



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2017 – 05:30 PM EST

PDB ID : 5KMS
Title : The structure of type II NADH dehydrogenase from *Caldalkalibacillus thermarum* complexed with NAD⁺ at 2.5 angstrom resolution.
Authors : Cook, G.M.; Aragao, D.; Nakatani, Y.
Deposited on : 2016-06-27
Resolution : 2.50 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

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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20028442

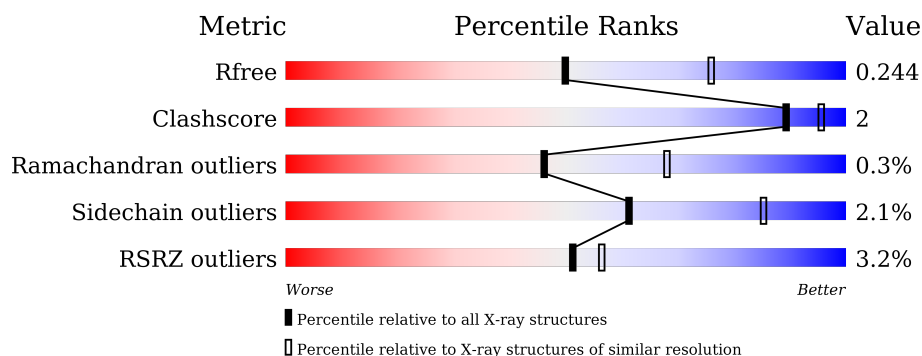
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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></div> <div>90% 7% .</div> </div>
1	B	405	<div> <div></div> <div>90% 7% .</div> </div>
1	C	405	<div> <div>2%</div> <div>92% 5% .</div> </div>
1	D	405	<div> <div>8%</div> <div>88% 9% .</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11969 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	A	394	Total	C	N	O	S	0	0	0
			2897	1859	496	533	9			
1	B	395	Total	C	N	O	S	0	0	0
			2911	1865	497	540	9			
1	C	394	Total	C	N	O	S	0	0	0
			2885	1842	494	541	8			
1	D	395	Total	C	N	O	S	0	0	0
			2805	1801	477	519	8			

There are 24 discrepancies between the modelled and reference sequences:

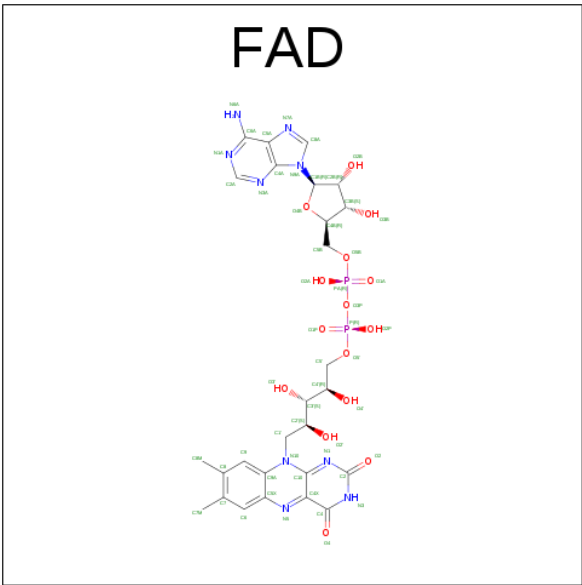
Chain	Residue	Modelled	Actual	Comment	Reference
A	400	HIS	-	expression tag	UNP F5L3B8
A	401	HIS	-	expression tag	UNP F5L3B8
A	402	HIS	-	expression tag	UNP F5L3B8
A	403	HIS	-	expression tag	UNP F5L3B8
A	404	HIS	-	expression tag	UNP F5L3B8
A	405	HIS	-	expression tag	UNP F5L3B8
B	400	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

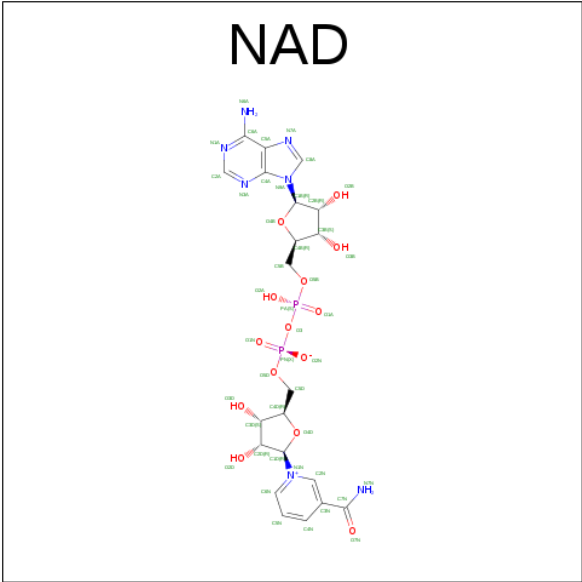
Chain	Residue	Modelled	Actual	Comment	Reference
D	403	HIS	-	expression tag	UNP F5L3B8
D	404	HIS	-	expression tag	UNP F5L3B8
D	405	HIS	-	expression tag	UNP F5L3B8

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



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

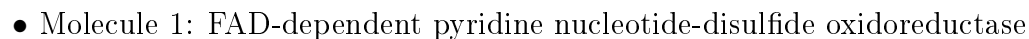


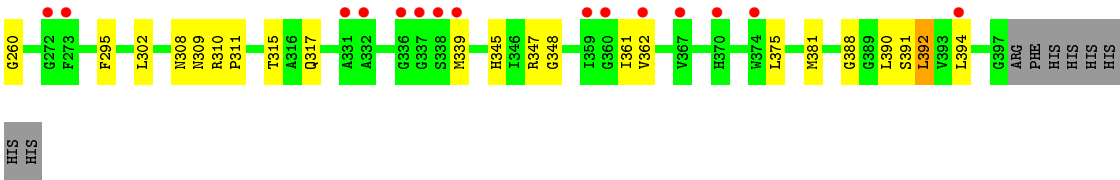
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	62	Total	O	0	0
			62	62		
4	C	62	Total	O	0	0
			62	62		
4	D	31	Total	O	0	0
			31	31		

- 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	72.88Å 114.01Å 130.64Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	47.89 – 2.50 47.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.89-2.50) 100.0 (47.89-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.214 , 0.244 0.216 , 0.244	Depositor DCC
R_{free} test set	3723 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.0	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	0.94	EDS
Total number of atoms	11969	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.22	0/2955	0.42	0/4029
1	B	0.22	0/2970	0.42	0/4050
1	C	0.22	0/2939	0.42	0/4006
1	D	0.22	0/2860	0.42	0/3911
All	All	0.22	0/11724	0.42	0/15996

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	2897	0	2837	14	0
1	B	2911	0	2833	14	0
1	C	2885	0	2810	10	0
1	D	2805	0	2669	18	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
3	A	44	0	24	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	60	0	0	0	0
4	B	62	0	0	0	0
4	C	62	0	0	0	0
4	D	31	0	0	0	0
All	All	11969	0	11297	55	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 2.

All (55) 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:D:89:GLN:NE2	1:D:100:TYR:O	2.22	0.71
1:A:6:ILE:HD11	1:A:334:ILE:HD11	1.77	0.66
1:C:302:LEU:HD11	1:C:311:PRO:HB3	1.79	0.63
1:C:6:ILE:HD11	1:C:334:ILE:HD11	1.85	0.59
1:D:317:GLN:OE1	1:D:347:ARG:N	2.37	0.58
1:B:89:GLN:NE2	1:B:100:TYR:O	2.38	0.56
1:B:201:PRO:HG2	1:C:82:VAL:HG12	1.89	0.54
1:B:79:ASP:HB3	1:B:93:LEU:HD23	1.89	0.53
1:A:302:LEU:HD11	1:A:311:PRO:HB3	1.91	0.53
1:A:89:GLN:NE2	1:A:100:TYR:O	2.42	0.53
1:B:258:TRP:CZ2	1:B:260:GLY:HA3	2.45	0.51
1:D:348:GLY:HA3	1:D:361:ILE:O	2.10	0.51
1:A:50:GLN:OE1	1:A:355:ARG:NH2	2.44	0.51
1:B:215:ALA:HB2	1:B:359:ILE:HD13	1.93	0.50
1:D:11:ALA:O	1:D:42:HIS:ND1	2.45	0.50
1:D:388:GLY:HA3	1:D:392:LEU:HD12	1.96	0.48
1:C:50:GLN:HB2	1:C:51:PRO:HD3	1.97	0.46
1:C:27:ASN:HB2	1:C:30:GLU:HG3	1.98	0.46
1:D:138:HIS:O	1:D:142:GLN:HG2	2.16	0.45
1:A:281:LYS:HB2	1:A:302:LEU:HD23	1.99	0.45
1:C:215:ALA:HB2	1:C:359:ILE:HD13	1.99	0.45
1:A:4:PRO:HD2	1:A:31:ALA:HA	1.99	0.45
1:D:258:TRP:CZ2	1:D:260:GLY:HA3	2.52	0.45
1:D:174:LEU:HD12	1:D:174:LEU:HA	1.89	0.45
1:D:45:THR:HA	1:D:48:LEU:HG	1.99	0.44
1:C:348:GLY:HA3	1:C:361:ILE:O	2.18	0.44
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.84	0.44
1:B:316:ALA:HB2	2:B:601:FAD:H2'	1.99	0.44
1:B:154:ASP:OD1	1:B:154:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:HA	1:C:311:PRO:HD3	1.90	0.43
1:D:308:ASN:C	1:D:310:ARG:H	2.22	0.43
1:B:333:LEU:HB2	1:B:339:MET:HE3	2.01	0.43
1:A:198:GLU:OE1	3:A:602:NAD:O2B	2.37	0.42
1:A:122:HIS:CE1	1:A:237:PRO:HG3	2.54	0.42
1:A:375:LEU:O	1:A:379:ILE:HG13	2.18	0.42
1:A:79:ASP:OD1	1:A:93:LEU:HB3	2.19	0.42
1:B:375:LEU:O	1:B:379:ILE:HG13	2.19	0.42
1:B:11:ALA:O	1:B:42:HIS:ND1	2.52	0.42
1:D:302:LEU:HD11	1:D:311:PRO:HB3	2.02	0.42
1:D:308:ASN:O	1:D:310:ARG:N	2.51	0.42
1:D:362:VAL:HG21	1:D:375:LEU:HD13	2.02	0.41
1:A:119:LEU:HA	1:A:119:LEU:HD12	1.87	0.41
1:A:355:ARG:NH1	1:A:355:ARG:HA	2.35	0.41
1:B:332:ALA:O	1:B:337:GLY:N	2.47	0.41
1:C:208:ASP:HA	1:C:209:PRO:HD3	1.87	0.41
1:A:310:ARG:HA	1:A:311:PRO:HD3	1.85	0.41
1:D:394:LEU:HD23	1:D:394:LEU:HA	1.92	0.41
1:D:154:ASP:N	1:D:154:ASP:OD1	2.54	0.41
1:B:138:HIS:O	1:B:142:GLN:HG2	2.21	0.41
1:C:308:ASN:C	1:C:310:ARG:H	2.24	0.41
1:D:295:PHE:HZ	1:D:339:MET:HE1	1.86	0.40
1:A:163:ALA:HB1	1:A:203:VAL:HG13	2.04	0.40
1:B:302:LEU:HD11	1:B:311:PRO:HB3	2.04	0.40
1:D:100:TYR:CD1	1:D:103:LEU:HB2	2.57	0.40
1:D:315:THR:HB	2:D:601:FAD:O2	2.22	0.40

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	392/405 (97%)	383 (98%)	6 (2%)	3 (1%)	24	41
1	B	393/405 (97%)	385 (98%)	8 (2%)	0	100	100
1	C	392/405 (97%)	385 (98%)	7 (2%)	0	100	100
1	D	393/405 (97%)	385 (98%)	7 (2%)	1 (0%)	46	68
All	All	1570/1620 (97%)	1538 (98%)	28 (2%)	4 (0%)	46	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	TYR
1	A	29	ASN
1	D	309	ASN
1	A	309	ASN

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	286/329 (87%)	279 (98%)	7 (2%)	57	82
1	B	287/329 (87%)	282 (98%)	5 (2%)	68	89
1	C	285/329 (87%)	282 (99%)	3 (1%)	80	94
1	D	261/329 (79%)	252 (97%)	9 (3%)	44	72
All	All	1119/1316 (85%)	1095 (98%)	24 (2%)	61	85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	TYR
1	A	156	LEU
1	A	180	GLU
1	A	343	LYS
1	A	355	ARG
1	A	378	LEU
1	A	381	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	121	GLU
1	B	156	LEU
1	B	378	LEU
1	B	381	MET
1	B	391	SER
1	C	156	LEU
1	C	238	GLU
1	C	394	LEU
1	D	26	LEU
1	D	30	GLU
1	D	92	THR
1	D	156	LEU
1	D	345	HIS
1	D	381	MET
1	D	390	LEU
1	D	391	SER
1	D	392	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	196	ASN
1	C	39	ASN
1	D	89	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

5 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	-	52,58,58	4.07	19 (36%)	52,89,89	2.69	11 (21%)
3	NAD	A	602	-	42,48,48	3.52	14 (33%)	46,73,73	1.66	5 (10%)
2	FAD	B	601	-	52,58,58	4.05	19 (36%)	52,89,89	2.74	11 (21%)
2	FAD	C	601	-	52,58,58	4.06	19 (36%)	52,89,89	2.76	12 (23%)
2	FAD	D	601	-	52,58,58	4.07	19 (36%)	52,89,89	2.70	11 (21%)

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	-	-	0/30/50/50	0/6/6/6
3	NAD	A	602	-	-	0/22/62/62	0/5/5/5
2	FAD	B	601	-	-	0/30/50/50	0/6/6/6
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
2	FAD	D	601	-	-	0/30/50/50	0/6/6/6

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C2B-C1B	-15.48	1.29	1.53
2	C	601	FAD	C2B-C1B	-15.45	1.29	1.53
2	B	601	FAD	C2B-C1B	-15.43	1.29	1.53
2	A	601	FAD	C2B-C1B	-15.22	1.29	1.53
3	A	602	NAD	C2D-C3D	-10.84	1.24	1.53
3	A	602	NAD	O4D-C1D	-10.21	1.26	1.41
3	A	602	NAD	O4B-C1B	-7.57	1.30	1.41
3	A	602	NAD	C3B-C4B	-7.16	1.33	1.53
2	B	601	FAD	O4B-C4B	-6.81	1.29	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	O4B-C4B	-6.77	1.29	1.45
2	A	601	FAD	O4B-C4B	-6.73	1.29	1.45
2	C	601	FAD	O4B-C4B	-6.67	1.29	1.45
3	A	602	NAD	O2B-C2B	-4.60	1.32	1.43
2	A	601	FAD	O4-C4	-3.65	1.15	1.24
2	C	601	FAD	O4-C4	-3.63	1.15	1.24
2	D	601	FAD	O4-C4	-3.63	1.15	1.24
2	B	601	FAD	O4-C4	-3.60	1.15	1.24
2	B	601	FAD	O4'-C4'	-2.67	1.37	1.43
2	C	601	FAD	O4'-C4'	-2.64	1.37	1.43
3	A	602	NAD	C5D-C4D	-2.61	1.43	1.51
2	D	601	FAD	O4'-C4'	-2.61	1.37	1.43
2	A	601	FAD	O4'-C4'	-2.60	1.37	1.43
3	A	602	NAD	O3B-C3B	2.42	1.48	1.43
3	A	602	NAD	C2B-C1B	2.51	1.57	1.53
3	A	602	NAD	O4D-C4D	2.59	1.51	1.45
3	A	602	NAD	C6A-N6A	2.69	1.45	1.34
2	B	601	FAD	C7M-C7	2.73	1.56	1.51
2	C	601	FAD	C7M-C7	2.75	1.56	1.51
2	D	601	FAD	C7M-C7	2.75	1.56	1.51
3	A	602	NAD	O2D-C2D	2.78	1.49	1.43
2	A	601	FAD	C7M-C7	2.79	1.56	1.51
2	B	601	FAD	C2A-N3A	2.84	1.37	1.32
2	C	601	FAD	C6A-N6A	2.84	1.45	1.34
2	D	601	FAD	C6A-N6A	2.89	1.46	1.34
2	B	601	FAD	C6A-N6A	2.90	1.46	1.34
2	A	601	FAD	C6A-N6A	2.91	1.46	1.34
2	A	601	FAD	C2A-N3A	2.91	1.37	1.32
2	D	601	FAD	C2A-N3A	2.91	1.37	1.32
2	C	601	FAD	C2A-N3A	2.93	1.37	1.32
2	A	601	FAD	C8M-C8	2.98	1.56	1.51
2	B	601	FAD	C8M-C8	2.98	1.56	1.51
2	D	601	FAD	C8M-C8	3.14	1.57	1.51
2	C	601	FAD	C8M-C8	3.14	1.57	1.51
2	D	601	FAD	C2-N3	3.99	1.46	1.38
2	A	601	FAD	C2-N3	4.00	1.46	1.38
2	D	601	FAD	C4-C4X	4.01	1.49	1.41
2	C	601	FAD	C2-N3	4.08	1.46	1.38
2	B	601	FAD	C2-N3	4.08	1.46	1.38
2	C	601	FAD	C4-C4X	4.09	1.49	1.41
2	B	601	FAD	C4-C4X	4.13	1.49	1.41
2	B	601	FAD	C2-N1	4.15	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C2-N1	4.17	1.46	1.38
2	A	601	FAD	C2-N1	4.19	1.46	1.38
2	A	601	FAD	C4-C4X	4.22	1.49	1.41
2	D	601	FAD	C2-N1	4.24	1.47	1.38
2	C	601	FAD	O2B-C2B	4.25	1.53	1.43
2	B	601	FAD	O2B-C2B	4.34	1.53	1.43
2	D	601	FAD	O2B-C2B	4.35	1.53	1.43
2	A	601	FAD	O2B-C2B	4.43	1.53	1.43
2	C	601	FAD	C10-N1	4.52	1.43	1.35
2	A	601	FAD	C10-N1	4.53	1.43	1.35
2	B	601	FAD	C10-N1	4.53	1.43	1.35
2	D	601	FAD	C10-N1	4.63	1.43	1.35
3	A	602	NAD	O3D-C3D	4.83	1.54	1.43
2	C	601	FAD	C9A-N10	5.05	1.46	1.38
2	B	601	FAD	C9A-N10	5.05	1.46	1.38
2	A	601	FAD	C9A-N10	5.12	1.46	1.38
2	D	601	FAD	C9A-N10	5.15	1.46	1.38
2	C	601	FAD	C10-N10	5.47	1.45	1.39
2	A	601	FAD	C10-N10	5.49	1.45	1.39
2	B	601	FAD	C10-N10	5.52	1.45	1.39
2	B	601	FAD	C4-N3	5.56	1.43	1.33
2	D	601	FAD	C10-N10	5.62	1.45	1.39
2	A	601	FAD	C4-N3	5.62	1.43	1.33
2	C	601	FAD	C4-N3	5.64	1.43	1.33
2	D	601	FAD	C4-N3	5.64	1.43	1.33
2	B	601	FAD	C4X-N5	6.22	1.42	1.33
2	D	601	FAD	C4X-N5	6.28	1.43	1.33
2	A	601	FAD	C4X-N5	6.31	1.43	1.33
2	C	601	FAD	C4X-N5	6.32	1.43	1.33
3	A	602	NAD	C2D-C1D	6.47	1.63	1.53
3	A	602	NAD	C7N-N7N	6.74	1.46	1.33
2	B	601	FAD	C5X-N5	8.53	1.48	1.35
2	D	601	FAD	C5X-N5	8.54	1.48	1.35
2	C	601	FAD	C5X-N5	8.61	1.48	1.35
2	A	601	FAD	C5X-N5	8.70	1.49	1.35
2	B	601	FAD	O4B-C1B	13.75	1.60	1.41
2	D	601	FAD	O4B-C1B	13.80	1.60	1.41
2	C	601	FAD	O4B-C1B	13.93	1.61	1.41
2	A	601	FAD	O4B-C1B	14.09	1.61	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	N3A-C2A-N1A	-11.51	119.83	128.87
2	B	601	FAD	N3A-C2A-N1A	-11.33	119.97	128.87
2	D	601	FAD	N3A-C2A-N1A	-11.25	120.03	128.87
2	A	601	FAD	N3A-C2A-N1A	-11.24	120.05	128.87
3	A	602	NAD	N3A-C2A-N1A	-8.79	121.97	128.87
2	B	601	FAD	N6A-C6A-N1A	-7.34	106.21	118.52
2	C	601	FAD	N6A-C6A-N1A	-7.06	106.67	118.52
2	A	601	FAD	N6A-C6A-N1A	-7.04	106.70	118.52
2	D	601	FAD	N6A-C6A-N1A	-7.01	106.75	118.52
2	C	601	FAD	C7M-C7-C6	-5.92	103.60	120.33
2	B	601	FAD	C7M-C7-C6	-5.89	103.69	120.33
2	A	601	FAD	C7M-C7-C6	-5.85	103.80	120.33
2	D	601	FAD	C7M-C7-C6	-5.85	103.80	120.33
2	A	601	FAD	N3-C2-N1	-4.71	119.76	127.69
2	B	601	FAD	N3-C2-N1	-4.71	119.77	127.69
2	C	601	FAD	N3-C2-N1	-4.69	119.79	127.69
2	D	601	FAD	N3-C2-N1	-4.66	119.84	127.69
2	C	601	FAD	C4B-O4B-C1B	-3.04	106.42	109.64
2	B	601	FAD	C4X-C4-N3	-3.00	119.60	123.52
2	D	601	FAD	C4X-C4-N3	-2.97	119.64	123.52
2	A	601	FAD	C4X-C4-N3	-2.95	119.67	123.52
2	C	601	FAD	C4X-C4-N3	-2.94	119.68	123.52
3	A	602	NAD	C4D-O4D-C1D	-2.87	106.60	109.64
2	D	601	FAD	C8M-C8-C7	-2.82	114.67	120.73
2	A	601	FAD	C8M-C8-C7	-2.81	114.69	120.73
2	B	601	FAD	C1B-N9A-C4A	-2.78	123.70	126.81
2	C	601	FAD	C8M-C8-C7	-2.73	114.84	120.73
2	B	601	FAD	C8M-C8-C7	-2.66	115.00	120.73
2	C	601	FAD	C1B-N9A-C4A	-2.57	123.94	126.81
2	D	601	FAD	C1B-N9A-C4A	-2.38	124.15	126.81
2	A	601	FAD	C1B-N9A-C4A	-2.16	124.40	126.81
3	A	602	NAD	C2D-C1D-N1N	-2.05	109.51	113.53
3	A	602	NAD	O4B-C1B-N9A	2.02	111.92	108.11
3	A	602	NAD	C2D-C3D-C4D	2.05	106.84	102.64
2	B	601	FAD	C4X-N5-C5X	2.67	119.87	116.72
2	D	601	FAD	C4X-N5-C5X	2.71	119.92	116.72
2	A	601	FAD	C4X-N5-C5X	2.77	119.99	116.72
2	C	601	FAD	C4X-N5-C5X	2.78	120.00	116.72
2	A	601	FAD	C5X-C9A-N10	3.57	120.25	117.58
2	C	601	FAD	C5X-C9A-N10	3.58	120.26	117.58
2	D	601	FAD	C5X-C9A-N10	3.82	120.44	117.58
2	B	601	FAD	C5X-C9A-N10	3.91	120.51	117.58
2	C	601	FAD	C4-N3-C2	5.45	119.71	115.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C4-N3-C2	5.51	119.76	115.16
2	A	601	FAD	C4-N3-C2	5.56	119.79	115.16
2	B	601	FAD	C4-N3-C2	5.60	119.83	115.16
2	D	601	FAD	C7M-C7-C8	7.18	136.18	120.73
2	A	601	FAD	C7M-C7-C8	7.19	136.19	120.73
2	B	601	FAD	C7M-C7-C8	7.25	136.33	120.73
2	C	601	FAD	C7M-C7-C8	7.34	136.52	120.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

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	394/405 (97%)	0.12	6 (1%) 76 79	31, 57, 83, 98	0
1	B	395/405 (97%)	0.09	6 (1%) 76 79	29, 54, 80, 102	0
1	C	394/405 (97%)	0.04	7 (1%) 71 75	31, 54, 80, 112	0
1	D	395/405 (97%)	0.47	32 (8%) 15 16	37, 71, 98, 108	0
All	All	1578/1620 (97%)	0.18	51 (3%) 51 56	29, 59, 89, 112	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	GLY	6.3
1	D	331	ALA	6.1
1	D	332	ALA	4.9
1	D	336	GLY	4.8
1	D	272	GLY	4.6
1	D	33	ILE	4.5
1	D	36	VAL	4.4
1	D	211	LEU	4.0
1	D	362	VAL	3.6
1	D	5	SER	3.5
1	D	34	THR	3.3
1	D	31	ALA	3.2
1	B	32	ASP	3.2
1	D	337	GLY	3.2
1	D	35	LEU	3.1
1	A	371	ALA	3.0
1	D	32	ASP	3.0
1	D	273	PHE	3.0
1	D	338	SER	3.0
1	B	368	TYR	2.8
1	D	86	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	84	ILE	2.8
1	D	7	VAL	2.7
1	A	368	TYR	2.7
1	D	374	TRP	2.7
1	C	378	LEU	2.6
1	D	394	LEU	2.6
1	D	6	ILE	2.5
1	D	367	VAL	2.5
1	D	29	ASN	2.4
1	A	362	VAL	2.4
1	C	349	THR	2.4
1	D	370	HIS	2.4
1	A	87	GLU	2.3
1	C	244	VAL	2.3
1	D	360	GLY	2.3
1	C	394	LEU	2.3
1	A	394	LEU	2.3
1	B	394	LEU	2.3
1	D	359	ILE	2.2
1	B	28	TYR	2.2
1	C	373	SER	2.2
1	D	339	MET	2.2
1	C	219	LEU	2.2
1	D	203	VAL	2.1
1	D	115	GLY	2.1
1	C	362	VAL	2.1
1	D	168	ILE	2.1
1	A	102	TYR	2.1
1	D	8	ILE	2.0
1	B	332	ALA	2.0

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. 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	B	601	53/53	0.97	0.18	0.73	25,40,50,55	0
3	NAD	A	602	44/44	0.93	0.16	0.25	50,64,72,79	0
2	FAD	A	601	53/53	0.97	0.16	0.15	33,45,53,57	0
2	FAD	C	601	53/53	0.98	0.15	-0.25	31,41,55,64	0
2	FAD	D	601	53/53	0.95	0.15	-0.38	45,55,69,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.