



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:31 PM GMT

PDB ID : 1KOL
Title : Crystal structure of formaldehyde dehydrogenase
Authors : Tanaka, N.; Kusakabe, Y.; Ito, K.; Yoshimoto, T.; Nakamura, K.T.
Deposited on : 2001-12-21
Resolution : 1.65 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

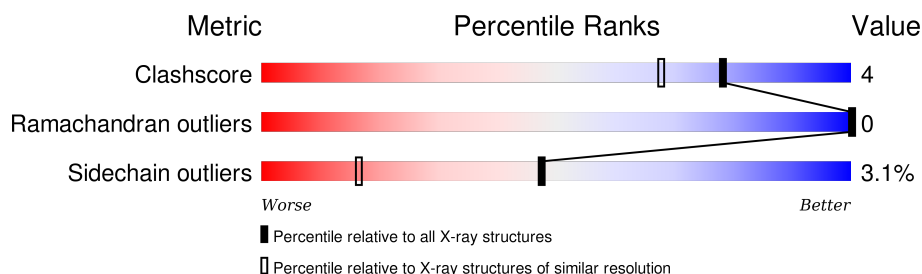
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	 90% 8% ..
1	B	398	 89% 10% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6937 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 formaldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			2934	1848	521	549	16			
1	B	396	Total	C	N	O	S	0	0	0
			2934	1848	521	549	16			

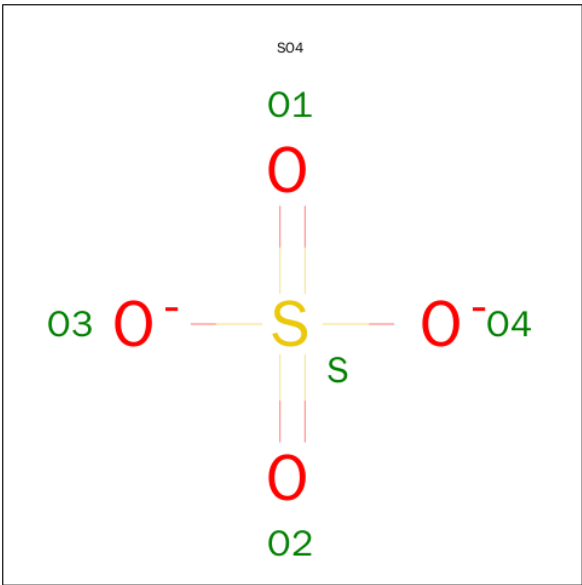
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	VAL	LEU	SEE REMARK 999	UNP P46154
B	139	VAL	LEU	SEE REMARK 999	UNP P46154

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

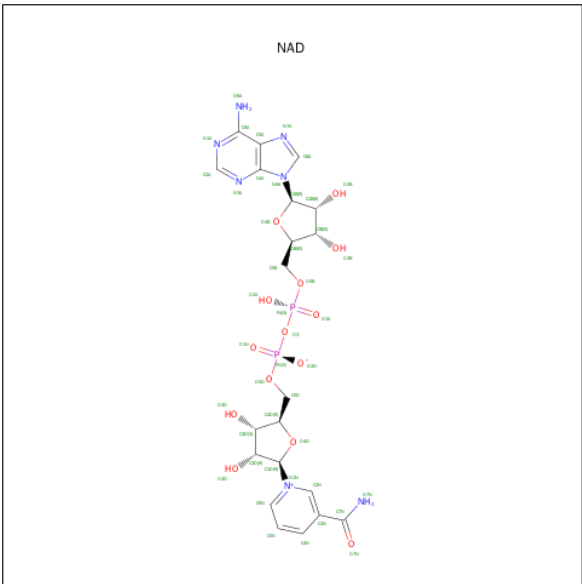
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

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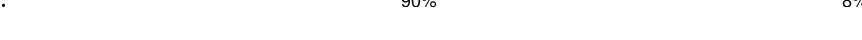
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	472	Total	O	0	0
			472	472		
5	B	495	Total	O	0	0
			495	495		

Note EDS was not executed.

- Chain A:  90% 8% ..
- 
- | Position | Amino Acid | Frequency (approx.) |
|----------|------------|---------------------|
| 1 | V361 | 0.25 |
| 2 | G2 | 0.25 |
| 3 | G3 | 0.25 |
| 4 | R4 | 0.25 |
| 9 | L9 | 0.25 |
| 15 | E15 | 0.25 |
| 13 | K13 | 0.25 |
| 26 | D26 | 0.25 |
| 27 | P27 | 0.25 |
| 30 | K30 | 0.25 |
| 34 | H34 | 0.25 |
| 43 | T43 | 0.25 |
| 46 | C46 | 0.25 |
| 58 | T58 | 0.25 |
| 68 | E68 | 0.25 |
| 88 | L88 | 0.25 |
| 143 | Y143 | 0.25 |
| 151 | L151 | 0.25 |
| 152 | P152 | 0.25 |
| 153 | D153 | 0.25 |
| 162 | R162 | 0.25 |
| 193 | G193 | 0.25 |
| 198 | G198 | 0.25 |
| 225 | H225 | 0.25 |
| 267 | R267 | 0.25 |
| 277 | E277 | 0.25 |
| 288 | Q288 | 0.25 |
| 291 | R291 | 0.25 |
| 299 | P299 | 0.25 |
| 316 | I316 | 0.25 |
| 319 | L319 | 0.25 |
| 345 | R345 | 0.25 |
| 355 | R355 | 0.25 |

- Chain B: 

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	85.69Å 85.69Å 190.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.65	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.65)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6937	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, 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	0.47	0/2991	1.10	9/4058 (0.2%)
1	B	0.48	0/2991	1.12	11/4058 (0.3%)
All	All	0.47	0/5982	1.11	20/8116 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	CD-NE-CZ	12.96	141.75	123.60
1	B	146	PHE	CB-CG-CD2	-7.52	115.54	120.80
1	B	101	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	B	355	ARG	CD-NE-CZ	7.06	133.48	123.60
1	A	162	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	291	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	345	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	291	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	267	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	374	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	B	206	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	A	4	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	374	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	206	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	355	ARG	CD-NE-CZ	5.29	131.00	123.60
1	B	374	ARG	N-CA-CB	5.25	120.04	110.60
1	B	101	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	B	374	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	88	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	206	ARG	NH1-CZ-NH2	5.09	125.00	119.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2934	0	2936	21	0
1	B	2934	0	2936	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	1	0
5	A	472	0	0	1	1
5	B	495	0	0	5	0
All	All	6937	0	5924	43	1

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 4.

All (43) 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:A:393:LYS:HA	1:A:393:LYS:HE3	1.56	0.85
1:A:34:HIS:HD2	1:A:143:TYR:H	1.31	0.77
1:B:34:HIS:HD2	1:B:143:TYR:H	1.37	0.72
1:A:374:ARG:HH21	1:A:374:ARG:HG2	1.55	0.71
1:A:34:HIS:CD2	1:A:143:TYR:H	2.08	0.71
1:B:277:GLU:HG2	5:B:2780:HOH:O	1.92	0.70
1:A:88:LEU:HG	1:A:151:LEU:HD12	1.76	0.65
1:A:393:LYS:CA	1:A:393:LYS:HE3	2.25	0.65
1:A:393:LYS:HE2	1:A:396:SER:OG	1.98	0.64
1:B:34:HIS:CD2	1:B:143:TYR:H	2.16	0.64
1:B:243:HIS:HB3	1:B:288:GLN:NE2	2.14	0.62
1:B:374:ARG:HG3	5:B:2855:HOH:O	2.01	0.61
1:B:243:HIS:HB3	1:B:288:GLN:HE22	1.70	0.56
1:A:26:ASP:HB2	1:A:27:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LYS:HE3	5:B:2808:HOH:O	2.07	0.54
1:A:288:GLN:HE21	1:A:288:GLN:HA	1.77	0.50
1:A:299:PRO:O	4:A:1403:NAD:H2N	2.13	0.49
1:B:299:PRO:O	4:B:2403:NAD:H2N	2.13	0.49
1:A:9:LEU:HD11	1:A:15:GLU:HB3	1.95	0.49
1:B:225:HIS:HE1	1:B:361:VAL:O	1.95	0.48
1:A:46:CYS:HB2	1:A:68:GLU:OE1	2.14	0.48
1:A:371:ASP:O	1:A:374:ARG:HG3	2.13	0.48
1:A:225:HIS:HE1	1:A:361:VAL:O	1.96	0.48
1:B:11:SER:O	1:B:13:LYS:HD2	2.14	0.47
1:B:227:LYS:HE3	5:B:2734:HOH:O	2.14	0.47
1:B:9:LEU:HD11	1:B:15:GLU:HB3	1.98	0.46
1:B:43:THR:HA	1:B:68:GLU:O	2.16	0.46
1:A:374:ARG:NH2	1:A:374:ARG:HG2	2.22	0.45
1:A:193:GLY:O	1:A:198:GLY:HA3	2.16	0.45
1:B:25:GLN:NE2	1:B:29:GLY:HA2	2.32	0.45
1:A:393:LYS:HA	1:A:393:LYS:CE	2.38	0.44
1:B:360:GLU:HG3	5:B:2511:HOH:O	2.18	0.44
1:B:374:ARG:O	1:B:378:GLU:HG3	2.19	0.43
1:B:293:ALA:HA	1:B:330:SER:O	2.19	0.43
1:B:203:ALA:HB2	1:B:361:VAL:HG11	2.00	0.42
1:B:26:ASP:HB2	1:B:27:PRO:CD	2.50	0.42
1:B:193:GLY:O	1:B:198:GLY:HA3	2.19	0.42
1:A:152:PRO:O	1:A:153:ASP:C	2.58	0.42
1:A:366:VAL:HA	1:A:388:VAL:O	2.20	0.41
1:B:46:CYS:HB2	1:B:68:GLU:OE1	2.20	0.41
1:B:78:ARG:HH11	1:B:78:ARG:HD3	1.70	0.41
1:A:277:GLU:HG2	5:A:1832:HOH:O	2.20	0.40
1:A:43:THR:HA	1:A:68:GLU:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1524:HOH:O	5:A:1630:HOH:O[4_555]	2.16	0.04

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	394/398 (99%)	382 (97%)	12 (3%)	0	100	100
1	B	394/398 (99%)	386 (98%)	8 (2%)	0	100	100
All	All	788/796 (99%)	768 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	303/304 (100%)	291 (96%)	12 (4%)	38	11
1	B	303/304 (100%)	296 (98%)	7 (2%)	58	30
All	All	606/608 (100%)	587 (97%)	19 (3%)	47	16

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	18	LYS
1	A	30	LYS
1	A	58	THR
1	A	153	ASP
1	A	267	ARG
1	A	288	GLN
1	A	316	ILE

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Mol	Chain	Res	Type
1	A	319	LEU
1	A	374	ARG
1	A	391	PRO
1	A	393	LYS
1	B	44	ASN
1	B	60	GLN
1	B	88	LEU
1	B	218	LEU
1	B	319	LEU
1	B	354	ASP
1	B	374	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	225	HIS
1	A	288	GLN
1	A	331	HIS
1	B	34	HIS
1	B	60	GLN
1	B	225	HIS
1	B	331	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
3	SO4	A	1003	-	4,4,4	0.96	0	6,6,6	0.22	0
4	NAD	A	1403	-	38,48,48	1.24	5 (13%)	47,73,73	2.02	11 (23%)
3	SO4	B	1002	-	4,4,4	0.93	0	6,6,6	0.20	0
4	NAD	B	2403	-	38,48,48	1.27	3 (7%)	47,73,73	2.07	10 (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
3	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	NAD	A	1403	-	-	0/22/62/62	0/5/5/5
3	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
4	NAD	B	2403	-	-	0/22/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1403	NAD	C2N-C3N	-2.14	1.35	1.39
4	A	1403	NAD	PN-O2N	-2.14	1.45	1.54
4	A	1403	NAD	C6N-N1N	2.16	1.41	1.35
4	B	2403	NAD	C6N-N1N	2.36	1.41	1.35
4	A	1403	NAD	O4D-C1D	2.44	1.44	1.41
4	B	2403	NAD	O4D-C1D	3.29	1.45	1.41
4	B	2403	NAD	C3N-C7N	3.67	1.56	1.50
4	A	1403	NAD	C3N-C7N	4.06	1.56	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1403	NAD	C5N-C4N-C3N	-7.33	111.11	120.33
4	B	2403	NAD	C5N-C4N-C3N	-6.87	111.69	120.33
4	B	2403	NAD	O4D-C1D-N1N	-4.86	102.79	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2403	NAD	C4B-O4B-C1B	-3.27	106.12	109.72
4	B	2403	NAD	C4N-C3N-C7N	-3.24	112.54	121.09
4	A	1403	NAD	C5N-C6N-N1N	-3.23	114.88	120.47
4	A	1403	NAD	C4N-C3N-C7N	-3.18	112.67	121.09
4	A	1403	NAD	C4B-O4B-C1B	-3.03	106.39	109.72
4	B	2403	NAD	C4D-O4D-C1D	-2.95	106.48	109.72
4	A	1403	NAD	C1B-N9A-C4A	-2.85	122.64	126.94
4	B	2403	NAD	C5N-C6N-N1N	-2.73	115.75	120.47
4	A	1403	NAD	O3-PN-O5D	-2.44	96.47	102.94
4	A	1403	NAD	O4D-C1D-N1N	-2.30	105.60	108.13
4	B	2403	NAD	C1B-N9A-C4A	-2.16	123.67	126.94
4	A	1403	NAD	C2B-C1B-N9A	2.02	117.38	114.29
4	A	1403	NAD	O7N-C7N-N7N	2.06	125.50	122.59
4	B	2403	NAD	C2B-C1B-N9A	2.63	118.30	114.29
4	A	1403	NAD	C2N-C3N-C4N	5.23	124.11	118.29
4	B	2403	NAD	C6N-C5N-C4N	5.32	127.48	119.44
4	B	2403	NAD	C2N-C3N-C4N	5.35	124.24	118.29
4	A	1403	NAD	C6N-C5N-C4N	5.47	127.70	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1403	NAD	1	0
4	B	2403	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.