



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:39 AM GMT

PDB ID : 4GAP
Title : Structure of the Ndi1 protein from *Saccharomyces cerevisiae* in complex with NAD⁺
Authors : Iwata, M.; Lee, Y.; Yamashita, T.; Yagi, T.; Iwata, S.; Cameron, A.D.; Maher, M.J.
Deposited on : 2012-07-25
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

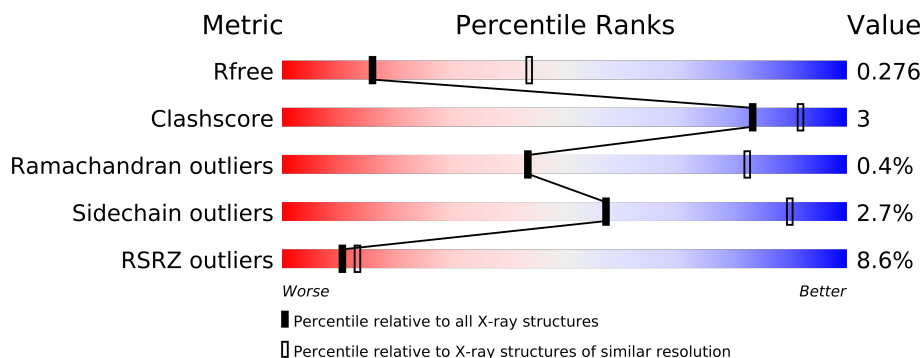
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAD	A	602	-	X
3	NAD	B	602	-	X

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7540 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Rotenone-insensitive NADH-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	1	0
			3673	2377	620	671	5			
1	B	463	Total	C	N	O	S	0	1	0
			3673	2377	620	671	5			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

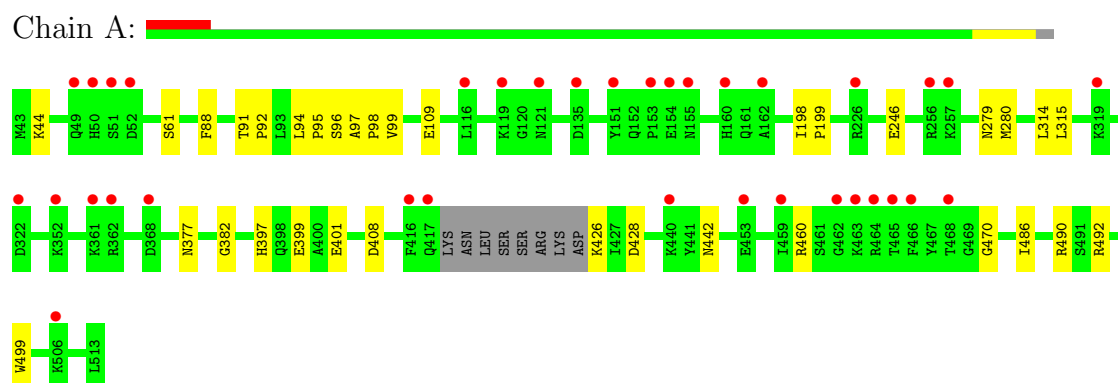


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

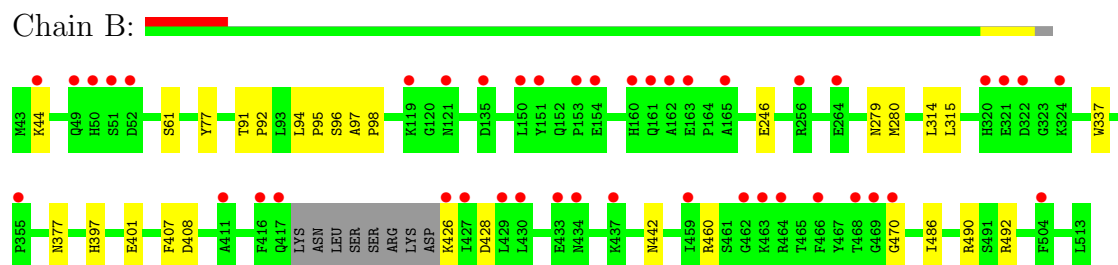
3 Residue-property plots

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.

- Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase



- Molecule 1: Rotenone-insensitive NADH-ubiquinone oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.01Å 164.48Å 70.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 2.90 39.84 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (39.84-2.90) 95.1 (39.84-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.237 , 0.277 0.237 , 0.276	Depositor DCC
R_{free} test set	1476 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 29028 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7540	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, FAD

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	0.41	1/3761 (0.0%)	0.50	0/5091
1	B	0.41	1/3761 (0.0%)	0.50	0/5091
All	All	0.41	2/7522 (0.0%)	0.50	0/10182

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	TRP	CD2-CE2	5.01	1.47	1.41
1	A	499	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3673	0	0	11	0
1	B	3673	0	0	9	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	3	0
All	All	7540	0	114	23	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (23) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:602:NAD:H4D	3:B:602:NAD:O2N	1.92	0.69
1:B:61:SER:N	2:B:601:FAD:HO3A	2.01	0.59
3:B:602:NAD:C4D	3:B:602:NAD:O2N	2.56	0.53
1:A:486:ILE:O	1:A:492:ARG:NH2	2.42	0.52
1:B:486:ILE:O	1:B:492:ARG:NH2	2.43	0.52
1:A:315:LEU:CD1	1:A:315:LEU:N	2.76	0.49
1:A:96:SER:OG	1:A:246:GLU:OE2	2.31	0.49
1:B:315:LEU:N	1:B:315:LEU:CD1	2.77	0.48
1:B:96:SER:OG	1:B:246:GLU:OE2	2.32	0.46
3:B:602:NAD:O2A	3:B:602:NAD:H3D	2.17	0.45
1:A:91:THR:N	1:A:92:PRO:CD	2.80	0.44
1:B:397:HIS:NE2	1:B:401:GLU:OE2	2.50	0.44
1:A:397:HIS:NE2	1:A:401:GLU:OE2	2.51	0.44
1:B:91:THR:N	1:B:92:PRO:CD	2.81	0.44
1:B:94:LEU:N	1:B:95:PRO:CD	2.82	0.43
1:A:94:LEU:N	1:A:95:PRO:CD	2.82	0.43
1:B:97:ALA:N	1:B:98:PRO:CD	2.83	0.41
1:A:61:SER:N	2:A:601:FAD:HO3A	2.18	0.41
1:B:77:TYR:OH	1:B:407:PHE:O	2.38	0.41
1:A:88:PHE:N	1:A:109:GLU:O	2.54	0.41
1:A:198:ILE:N	1:A:199:PRO:CD	2.84	0.41
1:A:382:GLY:N	1:A:399:GLU:OE1	2.54	0.40
1:A:97:ALA:N	1:A:98:PRO:CD	2.84	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	460/471 (98%)	437 (95%)	21 (5%)	2 (0%)	43	82
1	B	460/471 (98%)	436 (95%)	22 (5%)	2 (0%)	43	82
All	All	920/942 (98%)	873 (95%)	43 (5%)	4 (0%)	43	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	B	44	LYS
1	B	470	GLY
1	A	470	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	395/402 (98%)	384 (97%)	11 (3%)	56	90
1	B	395/402 (98%)	385 (98%)	10 (2%)	60	91
All	All	790/804 (98%)	769 (97%)	21 (3%)	57	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	A	279	ASN
1	A	280	MET
1	A	314	LEU
1	A	377	ASN
1	A	408	ASP
1	A	426	LYS
1	A	428	ASP
1	A	442	ASN
1	A	460	ARG
1	A	490	ARG

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Mol	Chain	Res	Type
1	B	279	ASN
1	B	280	MET
1	B	314	LEU
1	B	377	ASN
1	B	408	ASP
1	B	426	LYS
1	B	428	ASP
1	B	442	ASN
1	B	460	ARG
1	B	490	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	-	58,58,58	1.45	7 (12%)	85,89,89	1.88	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	A	602	-	48,48,48	0.90	2 (4%)	73,73,73	1.53	10 (13%)
2	FAD	B	601	-	58,58,58	1.48	8 (13%)	85,89,89	1.90	16 (18%)
3	NAD	B	602	-	48,48,48	0.95	2 (4%)	73,73,73	1.47	7 (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	-	-	0/34/50/50	0/1/6/6
3	NAD	A	602	-	-	0/30/62/62	0/3/5/5
2	FAD	B	601	-	-	0/34/50/50	0/1/6/6
3	NAD	B	602	-	-	0/30/62/62	0/3/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4-C4X	5.03	1.49	1.41
2	B	601	FAD	C4-C4X	4.77	1.49	1.41
2	A	601	FAD	C4X-C10	4.61	1.48	1.40
2	B	601	FAD	C4X-C10	4.32	1.48	1.40
2	A	601	FAD	C9A-C5X	3.80	1.50	1.42
2	B	601	FAD	C9A-C5X	3.68	1.50	1.42
2	B	601	FAD	C4A-N9A	-3.26	1.33	1.37
3	B	602	NAD	C5A-C4A	3.19	1.47	1.40
3	A	602	NAD	C5A-C4A	2.93	1.47	1.40
3	A	602	NAD	C4A-N9A	-2.91	1.33	1.37
2	B	601	FAD	C9A-N10	2.91	1.43	1.38
2	B	601	FAD	C5A-C4A	2.88	1.47	1.40
2	A	601	FAD	C5A-C4A	2.85	1.46	1.40
2	A	601	FAD	C8-C7	2.81	1.49	1.40
2	A	601	FAD	C4A-N9A	-2.75	1.33	1.37
2	B	601	FAD	C8-C7	2.71	1.48	1.40
3	B	602	NAD	C4A-N9A	-2.65	1.33	1.37
2	A	601	FAD	C9A-N10	2.54	1.42	1.38
2	B	601	FAD	C4-N3	-2.17	1.33	1.37

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N3A-C2A-N1A	-7.54	122.40	128.71
2	B	601	FAD	N3A-C2A-N1A	-7.13	122.75	128.71
3	A	602	NAD	N3A-C2A-N1A	-7.06	122.80	128.71
3	B	602	NAD	N3A-C2A-N1A	-6.86	122.97	128.71
2	A	601	FAD	C2-N1-C10	6.26	121.29	114.98
2	B	601	FAD	C2-N1-C10	6.07	121.10	114.98
3	B	602	NAD	N3A-C4A-N9A	5.25	134.91	125.43
3	A	602	NAD	N3A-C4A-N9A	5.18	134.78	125.43
2	A	601	FAD	N3A-C4A-N9A	5.03	134.52	125.43
2	B	601	FAD	C1'-N10-C9A	5.01	123.75	118.87
2	B	601	FAD	N3A-C4A-N9A	4.75	134.01	125.43
2	B	601	FAD	C4X-N5-C5X	4.56	121.81	116.69
2	A	601	FAD	C4X-C10-N1	-4.47	118.26	122.73
2	B	601	FAD	C4X-C10-N1	-4.27	118.47	122.73
2	A	601	FAD	C1'-N10-C9A	4.01	122.77	118.87
2	A	601	FAD	C4X-N5-C5X	3.83	120.99	116.69
2	B	601	FAD	C4A-C5A-N7A	-3.79	106.28	109.52
2	A	601	FAD	C9A-N10-C10	-3.78	118.05	121.77
2	B	601	FAD	C8A-N9A-C4A	3.25	109.38	106.90
2	B	601	FAD	C1B-N9A-C4A	-3.21	121.09	126.64
3	B	602	NAD	C4A-C5A-N7A	-3.14	106.83	109.52
3	B	602	NAD	C5A-C4A-N3A	-3.13	118.89	125.70
3	A	602	NAD	C4A-C5A-N7A	-3.07	106.89	109.52
3	A	602	NAD	C8A-N9A-C4A	3.06	109.23	106.90
2	A	601	FAD	C4A-C5A-N7A	-3.04	106.92	109.52
3	B	602	NAD	PN-O3-PA	-3.03	119.92	132.95
2	A	601	FAD	C5A-C4A-N3A	-2.96	119.26	125.70
3	A	602	NAD	C5A-C4A-N3A	-2.94	119.29	125.70
3	A	602	NAD	O4B-C1B-N9A	2.83	111.07	108.44
2	A	601	FAD	P-O3P-PA	-2.81	123.43	131.68
2	B	601	FAD	C4X-C10-N10	-2.79	119.12	120.51
2	B	601	FAD	C5A-C4A-N3A	-2.77	119.67	125.70
2	B	601	FAD	C9A-N10-C10	-2.76	119.06	121.77
3	A	602	NAD	PN-O3-PA	-2.63	121.65	132.95
2	A	601	FAD	C2A-N3A-C4A	2.59	121.40	114.01
2	A	601	FAD	C8A-N9A-C4A	2.58	108.87	106.90
3	A	602	NAD	O4D-C1D-N1N	2.58	110.59	107.95
2	B	601	FAD	C4'-C3'-C2'	-2.56	107.47	113.25
2	A	601	FAD	C1B-N9A-C4A	-2.55	122.23	126.64
3	B	602	NAD	C2A-N3A-C4A	2.46	121.01	114.01
2	B	601	FAD	N1-C10-N10	2.45	122.41	115.97
2	B	601	FAD	C2A-N3A-C4A	2.42	120.90	114.01
3	A	602	NAD	C2A-N3A-C4A	2.41	120.86	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C5X-C9A-N10	2.35	119.12	116.80
2	A	601	FAD	N1-C10-N10	2.30	122.02	115.97
3	B	602	NAD	C8A-N9A-C4A	2.26	108.63	106.90
2	B	601	FAD	P-O3P-PA	-2.21	125.19	131.68
2	A	601	FAD	O4B-C1B-N9A	-2.16	106.43	108.44
2	A	601	FAD	C2B-C1B-N9A	2.13	118.73	113.27
3	A	602	NAD	C2A-N1A-C6A	2.02	122.41	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	463/471 (98%)	0.41	35 (7%) 14 17	32, 59, 96, 121	0
1	B	463/471 (98%)	0.47	43 (9%) 9 11	33, 58, 110, 147	0
All	All	926/942 (98%)	0.44	78 (8%) 11 14	32, 59, 103, 147	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	HIS	10.5
1	B	427	ILE	8.6
1	B	50	HIS	8.2
1	B	151	TYR	7.8
1	A	49	GLN	7.3
1	B	49	GLN	6.9
1	B	463	LYS	6.3
1	B	417	GLN	6.3
1	B	430	LEU	6.0
1	B	52	ASP	5.9
1	B	153	PRO	5.7
1	A	468	THR	5.5
1	B	162	ALA	5.2
1	A	52	ASP	5.1
1	B	468	THR	5.0
1	A	51	SER	4.8
1	A	155	ASN	4.5
1	A	417	GLN	4.5
1	B	51	SER	4.4
1	A	462	GLY	4.3
1	A	154	GLU	4.2
1	A	322	ASP	3.9
1	B	321	GLU	3.9
1	A	135	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	119	LYS	3.7
1	B	150	LEU	3.7
1	A	153	PRO	3.7
1	B	469	GLY	3.6
1	A	119	LYS	3.6
1	B	256	ARG	3.6
1	B	322	ASP	3.5
1	A	319	LYS	3.4
1	B	411	ALA	3.4
1	A	416	PHE	3.3
1	A	116	LEU	3.3
1	B	464	ARG	3.3
1	A	361	LYS	3.3
1	A	151	TYR	3.2
1	B	433	GLU	3.2
1	B	429	LEU	3.1
1	B	163	GLU	3.1
1	B	462	GLY	3.0
1	B	264	GLU	3.0
1	A	362	ARG	2.9
1	A	453	GLU	2.9
1	B	154	GLU	2.8
1	A	257	LYS	2.8
1	B	165	ALA	2.8
1	A	464	ARG	2.7
1	A	160	HIS	2.7
1	A	463	LYS	2.7
1	B	426	LYS	2.7
1	B	324	LYS	2.6
1	B	355	PRO	2.6
1	A	506	LYS	2.6
1	B	135	ASP	2.6
1	A	440	LYS	2.6
1	B	161	GLN	2.6
1	A	256	ARG	2.5
1	A	465	THR	2.5
1	A	459	ILE	2.4
1	B	504	PHE	2.4
1	B	459	ILE	2.4
1	A	226	ARG	2.4
1	A	466	PHE	2.4
1	B	466	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	470	GLY	2.4
1	A	352	LYS	2.3
1	B	434	ASN	2.3
1	B	44	LYS	2.3
1	B	416	PHE	2.2
1	A	368	ASP	2.2
1	B	320	HIS	2.1
1	B	437	LYS	2.1
1	A	121	ASN	2.1
1	B	121	ASN	2.1
1	A	162	ALA	2.0
1	B	160	HIS	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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAD	A	602	44/44	0.43	6.22	40,44,47,47	44
3	NAD	B	602	44/44	0.44	5.81	31,38,43,45	44
2	FAD	A	601	53/53	0.23	0.82	34,41,55,59	0
2	FAD	B	601	53/53	0.18	-0.13	30,37,41,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.