Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:02 PM GMT

PDB ID	:	1DQS
Title	:	CRYSTAL STRUCTURE OF DEHYDROQUINATE SYNTHASE (DHQS) COMPLEXED WITH CARBAPHOSPHONATE, NAD+ AND ZN2+
Authors	:	Carpenter, E.P.; Hawkins, A.R.; Frost, J.W.; Brown, K.A.
Deposited on	:	1998-04-09
Resolution	:	1.80 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 (i) symbol.

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

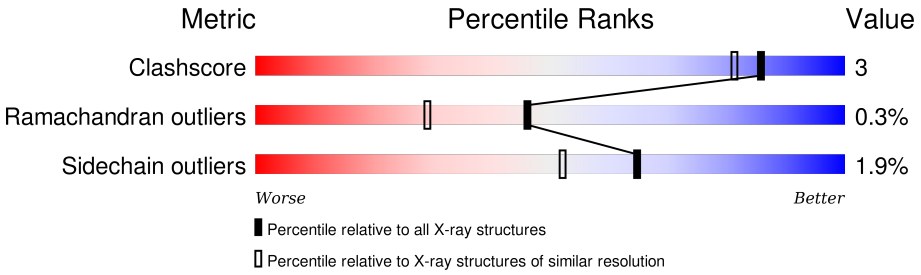
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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 <=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	393	86% 11% ·
1	B	393	89% 8% ·

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6539 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 PROTEIN (3-DEHYDROQUINATE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2843	1813	488	530	12			
1	B	380	Total	C	N	O	S	0	0	0
			2853	1820	484	537	12			

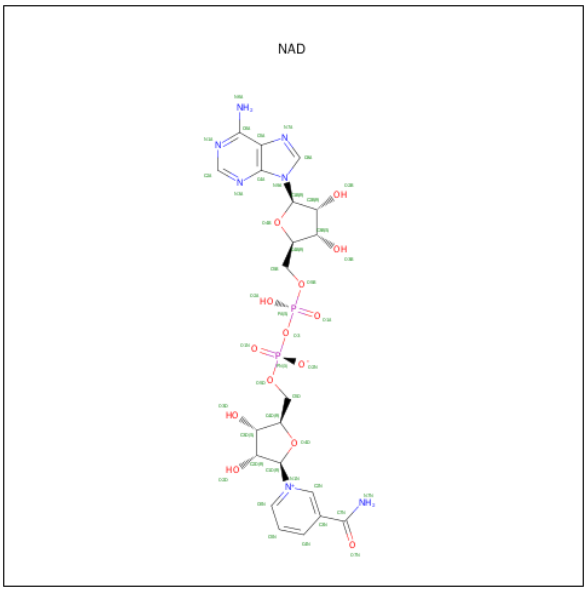
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

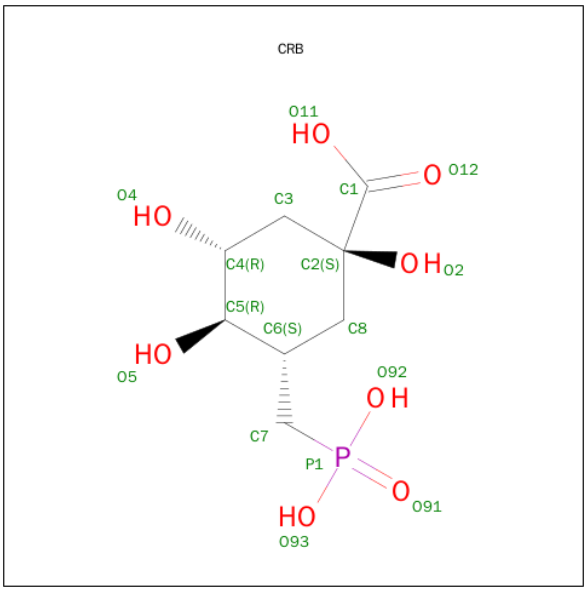
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 5 is [1R-(1ALPHA,3BETA,4ALPHA,5BETA)]-5-(PHOSPHONOMETHYL)-1 ,3,4-TRIHYDROXYCYCLOHEXANE-1-CARBOXYLIC ACID (three-letter code: CRB) (formula: $C_8H_{15}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			17	8	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			17	8	8	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	359	Total	O	0	0
			359	359		
6	B	359	Total	O	0	0
			359	359		

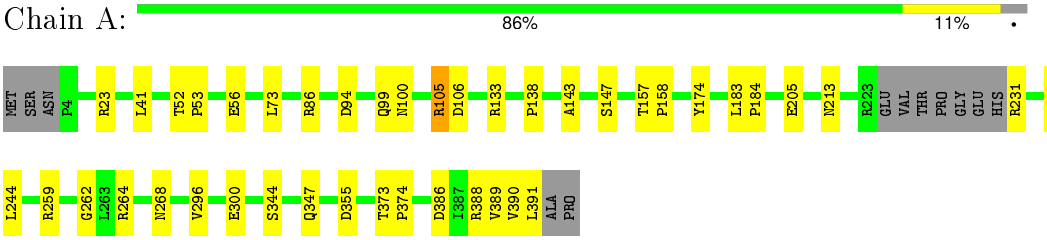
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

Note EDS was not executed.

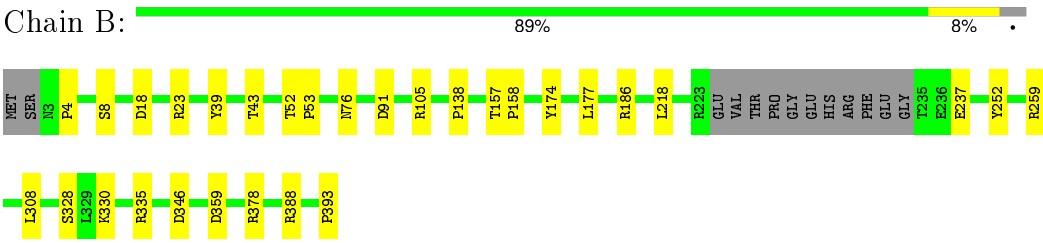
- Molecule 1: PROTEIN (3-DEHYDROQUINATE SYNTHASE)

Chain A:



- Molecule 1: PROTEIN (3-DEHYDROQUINATE SYNTHASE)

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.68Å 80.81Å 143.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.80	Depositor
% Data completeness (in resolution range)	91.2 (25.00-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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: CRB, ZN, NAD, CL

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	0.62	0/2890	1.18	11/3926 (0.3%)
1	B	0.63	0/2899	1.21	12/3936 (0.3%)
All	All	0.62	0/5789	1.19	23/7862 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	259	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	A	264	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	B	186	ARG	NE-CZ-NH2	8.41	124.51	120.30
1	B	378	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	A	388	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	264	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	133	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	A	259	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	B	388	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	A	106	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	133	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	B	346	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	39	TYR	CB-CG-CD2	6.29	124.77	121.00
1	A	105	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	A	23	ARG	CD-NE-CZ	5.88	131.83	123.60
1	B	91	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	39	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	186	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	B	335	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	23	ARG	CD-NE-CZ	5.40	131.17	123.60
1	B	8	SER	N-CA-CB	-5.31	102.53	110.50
1	A	94	ASP	CB-CG-OD2	-5.19	113.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	355	ASP	CB-CG-OD2	-5.11	113.70	118.30

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	2843	0	2864	21	0
1	B	2853	0	2902	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	1	0
5	A	17	0	10	1	0
5	B	17	0	10	1	0
6	A	359	0	0	3	0
6	B	359	0	0	2	0
All	All	6539	0	5838	33	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 3.

All (33) 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:386:ASP:O	1:A:389:VAL:HG22	1.57	1.03
1:B:177:LEU:HD23	6:B:1148:HOH:O	1.79	0.82
1:A:231:ARG:HG2	6:A:834:HOH:O	1.84	0.76
1:A:344:SER:H	1:A:347:GLN:HE21	1.38	0.71
1:A:52:THR:O	1:A:56:GLU:HG3	1.92	0.70
1:A:389:VAL:HG23	1:A:390:VAL:HG13	1.82	0.62
1:A:344:SER:H	1:A:347:GLN:NE2	2.04	0.55
1:B:138:PRO:HD2	1:B:174:TYR:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:N	1:A:53:PRO:CD	2.73	0.52
1:A:157:THR:HB	1:A:158:PRO:CD	2.41	0.51
1:A:73:LEU:HD13	1:A:99:GLN:HG3	1.93	0.51
1:B:52:THR:N	1:B:53:PRO:CD	2.75	0.50
4:A:400:NAD:C4N	5:A:401:CRB:H5	2.45	0.47
4:B:400:NAD:C4N	5:B:401:CRB:H5	2.46	0.46
1:B:43:THR:CG2	1:B:76:ASN:HD22	2.29	0.45
1:B:157:THR:HB	1:B:158:PRO:CD	2.48	0.43
1:A:143:ALA:HA	1:A:147:SER:OG	2.19	0.43
1:A:86:ARG:HH11	1:A:86:ARG:HD2	1.70	0.43
1:B:359:ASP:HB2	6:B:1123:HOH:O	2.19	0.43
1:B:105:ARG:HD3	1:B:105:ARG:HH11	1.66	0.42
1:A:296:VAL:O	1:A:300:GLU:HG3	2.20	0.42
1:A:183:LEU:HA	1:A:184:PRO:HD3	1.91	0.42
1:A:41:LEU:HD23	1:A:41:LEU:C	2.40	0.42
1:A:213:ASN:OD1	1:A:242:ARG:HD2	2.20	0.41
1:B:157:THR:HB	1:B:158:PRO:HD2	2.03	0.41
1:A:105:ARG:NH1	6:A:857:HOH:O	2.52	0.41
1:A:157:THR:HB	1:A:158:PRO:HD2	2.02	0.41
1:A:373:THR:HA	1:A:374:PRO:HD3	1.80	0.41
1:A:205:GLU:HG3	6:A:820:HOH:O	2.20	0.41
1:B:4:PRO:HB3	1:B:18:ASP:HB2	2.02	0.41
1:A:389:VAL:HG23	1:A:390:VAL:N	2.36	0.40
1:B:330:LYS:HE3	1:B:393:PRO:HB2	2.04	0.40
1:A:138:PRO:HD2	1:A:174:TYR:O	2.22	0.40

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	377/393 (96%)	368 (98%)	8 (2%)	1 (0%)	46 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	376/393 (96%)	366 (97%)	9 (2%)	1 (0%)	46 29
All	All	753/786 (96%)	734 (98%)	17 (2%)	2 (0%)	46 29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	GLY
1	B	262	GLY

5.3.2 Protein sidechains (i)

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	292/326 (90%)	287 (98%)	5 (2%)	68 57
1	B	298/326 (91%)	292 (98%)	6 (2%)	63 49
All	All	590/652 (90%)	579 (98%)	11 (2%)	65 52

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	235	THR
1	A	244	LEU
1	A	268	ASN
1	A	391	LEU
1	B	218	LEU
1	B	237	GLU
1	B	252	TYR
1	B	268	ASN
1	B	308	LEU
1	B	328	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	347	GLN
1	B	76	ASN
1	B	100	ASN
1	B	384	ASN

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

Of 7 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
4	NAD	A	400	-	38,48,48	1.48	4 (10%)	47,73,73	2.12	12 (25%)
5	CRB	A	401	2	13,17,17	1.48	1 (7%)	17,27,27	1.04	2 (11%)
4	NAD	B	400	-	38,48,48	1.43	5 (13%)	47,73,73	2.04	11 (23%)
5	CRB	B	401	2	13,17,17	1.32	1 (7%)	17,27,27	0.99	2 (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
4	NAD	A	400	-	-	0/22/62/62	0/5/5/5
5	CRB	A	401	2	-	0/5/29/29	0/1/1/1
4	NAD	B	400	-	-	0/22/62/62	0/5/5/5
5	CRB	B	401	2	-	0/5/29/29	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	NAD	C4A-N3A	2.21	1.38	1.35
4	A	400	NAD	C6N-N1N	2.33	1.41	1.35
4	B	400	NAD	C6N-N1N	2.43	1.42	1.35
4	B	400	NAD	C3N-C7N	2.83	1.55	1.50
5	B	401	CRB	P1-C7	3.07	1.82	1.79
4	A	400	NAD	C3N-C7N	3.24	1.55	1.50
4	B	400	NAD	O4B-C1B	3.48	1.45	1.41
4	A	400	NAD	O4D-C1D	3.85	1.46	1.41
4	B	400	NAD	O4D-C1D	4.12	1.46	1.41
5	A	401	CRB	P1-C7	4.29	1.83	1.79
4	A	400	NAD	O4B-C1B	5.36	1.48	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	400	NAD	C5N-C4N-C3N	-6.59	112.04	120.33
4	A	400	NAD	C5N-C4N-C3N	-5.80	113.04	120.33
4	A	400	NAD	O4D-C1D-N1N	-4.50	103.18	108.13
4	A	400	NAD	O4B-C1B-N9A	-4.13	99.45	108.10
4	B	400	NAD	O4B-C1B-N9A	-3.79	100.16	108.10
4	B	400	NAD	O4D-C1D-N1N	-3.63	104.14	108.13
4	A	400	NAD	C5N-C6N-N1N	-3.35	114.67	120.47
4	A	400	NAD	C4N-C3N-C7N	-3.19	112.66	121.09
4	B	400	NAD	C5N-C6N-N1N	-2.83	115.58	120.47
4	A	400	NAD	C3N-C7N-N7N	-2.68	114.89	117.82
4	B	400	NAD	C4N-C3N-C7N	-2.62	114.17	121.09
4	A	400	NAD	C4D-O4D-C1D	-2.49	106.98	109.72
4	B	400	NAD	O3-PN-O5D	-2.12	97.31	102.94
5	B	401	CRB	C3-C4-C5	-2.08	108.93	110.84
5	A	401	CRB	O4-C4-C5	2.03	114.21	110.12
5	B	401	CRB	O5-C5-C6	2.33	113.95	110.07
4	B	400	NAD	O2N-PN-O1N	2.37	125.39	112.53
4	B	400	NAD	N3A-C2A-N1A	2.72	130.98	128.89
5	A	401	CRB	C8-C2-C3	2.83	113.47	110.33
4	A	400	NAD	C4A-C5A-N7A	2.85	112.10	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	400	NAD	C2B-C1B-N9A	3.42	119.52	114.29
4	A	400	NAD	C4B-O4B-C1B	3.43	113.49	109.72
4	B	400	NAD	C2B-C1B-N9A	4.06	120.50	114.29
4	A	400	NAD	C2N-C3N-C4N	4.31	123.08	118.29
4	B	400	NAD	C2N-C3N-C4N	4.71	123.53	118.29
4	A	400	NAD	C6N-C5N-C4N	5.36	127.53	119.44
4	B	400	NAD	C6N-C5N-C4N	5.40	127.60	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	400	NAD	1	0
5	A	401	CRB	1	0
4	B	400	NAD	1	0
5	B	401	CRB	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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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