



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:34 am GMT

PDB ID : 1ORR  
Title : Crystal Structure of CDP-Tyvelose 2-Epimerase complexed with NAD and CDP  
Authors : Koropatkin, N.M.; Liu, H.; Holden, H.M.  
Deposited on : 2003-03-14  
Resolution : 1.50 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](mailto: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.

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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 : trunk28620  
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) : recalc28949

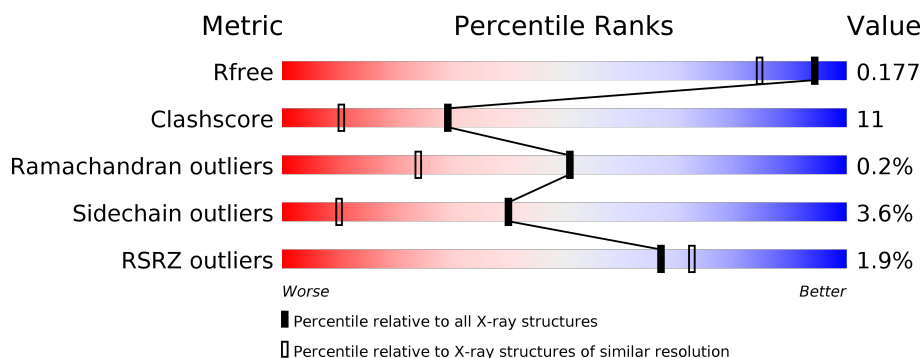
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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))
$R_{free}$	100719	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (1.50-1.50)

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  $\geq 3$ , 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	347	<div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	347	<div> <div>2%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	C	347	<div> <div>5%</div> <div>68%</div> <div>25%</div> <div>• •</div> </div>
1	D	347	<div> <div>2%</div> <div>67%</div> <div>25%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12059 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 CDP-tyvelose-2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	11	0
			2706	1712	458	520	16			
1	B	338	Total	C	N	O	S	0	4	0
			2676	1695	451	514	16			
1	C	335	Total	C	N	O	S	0	6	0
			2661	1686	448	511	16			
1	D	336	Total	C	N	O	S	0	5	0
			2661	1685	450	510	16			

There are 40 discrepancies between the modelled and reference sequences:

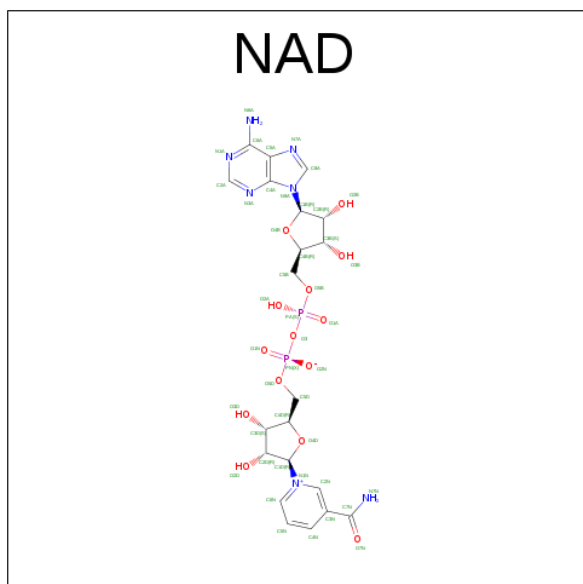
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P14169
A	2	ALA	-	CLONING ARTIFACT	UNP P14169
A	340	LEU	-	EXPRESSION TAG	UNP P14169
A	341	GLU	-	EXPRESSION TAG	UNP P14169
A	342	HIS	-	EXPRESSION TAG	UNP P14169
A	343	HIS	-	EXPRESSION TAG	UNP P14169
A	344	HIS	-	EXPRESSION TAG	UNP P14169
A	345	HIS	-	EXPRESSION TAG	UNP P14169
A	346	HIS	-	EXPRESSION TAG	UNP P14169
A	347	HIS	-	EXPRESSION TAG	UNP P14169
B	1	MET	-	CLONING ARTIFACT	UNP P14169
B	2	ALA	-	CLONING ARTIFACT	UNP P14169
B	340	LEU	-	EXPRESSION TAG	UNP P14169
B	341	GLU	-	EXPRESSION TAG	UNP P14169
B	342	HIS	-	EXPRESSION TAG	UNP P14169
B	343	HIS	-	EXPRESSION TAG	UNP P14169
B	344	HIS	-	EXPRESSION TAG	UNP P14169
B	345	HIS	-	EXPRESSION TAG	UNP P14169
B	346	HIS	-	EXPRESSION TAG	UNP P14169
B	347	HIS	-	EXPRESSION TAG	UNP P14169
C	1	MET	-	CLONING ARTIFACT	UNP P14169

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	CLONING ARTIFACT	UNP P14169
C	340	LEU	-	EXPRESSION TAG	UNP P14169
C	341	GLU	-	EXPRESSION TAG	UNP P14169
C	342	HIS	-	EXPRESSION TAG	UNP P14169
C	343	HIS	-	EXPRESSION TAG	UNP P14169
C	344	HIS	-	EXPRESSION TAG	UNP P14169
C	345	HIS	-	EXPRESSION TAG	UNP P14169
C	346	HIS	-	EXPRESSION TAG	UNP P14169
C	347	HIS	-	EXPRESSION TAG	UNP P14169
D	1	MET	-	CLONING ARTIFACT	UNP P14169
D	2	ALA	-	CLONING ARTIFACT	UNP P14169
D	340	LEU	-	EXPRESSION TAG	UNP P14169
D	341	GLU	-	EXPRESSION TAG	UNP P14169
D	342	HIS	-	EXPRESSION TAG	UNP P14169
D	343	HIS	-	EXPRESSION TAG	UNP P14169
D	344	HIS	-	EXPRESSION TAG	UNP P14169
D	345	HIS	-	EXPRESSION TAG	UNP P14169
D	346	HIS	-	EXPRESSION TAG	UNP P14169
D	347	HIS	-	EXPRESSION TAG	UNP P14169

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



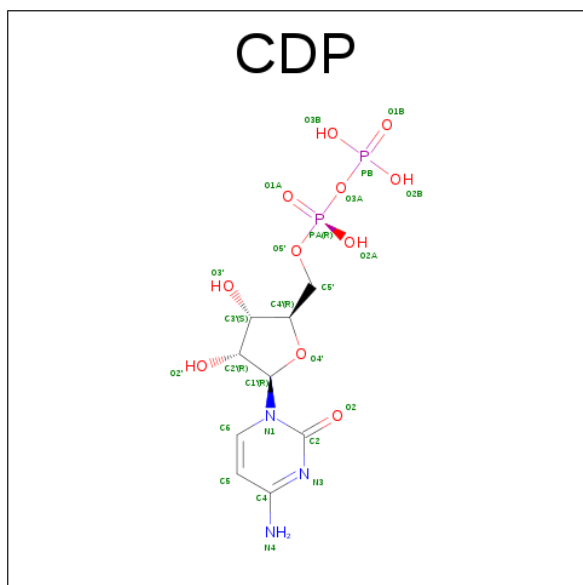
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			44	21	7	14	2	

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

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula:  $C_9H_{15}N_3O_{11}P_2$ ).

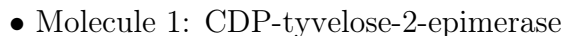
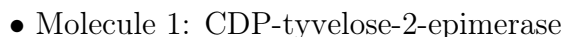


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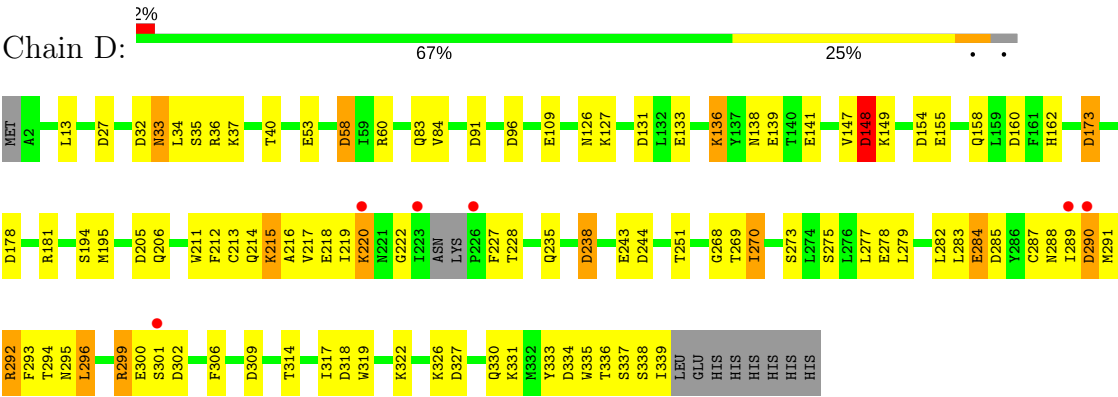
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	259	Total	O	0	0
			259	259		
4	D	233	Total	O	0	0
			233	233		



- Molecule 1: CDP-tyvelose-2-epimerase



● Molecule 1: CDP-tyvelose-2-epimerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.00Å 168.10Å 89.60Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 47.01 – 1.46	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-1.50) 95.4 (47.01-1.46)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.75 (at 1.46Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.178 , 0.229 0.175 , 0.177	Depositor DCC
$R_{free}$ test set	20900 reflections (11.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.6	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 80.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDP, 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	0.87	10/2828 (0.4%)	1.31	43/3830 (1.1%)
1	B	0.88	8/2761 (0.3%)	1.30	32/3738 (0.9%)
1	C	0.87	12/2757 (0.4%)	1.32	42/3729 (1.1%)
1	D	0.90	10/2740 (0.4%)	1.32	42/3704 (1.1%)
All	All	0.88	40/11086 (0.4%)	1.31	159/15001 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	0
All	All	2	0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	218	GLU	CD-OE2	7.30	1.33	1.25
1	D	278	GLU	CD-OE2	7.02	1.33	1.25
1	C	155	GLU	CD-OE2	6.87	1.33	1.25
1	C	284	GLU	CD-OE2	6.69	1.33	1.25
1	D	133	GLU	CD-OE2	6.65	1.32	1.25

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	A	292	ARG	NE-CZ-NH1	9.43	125.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	A	302	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	96	ASP	CB-CG-OD2	-8.21	110.91	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	300	GLU	CA
1	C	299	ARG	CA

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	2706	0	2639	67	0
1	B	2676	0	2612	49	0
1	C	2661	0	2592	68	0
1	D	2661	0	2584	60	0
2	A	44	0	26	4	0
2	B	44	0	26	0	0
2	C	44	0	26	3	0
2	D	44	0	26	1	0
3	A	25	0	12	0	0
3	B	25	0	12	0	0
3	C	25	0	12	1	0
3	D	25	0	12	1	0
4	A	310	0	0	12	0
4	B	277	0	0	5	0
4	C	259	0	0	4	0
4	D	233	0	0	6	0
All	All	12059	0	10579	233	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 11.

The worst 5 of 233 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:125[C]:THR:HG22	1:C:127:LYS:H	1.00	1.11
1:C:218:GLU:HA	1:C:223:ILE:HD12	1.34	1.05
1:C:218:GLU:HB3	1:C:223:ILE:HB	1.42	0.99
1:B:134:GLN:H	1:B:134:GLN:HE21	1.14	0.94
1:C:125[C]:THR:HG22	1:C:127:LYS:N	1.85	0.90

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	350/347 (101%)	339 (97%)	11 (3%)	0	100	100
1	B	342/347 (99%)	332 (97%)	10 (3%)	0	100	100
1	C	337/347 (97%)	325 (96%)	11 (3%)	1 (0%)	44	19
1	D	337/347 (97%)	319 (95%)	17 (5%)	1 (0%)	44	19
All	All	1366/1388 (98%)	1315 (96%)	49 (4%)	2 (0%)	51	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	GLY
1	D	301	SER

### 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	306/301 (102%)	300 (98%)	6 (2%)	60	28
1	B	298/301 (99%)	289 (97%)	9 (3%)	46	14
1	C	297/301 (99%)	284 (96%)	13 (4%)	33	6
1	D	294/301 (98%)	278 (95%)	16 (5%)	26	4
All	All	1195/1204 (99%)	1151 (96%)	44 (4%)	40	9

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	281	LYS
1	C	299	ARG
1	D	322[B]	LYS
1	C	282	LEU
1	C	288	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	330	GLN
1	C	44	HIS
1	D	33	ASN
1	B	200	GLN
1	B	206	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

8 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	NAD	A	1200	-	41,48,48	1.81	6 (14%)	43,73,73	1.78	5 (11%)
3	CDP	A	1201	-	22,26,26	1.38	5 (22%)	23,40,40	1.35	2 (8%)
2	NAD	B	1300	-	41,48,48	1.86	6 (14%)	43,73,73	1.73	7 (16%)
3	CDP	B	1301	-	22,26,26	1.38	5 (22%)	23,40,40	1.26	2 (8%)
2	NAD	C	1400	-	41,48,48	2.06	8 (19%)	43,73,73	1.48	3 (6%)
3	CDP	C	1401	-	22,26,26	1.49	5 (22%)	23,40,40	1.43	3 (13%)
2	NAD	D	1500	-	41,48,48	1.88	5 (12%)	43,73,73	1.64	4 (9%)
3	CDP	D	1501	-	22,26,26	1.37	3 (13%)	23,40,40	1.41	4 (17%)

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	NAD	A	1200	-	-	0/22/62/62	0/5/5/5
3	CDP	A	1201	-	-	0/12/32/32	0/2/2/2
2	NAD	B	1300	-	-	0/22/62/62	0/5/5/5
3	CDP	B	1301	-	-	0/12/32/32	0/2/2/2
2	NAD	C	1400	-	-	0/22/62/62	0/5/5/5
3	CDP	C	1401	-	-	0/12/32/32	0/2/2/2
2	NAD	D	1500	-	-	0/22/62/62	0/5/5/5
3	CDP	D	1501	-	-	0/12/32/32	0/2/2/2

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1300	NAD	C3N-C7N	-4.11	1.44	1.50
2	A	1200	NAD	C3N-C7N	-3.15	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1200	NAD	O4B-C1B	-2.98	1.37	1.41
3	C	1401	CDP	C6-C5	-2.91	1.31	1.38
2	D	1500	NAD	C6N-C5N	-2.90	1.32	1.38

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1200	NAD	C5N-C4N-C3N	-8.79	110.01	120.35
2	B	1300	NAD	C5N-C4N-C3N	-6.95	112.18	120.35
2	C	1400	NAD	C5N-C4N-C3N	-6.71	112.45	120.35
2	D	1500	NAD	C5N-C4N-C3N	-4.98	114.50	120.35
2	D	1500	NAD	O7N-C7N-C3N	-4.35	114.54	119.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1200	NAD	4	0
2	C	1400	NAD	3	0
3	C	1401	CDP	1	0
2	D	1500	NAD	1	0
3	D	1501	CDP	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	338/347 (97%)	-0.63	1 (0%) 93 94	11, 18, 48, 75	0
1	B	338/347 (97%)	-0.66	2 (0%) 89 91	11, 19, 50, 95	0
1	C	335/347 (96%)	-0.20	17 (5%) 29 32	11, 21, 57, 95	0
1	D	336/347 (96%)	-0.34	6 (1%) 69 74	11, 20, 58, 90	0
All	All	1347/1388 (97%)	-0.46	26 (1%) 67 72	11, 19, 55, 95	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	ILE	7.0
1	D	289	ILE	5.2
1	C	333	TYR	4.1
1	C	339	ILE	3.7
1	C	282	LEU	3.6

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CDP	A	1201	25/25	0.97	0.07	0.03	14,21,45,100	0
3	CDP	D	1501	25/25	0.96	0.07	-0.00	15,22,62,100	0
3	CDP	B	1301	25/25	0.97	0.06	-0.24	15,23,32,100	0
2	NAD	B	1300	44/44	0.99	0.05	-0.27	12,15,28,95	0
2	NAD	A	1200	44/44	0.99	0.05	-0.39	11,15,24,37	0
2	NAD	D	1500	44/44	0.99	0.05	-0.53	11,15,18,23	0
3	CDP	C	1401	25/25	0.95	0.08	-0.76	19,25,100,100	0
2	NAD	C	1400	44/44	0.99	0.05	-0.88	11,16,26,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.