> </div>
1	B	405	<div> <div>85%</div> <div>11%</div> <div>••</div> </div>
1	C	405	<div> <div>%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
1	D	405	<div> <div>86%</div> <div>11%</div> <div>•</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11468 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 FAD-dependent pyridine nucleotide-disulfide oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	394	Total	C	N	O	S	0	0	0
			2845	1823	489	525	8			
1	A	393	Total	C	N	O	S	0	0	0
			2815	1809	485	513	8			
1	C	391	Total	C	N	O	S	0	0	0
			2640	1684	458	491	7			
1	D	394	Total	C	N	O	S	0	0	0
			2807	1798	483	518	8			

There are 24 discrepancies between the modelled and reference sequences:

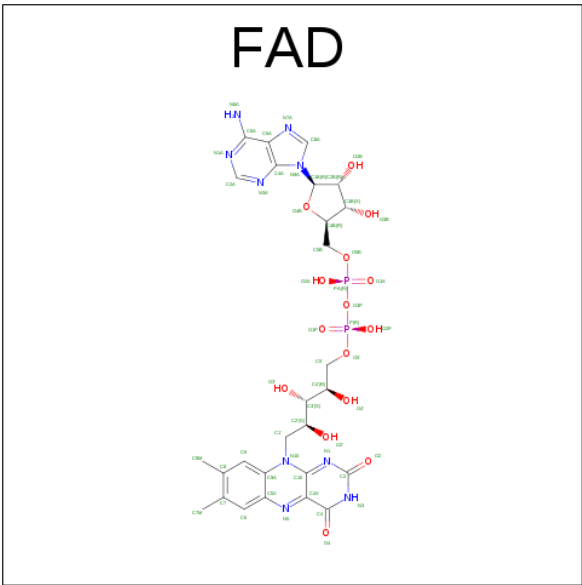
Chain	Residue	Modelled	Actual	Comment	Reference
B	400	HIS	-	expression tag	UNP F5L3B8
B	401	HIS	-	expression tag	UNP F5L3B8
B	402	HIS	-	expression tag	UNP F5L3B8
B	403	HIS	-	expression tag	UNP F5L3B8
B	404	HIS	-	expression tag	UNP F5L3B8
B	405	HIS	-	expression tag	UNP F5L3B8
A	400	HIS	-	expression tag	UNP F5L3B8
A	401	HIS	-	expression tag	UNP F5L3B8
A	402	HIS	-	expression tag	UNP F5L3B8
A	403	HIS	-	expression tag	UNP F5L3B8
A	404	HIS	-	expression tag	UNP F5L3B8
A	405	HIS	-	expression tag	UNP F5L3B8
C	400	HIS	-	expression tag	UNP F5L3B8
C	401	HIS	-	expression tag	UNP F5L3B8
C	402	HIS	-	expression tag	UNP F5L3B8
C	403	HIS	-	expression tag	UNP F5L3B8
C	404	HIS	-	expression tag	UNP F5L3B8
C	405	HIS	-	expression tag	UNP F5L3B8
D	400	HIS	-	expression tag	UNP F5L3B8
D	401	HIS	-	expression tag	UNP F5L3B8
D	402	HIS	-	expression tag	UNP F5L3B8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	403	HIS	-	expression tag	UNP F5L3B8
D	404	HIS	-	expression tag	UNP F5L3B8
D	405	HIS	-	expression tag	UNP F5L3B8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

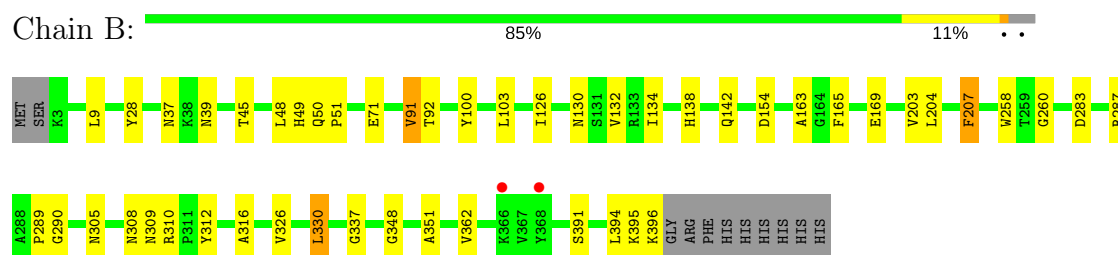
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	O	0	0
			3	3		
4	A	8	Total	O	0	0
			8	8		
4	C	3	Total	O	0	0
			3	3		
4	D	3	Total	O	0	0
			3	3		

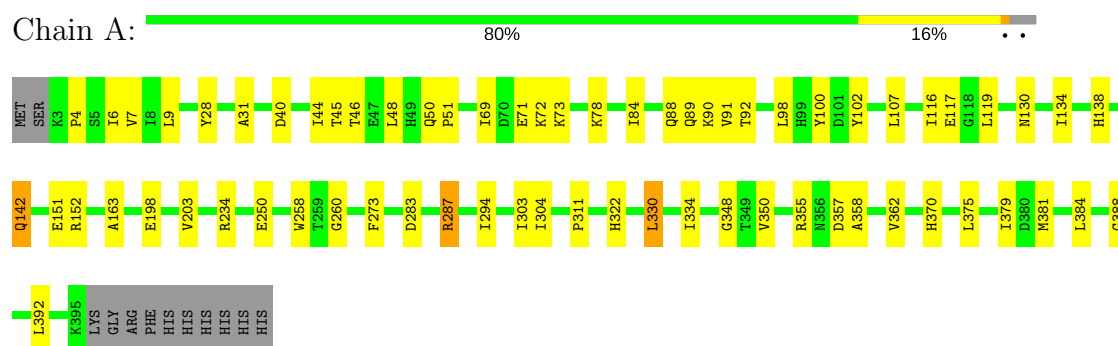
3 Residue-property plots [i](#)

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.

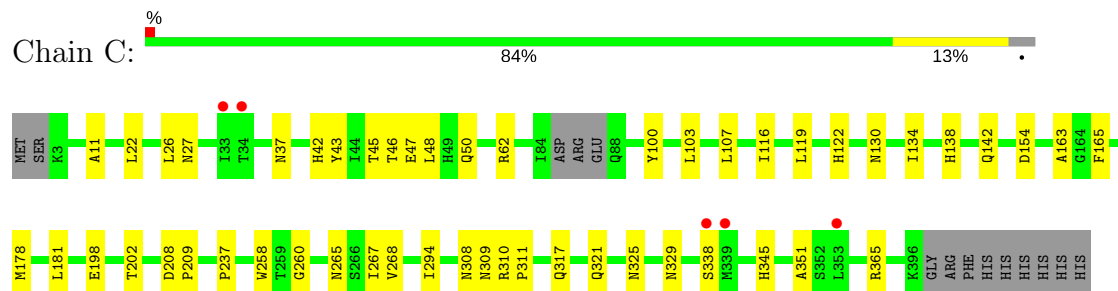
- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase

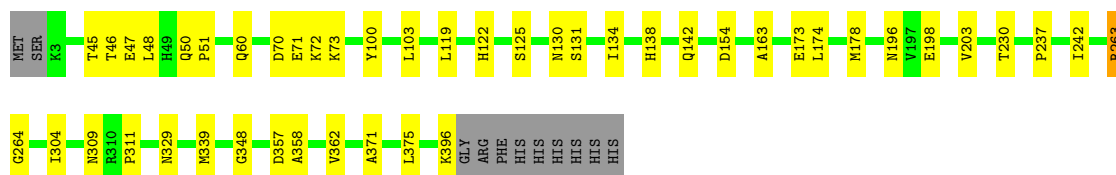


- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.06Å 114.21Å 130.96Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	43.64 – 3.00 43.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.64-3.00) 99.0 (43.64-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.237 , 0.254 0.238 , 0.253	Depositor DCC
R_{free} test set	2132 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11468	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: FAD, 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	0.21	0/2873	0.42	0/3930
1	B	0.21	0/2902	0.42	0/3967
1	C	0.21	0/2688	0.42	0/3689
1	D	0.21	0/2861	0.40	0/3910
All	All	0.21	0/11324	0.42	0/15496

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	2815	0	2681	34	0
1	B	2845	0	2720	23	0
1	C	2640	0	2385	26	0
1	D	2807	0	2678	26	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	44	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	24	0	0
3	D	44	0	25	1	0
4	A	8	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
All	All	11468	0	10662	110	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 110 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:C:11:ALA:H	1:C:37:ASN:HD22	1.32	0.76
1:D:125:SER:O	1:D:131:SER:OG	2.07	0.70
1:C:325:ASN:ND2	1:C:329:ASN:OD1	2.24	0.70
1:C:103:LEU:HB3	1:C:294:ILE:HG13	1.74	0.69
1:A:348:GLY:HA3	1:A:362:VAL:HA	1.76	0.68

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	391/405 (96%)	379 (97%)	9 (2%)	3 (1%)	22 64
1	B	392/405 (97%)	380 (97%)	7 (2%)	5 (1%)	14 51
1	C	387/405 (96%)	378 (98%)	7 (2%)	2 (0%)	32 74
1	D	392/405 (97%)	384 (98%)	6 (2%)	2 (0%)	32 74
All	All	1562/1620 (96%)	1521 (97%)	29 (2%)	12 (1%)	22 64

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	GLU
1	A	89	GLN
1	D	71	GLU
1	B	309	ASN
1	B	337	GLY

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	262/329 (80%)	256 (98%)	6 (2%)	56	85
1	B	270/329 (82%)	265 (98%)	5 (2%)	62	88
1	C	222/329 (68%)	217 (98%)	5 (2%)	56	85
1	D	263/329 (80%)	261 (99%)	2 (1%)	85	95
All	All	1017/1316 (77%)	999 (98%)	18 (2%)	64	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	ARG
1	A	330	LEU
1	C	317	GLN
1	A	142	GLN
1	A	250	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	GLN
1	C	122	HIS
1	D	89	GLN
1	A	370	HIS
1	D	88	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 ⓘ

7 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	FAD	A	601	-	51,58,58	4.09	18 (35%)	54,89,89	2.71	12 (22%)
3	NAD	A	602	-	41,48,48	3.64	14 (34%)	43,73,73	1.64	3 (6%)
2	FAD	B	601	-	51,58,58	4.08	18 (35%)	54,89,89	2.72	11 (20%)
2	FAD	C	601	-	51,58,58	4.08	18 (35%)	54,89,89	2.69	13 (24%)
3	NAD	C	602	-	41,48,48	3.65	14 (34%)	43,73,73	1.59	6 (13%)
2	FAD	D	601	-	51,58,58	4.08	18 (35%)	54,89,89	2.72	12 (22%)
3	NAD	D	602	-	41,48,48	3.65	14 (34%)	43,73,73	1.60	4 (9%)

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	FAD	A	601	-	-	0/28/50/50	0/6/6/6
3	NAD	A	602	-	-	0/22/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	601	-	-	0/28/50/50	0/6/6/6
2	FAD	C	601	-	-	0/28/50/50	0/6/6/6
3	NAD	C	602	-	-	0/22/62/62	0/5/5/5
2	FAD	D	601	-	-	0/28/50/50	0/6/6/6
3	NAD	D	602	-	-	0/22/62/62	0/5/5/5

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C2B-C1B	-15.32	1.29	1.53
2	D	601	FAD	C2B-C1B	-15.29	1.29	1.53
2	B	601	FAD	C2B-C1B	-15.23	1.29	1.53
2	C	601	FAD	C2B-C1B	-15.16	1.29	1.53
3	D	602	NAD	C2D-C3D	-11.13	1.23	1.53

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	N3A-C2A-N1A	-10.31	119.88	128.86
2	D	601	FAD	N3A-C2A-N1A	-10.23	119.95	128.86
2	A	601	FAD	N3A-C2A-N1A	-10.22	119.95	128.86
2	C	601	FAD	N3A-C2A-N1A	-10.10	120.07	128.86
3	D	602	NAD	N3A-C2A-N1A	-8.18	121.74	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	1	0
3	A	602	NAD	2	0
2	B	601	FAD	1	0
2	C	601	FAD	2	0
2	D	601	FAD	1	0
3	D	602	NAD	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	393/405 (97%)	-0.21	0 100 100	50, 73, 102, 117	0
1	B	394/405 (97%)	-0.21	2 (0%) 90 74	52, 73, 97, 125	0
1	C	391/405 (96%)	-0.09	5 (1%) 77 51	58, 84, 114, 127	0
1	D	394/405 (97%)	-0.23	0 100 100	57, 72, 93, 102	0
All	All	1572/1620 (97%)	-0.19	7 (0%) 92 77	50, 75, 105, 127	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	THR	3.6
1	C	33	ILE	3.0
1	C	338	SER	3.0
1	B	366	LYS	2.9
1	B	368	TYR	2.4

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	C	601	53/53	0.94	0.21	-0.07	72,80,87,95	0
3	NAD	C	602	44/44	0.90	0.19	-0.19	79,84,95,105	0
2	FAD	B	601	53/53	0.96	0.18	-0.33	52,59,65,75	0
3	NAD	D	602	44/44	0.93	0.18	-0.43	69,72,78,88	0
2	FAD	D	601	53/53	0.96	0.17	-0.71	57,62,73,77	0
3	NAD	A	602	44/44	0.94	0.17	-0.74	61,66,69,84	0
2	FAD	A	601	53/53	0.95	0.17	-0.79	57,63,73,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.