



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:58 PM GMT

PDB ID : 1DFI  
Title : X-RAY STRUCTURE OF ESCHERICHIA COLI ENOYL REDUCTASE  
WITH BOUND NAD  
Authors : Baldock, C.; Rafferty, J.B.; Rice, D.W.  
Deposited on : 1997-01-16  
Resolution : 2.09 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](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.

---

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

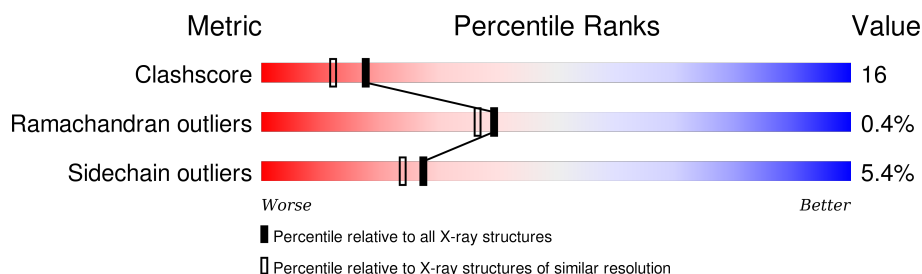
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	
1	D	261	

## 2 Entry composition [i](#)

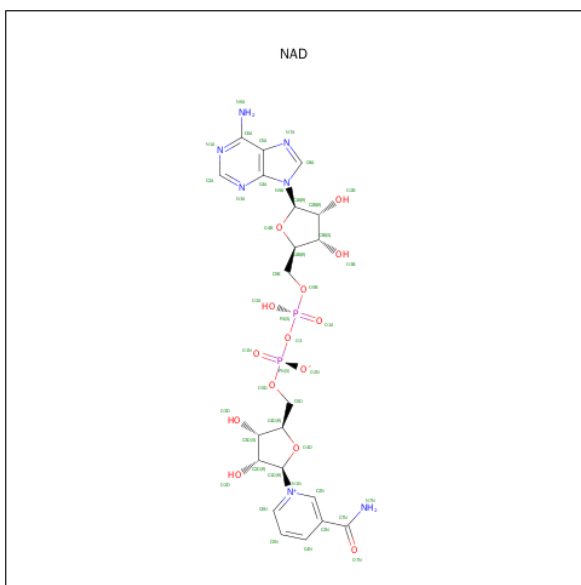
There are 3 unique types of molecules in this entry. The entry contains 7839 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENOYL ACYL CARRIER PROTEIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1834	1155	315	351	13			
1	B	247	Total	C	N	O	S	0	0	0
			1834	1155	315	351	13			
1	C	247	Total	C	N	O	S	0	0	0
			1834	1155	315	351	13			
1	D	247	Total	C	N	O	S	0	0	0
			1834	1155	315	351	13			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 water.

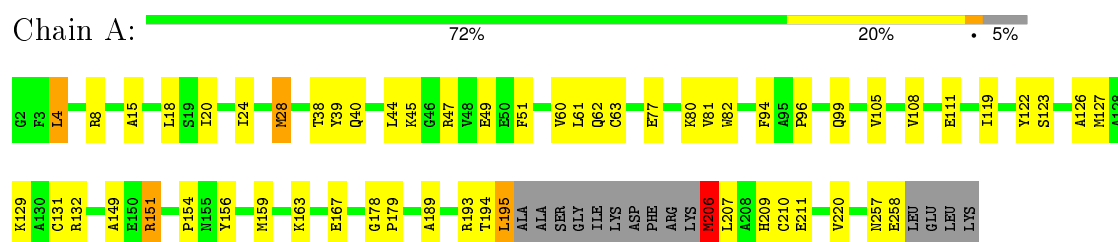
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	84	Total	O	0	0
			84	84		
3	C	80	Total	O	0	0
			80	80		
3	D	73	Total	O	0	0
			73	73		

### 3 Residue-property plots

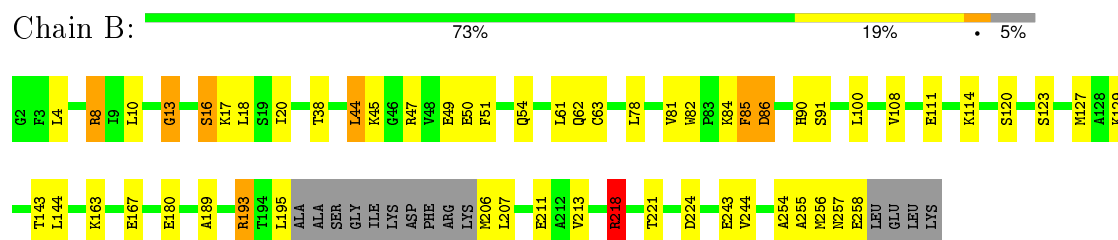
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

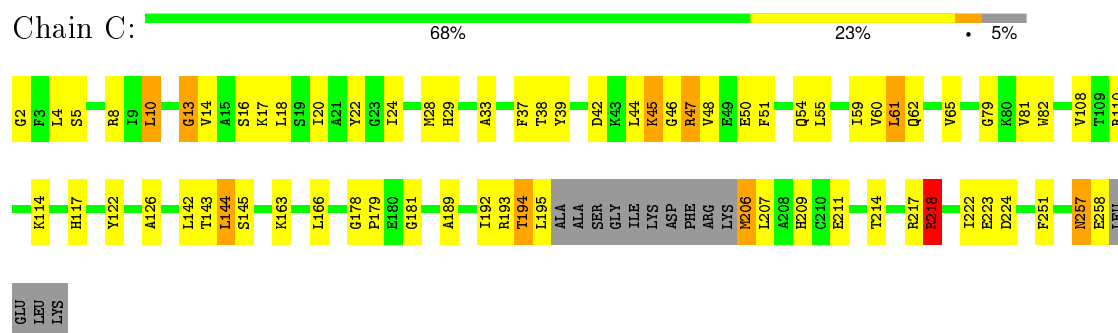
#### • Molecule 1: ENOYL ACYL CARRIER PROTEIN REDUCTASE



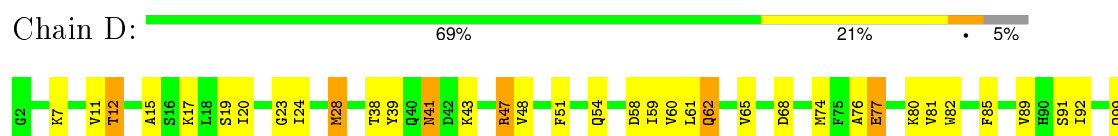
#### • Molecule 1: ENOYL ACYL CARRIER PROTEIN REDUCTASE

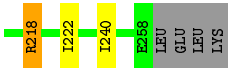
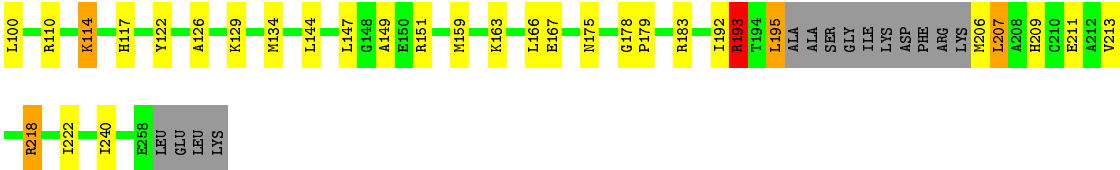


#### • Molecule 1: ENOYL ACYL CARRIER PROTEIN REDUCTASE



#### • Molecule 1: ENOYL ACYL CARRIER PROTEIN REDUCTASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.00 Å   81.20 Å   79.00 Å 90.00°   92.90°   90.00°	Depositor
Resolution (Å)	10.00 – 2.09	Depositor
% Data completeness (in resolution range)	93.0 (10.00-2.09)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7839	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 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

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	0.76	0/1864	0.83	4/2519 (0.2%)
1	B	1.04	1/1864 (0.1%)	0.97	5/2519 (0.2%)
1	C	0.76	1/1864 (0.1%)	0.86	2/2519 (0.1%)
1	D	0.82	2/1864 (0.1%)	0.91	6/2519 (0.2%)
All	All	0.86	4/7456 (0.1%)	0.89	17/10076 (0.2%)

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	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	PHE	C-N	28.54	1.99	1.34
1	D	11	VAL	C-N	-11.26	1.08	1.34
1	C	10	LEU	C-N	6.36	1.48	1.34
1	D	77	GLU	CD-OE2	5.58	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	PHE	C-N-CA	-19.27	73.52	121.70
1	B	13	GLY	O-C-N	-11.89	103.68	122.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	GLY	O-C-N	-10.52	105.86	122.70
1	D	218	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	193	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	D	218	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	D	11	VAL	C-N-CA	6.61	138.23	121.70
1	A	151	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	C	218	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	74	MET	CG-SD-CE	5.92	109.67	100.20
1	B	218	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	159	MET	CG-SD-CE	5.85	109.56	100.20
1	D	28	MET	CG-SD-CE	5.77	109.44	100.20
1	A	206	MET	CG-SD-CE	5.77	109.43	100.20
1	A	28	MET	CG-SD-CE	5.68	109.30	100.20
1	B	8	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	85	PHE	O-C-N	5.11	130.88	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	13	GLY	Mainchain
1	C	13	GLY	Mainchain
1	D	167	GLU	Mainchain

## 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	1834	0	1816	49	0
1	B	1834	0	1815	47	0
1	C	1834	0	1816	73	0
1	D	1834	0	1815	70	0
2	A	44	0	25	6	0
2	B	44	0	25	10	0
2	C	44	0	24	7	0
2	D	44	0	24	4	0
3	A	90	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	84	0	0	1	0
3	C	80	0	0	4	0
3	D	73	0	0	2	0
All	All	7839	0	7360	237	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 16.

All (237) 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:B:85:PHE:C	1:B:86:ASP:HA	1.58	1.21
1:A:156:TYR:N	3:A:581:HOH:O	1.69	1.20
1:B:85:PHE:C	1:B:86:ASP:CA	2.11	1.18
1:B:85:PHE:C	1:B:86:ASP:N	1.99	1.16
1:D:192:ILE:HB	1:D:195:LEU:CD2	1.75	1.16
1:D:61:LEU:HD22	1:D:77:GLU:OE2	1.48	1.13
1:B:85:PHE:O	1:B:86:ASP:HA	1.57	1.04
1:D:47:ARG:HG2	1:D:51:PHE:CZ	1.92	1.04
1:D:206:MET:O	1:D:209:HIS:HB3	1.59	1.02
1:D:61:LEU:CD2	1:D:77:GLU:OE2	2.07	1.00
1:D:47:ARG:HG2	1:D:51:PHE:HZ	1.28	0.94
1:D:192:ILE:HB	1:D:195:LEU:HD23	1.48	0.94
1:A:20:ILE:HG13	1:A:195:LEU:CD2	1.98	0.93
1:D:207:LEU:HD12	1:D:207:LEU:N	1.85	0.92
1:C:29:HIS:ND1	3:C:553:HOH:O	2.03	0.92
1:C:22:TYR:OH	1:C:54:GLN:OE1	1.88	0.91
1:C:42:ASP:HB2	3:C:561:HOH:O	1.72	0.88
1:C:59:ILE:HG22	1:C:61:LEU:HD11	1.57	0.87
1:D:23:GLY:HA3	1:D:222:ILE:HG22	1.55	0.87
1:D:47:ARG:HG3	1:D:47:ARG:HH11	1.38	0.87
1:D:47:ARG:CG	1:D:47:ARG:HH11	1.87	0.87
1:A:20:ILE:HG13	1:A:195:LEU:HD21	1.58	0.86
1:D:192:ILE:HB	1:D:195:LEU:HD22	1.58	0.86
1:B:163:LYS:NZ	2:B:501:NAD:O2D	2.09	0.86
1:B:193:ARG:HG3	1:B:207:LEU:HD13	1.56	0.85
1:D:193:ARG:HH22	1:D:211:GLU:CD	1.79	0.85
1:C:194:THR:OG1	1:C:195:LEU:N	2.08	0.84
2:A:501:NAD:H2N	2:A:501:NAD:O1N	1.78	0.83
1:C:108:VAL:O	1:D:129:LYS:HE3	1.79	0.83
1:D:207:LEU:CD1	1:D:207:LEU:N	2.43	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ASN:OD1	1:D:43:LYS:HB3	1.79	0.81
1:D:206:MET:HG2	1:D:207:LEU:HD12	1.62	0.81
1:C:206:MET:HG3	1:C:207:LEU:N	1.94	0.80
1:D:207:LEU:CD1	1:D:207:LEU:H	1.95	0.80
1:A:195:LEU:HD21	2:A:501:NAD:O2N	1.83	0.79
1:C:206:MET:O	1:C:209:HIS:HB3	1.84	0.78
1:A:154:PRO:O	3:A:581:HOH:O	2.02	0.77
1:D:193:ARG:NH2	1:D:211:GLU:CD	2.37	0.77
1:C:44:LEU:HD13	1:C:47:ARG:NH2	1.99	0.77
1:C:59:ILE:HG22	1:C:61:LEU:CD1	2.14	0.76
1:D:193:ARG:NH2	1:D:211:GLU:OE2	2.19	0.75
1:C:59:ILE:CG2	1:C:61:LEU:HD11	2.16	0.75
1:C:10:LEU:HD11	1:C:38:THR:HG23	1.70	0.73
1:B:78:LEU:O	1:B:81:VAL:HG12	1.87	0.73
1:B:20:ILE:N	2:B:501:NAD:O2N	2.20	0.71
1:C:61:LEU:N	1:C:61:LEU:HD12	2.06	0.71
2:D:501:NAD:H2N	2:D:501:NAD:O1N	1.90	0.71
1:D:206:MET:CE	1:D:207:LEU:HD11	2.22	0.69
1:C:10:LEU:HD11	1:C:38:THR:CG2	2.24	0.68
1:D:23:GLY:HA3	1:D:222:ILE:CG2	2.24	0.67
1:A:108:VAL:O	1:B:129:LYS:HE3	1.93	0.67
2:C:501:NAD:O1N	2:C:501:NAD:H2N	1.95	0.66
1:C:47:ARG:HG2	1:C:51:PHE:CZ	2.31	0.66
1:D:206:MET:HE2	1:D:207:LEU:CD1	2.27	0.65
1:C:60:VAL:C	1:C:61:LEU:HD12	2.18	0.64
1:D:12:THR:HG22	1:D:91:SER:H	1.62	0.64
1:B:218:ARG:NH2	1:B:224:ASP:OD2	2.26	0.64
1:B:207:LEU:O	1:B:211:GLU:HG3	1.98	0.64
1:D:38:THR:HA	1:D:61:LEU:O	1.99	0.63
1:A:156:TYR:HB2	3:A:581:HOH:O	1.97	0.63
1:B:254:ALA:HB1	1:B:257:ASN:OD1	1.99	0.63
1:D:206:MET:HE2	1:D:207:LEU:HD11	1.81	0.63
1:C:189:ALA:HB3	2:C:501:NAD:H5N	1.80	0.63
1:D:12:THR:HB	1:D:89:VAL:O	1.99	0.61
1:A:24:ILE:O	1:A:28:MET:HG3	2.00	0.61
1:D:206:MET:CG	1:D:207:LEU:HD12	2.31	0.61
1:C:110:ARG:NH2	1:D:68:ASP:OD1	2.30	0.61
1:C:24:ILE:O	1:C:28:MET:HG3	2.01	0.61
1:A:156:TYR:CA	3:A:581:HOH:O	2.34	0.61
1:D:76:ALA:O	1:D:80:LYS:HD2	2.01	0.60
1:B:38:THR:HA	1:B:61:LEU:O	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HA	1:D:222:ILE:HG23	1.83	0.60
1:B:144:LEU:HB3	2:B:501:NAD:H1D	1.83	0.60
1:B:86:ASP:OD1	1:B:86:ASP:N	2.35	0.60
1:A:77:GLU:OE1	1:A:80:LYS:HE3	2.01	0.60
1:A:39:TYR:CZ	1:A:62:GLN:HB2	2.37	0.60
2:A:501:NAD:O3D	3:A:591:HOH:O	2.15	0.60
1:B:20:ILE:HG13	1:B:195:LEU:HD21	1.84	0.60
1:A:122:TYR:CE2	1:A:126:ALA:HB2	2.36	0.60
1:B:8:ARG:O	1:B:86:ASP:N	2.35	0.59
1:A:20:ILE:HG13	1:A:195:LEU:HD23	1.82	0.59
1:A:38:THR:HA	1:A:61:LEU:O	2.01	0.59
1:B:47:ARG:O	1:B:50:GLU:HB3	2.01	0.59
1:C:51:PHE:O	1:C:54:GLN:HB3	2.02	0.59
1:B:144:LEU:HB2	2:B:501:NAD:O3D	2.02	0.59
1:C:8:ARG:HG2	1:C:82:TRP:CE2	2.37	0.59
1:B:20:ILE:HB	2:B:501:NAD:O2N	2.03	0.58
1:D:207:LEU:H	1:D:207:LEU:HD13	1.68	0.57
1:A:45:LYS:O	1:A:49:GLU:HG3	2.04	0.57
1:C:144:LEU:HD23	1:C:144:LEU:N	2.19	0.57
1:A:47:ARG:HG2	1:A:51:PHE:CE2	2.40	0.57
1:D:159:MET:CE	1:D:163:LYS:HE2	2.35	0.57
1:C:206:MET:HG3	1:C:207:LEU:H	1.69	0.57
1:C:61:LEU:N	1:C:61:LEU:CD1	2.67	0.57
1:D:61:LEU:HD22	1:D:77:GLU:CD	2.25	0.57
1:D:175:ASN:ND2	3:D:557:HOH:O	2.38	0.57
1:C:38:THR:HA	1:C:61:LEU:O	2.05	0.56
1:B:189:ALA:HB3	2:B:501:NAD:H5N	1.86	0.56
1:C:189:ALA:HB3	2:C:501:NAD:C5N	2.35	0.56
1:D:39:TYR:CZ	1:D:62:GLN:HB2	2.40	0.56
1:A:193:ARG:HG3	1:A:207:LEU:HD13	1.87	0.56
1:C:222:ILE:HG13	1:C:223:GLU:OE2	2.05	0.56
1:A:123:SER:O	1:A:127:MET:HG3	2.05	0.55
1:C:143:THR:C	1:C:144:LEU:HD23	2.27	0.55
1:D:61:LEU:HD21	1:D:77:GLU:OE2	2.02	0.55
1:D:48:VAL:HA	1:D:51:PHE:CD2	2.42	0.55
1:C:144:LEU:N	1:C:144:LEU:CD2	2.69	0.55
1:D:7:LYS:HE3	3:D:560:HOH:O	2.05	0.55
1:D:19:SER:HB2	2:D:501:NAD:O2A	2.07	0.54
1:D:47:ARG:HG3	1:D:47:ARG:NH1	2.11	0.54
1:C:2:GLY:N	1:C:5:SER:HG	2.05	0.54
1:B:163:LYS:O	1:B:167:GLU:HG3	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:HG12	1:D:82:TRP:CD1	2.44	0.53
1:C:39:TYR:HB3	1:C:48:VAL:HG21	1.90	0.53
1:D:149:ALA:HB2	1:D:163:LYS:HB3	1.92	0.52
1:B:44:LEU:HD13	1:B:44:LEU:N	2.24	0.52
1:C:144:LEU:HB3	2:C:501:NAD:H1D	1.91	0.52
1:A:209:HIS:CE1	1:A:258:GLU:HG2	2.45	0.52
1:C:44:LEU:O	1:C:45:LYS:C	2.48	0.51
1:B:123:SER:O	1:B:127:MET:HG3	2.11	0.51
1:A:20:ILE:CG1	1:A:195:LEU:HD23	2.40	0.51
1:C:14:VAL:HG21	1:C:37:PHE:HE1	1.76	0.51
1:D:48:VAL:HA	1:D:51:PHE:HD2	1.76	0.51
1:A:15:ALA:HA	1:A:44:LEU:HD21	1.93	0.51
1:B:20:ILE:HG13	1:B:195:LEU:CD2	2.41	0.50
1:C:122:TYR:CE2	1:C:126:ALA:HB2	2.46	0.50
1:B:206:MET:O	1:B:206:MET:HG2	2.10	0.50
1:B:10:LEU:HD11	1:B:38:THR:HG23	1.92	0.50
1:B:62:GLN:HG2	1:B:63:CYS:N	2.24	0.50
1:C:163:LYS:NZ	2:C:501:NAD:O2D	2.41	0.50
1:A:20:ILE:CG1	1:A:195:LEU:CD2	2.82	0.49
2:A:501:NAD:C5D	2:A:501:NAD:O5B	2.60	0.49
1:A:18:LEU:HD22	1:A:194:THR:HB	1.94	0.49
1:D:159:MET:HE1	1:D:163:LYS:HE2	1.94	0.49
1:A:129:LYS:HE3	1:B:108:VAL:O	2.13	0.49
1:C:251:PHE:CG	3:C:573:HOH:O	2.64	0.49
1:C:206:MET:CG	1:C:207:LEU:N	2.73	0.49
1:A:94:PHE:HB3	1:A:119:ILE:HG21	1.95	0.49
1:D:24:ILE:O	1:D:28:MET:HG3	2.13	0.48
1:C:206:MET:O	1:C:209:HIS:N	2.45	0.48
1:C:207:LEU:O	1:C:211:GLU:HG3	2.13	0.48
1:B:221:THR:O	1:B:224:ASP:HB2	2.14	0.48
1:D:85:PHE:CE1	1:D:134:MET:HE2	2.48	0.48
1:B:91:SER:OG	2:B:501:NAD:H4D	2.14	0.48
1:A:8:ARG:NH1	1:A:82:TRP:CD1	2.76	0.48
1:B:45:LYS:O	1:B:49:GLU:HB2	2.14	0.47
1:C:20:ILE:HD11	1:C:192:ILE:HD12	1.96	0.47
1:C:145:SER:O	2:C:501:NAD:H6N	2.13	0.47
1:B:189:ALA:HB3	2:B:501:NAD:C5N	2.44	0.47
1:C:51:PHE:O	1:C:55:LEU:HG	2.14	0.47
1:C:222:ILE:CG1	1:C:223:GLU:OE2	2.63	0.47
1:A:149:ALA:HB2	1:A:163:LYS:HB3	1.97	0.47
1:C:79:GLY:HA2	1:C:82:TRP:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:MET:HG2	1:D:207:LEU:N	2.29	0.47
1:B:81:VAL:CG1	1:B:82:TRP:N	2.78	0.47
1:D:12:THR:HG23	1:D:92:ILE:HD11	1.96	0.46
1:A:220:VAL:HG22	3:A:559:HOH:O	2.15	0.46
1:D:178:GLY:N	1:D:179:PRO:CD	2.78	0.46
1:C:16:SER:OG	1:C:17:LYS:N	2.45	0.46
1:A:77:GLU:OE1	1:A:77:GLU:HA	2.15	0.46
1:C:178:GLY:N	1:C:179:PRO:CD	2.78	0.46
1:A:96:PRO:O	1:A:99:GLN:HB2	2.15	0.46
1:C:17:LYS:HB3	1:C:17:LYS:HE2	1.67	0.46
1:B:255:ALA:O	1:B:256:MET:HB2	2.16	0.46
1:D:47:ARG:NH1	1:D:47:ARG:CG	2.59	0.46
1:D:122:TYR:CE2	1:D:126:ALA:HB2	2.51	0.46
1:A:8:ARG:HD3	1:A:82:TRP:CE2	2.52	0.45
1:C:181:GLY:O	3:C:533:HOH:O	2.20	0.45
1:B:51:PHE:O	1:B:54:GLN:HB2	2.16	0.45
1:D:206:MET:HE3	1:D:207:LEU:HD11	1.97	0.45
1:C:44:LEU:O	1:C:46:GLY:N	2.49	0.45
1:D:183:ARG:HD2	1:D:240:ILE:O	2.16	0.45
1:A:178:GLY:N	1:A:179:PRO:CD	2.79	0.45
1:C:214:THR:O	1:C:217:ARG:N	2.44	0.45
1:C:39:TYR:CZ	1:C:62:GLN:HB2	2.52	0.45
1:D:206:MET:HB3	1:D:206:MET:HE2	1.67	0.45
1:C:44:LEU:HD13	1:C:47:ARG:CZ	2.46	0.45
1:C:142:LEU:HG	1:C:143:THR:N	2.32	0.45
1:A:156:TYR:CB	3:A:581:HOH:O	2.54	0.45
1:C:22:TYR:CZ	1:C:54:GLN:OE1	2.68	0.45
1:C:39:TYR:CE1	1:C:60:VAL:HG12	2.52	0.45
1:C:143:THR:C	1:C:144:LEU:CD2	2.85	0.45
1:C:44:LEU:HD13	1:C:44:LEU:HA	1.85	0.44
1:A:149:ALA:HB2	1:A:163:LYS:CB	2.48	0.44
2:B:501:NAD:O5B	2:B:501:NAD:H51N	2.17	0.44
1:B:213:VAL:O	1:B:213:VAL:HG12	2.16	0.44
1:D:207:LEU:O	1:D:211:GLU:HG3	2.18	0.44
1:A:49:GLU:HA	1:A:60:VAL:HG21	1.98	0.44
1:A:108:VAL:O	1:B:129:LYS:CE	2.64	0.44
1:A:45:LYS:HE3	1:A:49:GLU:OE2	2.18	0.44
1:C:47:ARG:HG2	1:C:51:PHE:HZ	1.79	0.44
1:D:60:VAL:O	1:D:61:LEU:HD23	2.18	0.44
1:C:65:VAL:HG22	2:C:501:NAD:N1A	2.33	0.44
1:A:62:GLN:HG2	1:A:63:CYS:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:HG3	1:B:244:VAL:N	2.33	0.43
1:C:257:ASN:O	1:C:258:GLU:C	2.55	0.43
1:B:257:ASN:O	1:B:258:GLU:HB2	2.19	0.43
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.65	0.43
1:B:8:ARG:NH2	3:B:524:HOH:O	1.89	0.43
1:A:207:LEU:O	1:A:211:GLU:HG3	2.19	0.43
1:D:206:MET:O	1:D:209:HIS:CB	2.47	0.43
1:B:213:VAL:O	1:B:213:VAL:CG1	2.65	0.43
1:A:131:CYS:O	1:A:132:ARG:C	2.57	0.43
1:B:81:VAL:HG13	1:B:82:TRP:N	2.33	0.43
1:C:218:ARG:NH2	1:C:224:ASP:OD2	2.47	0.43
1:A:40:GLN:HG3	2:A:501:NAD:C2A	2.49	0.43
1:A:206:MET:O	1:A:209:HIS:N	2.50	0.43
1:D:147:LEU:HD12	1:D:147:LEU:HA	1.83	0.43
1:D:15:ALA:HB2	2:D:501:NAD:O3B	2.19	0.42
1:D:51:PHE:O	1:D:54:GLN:HB2	2.19	0.42
1:C:47:ARG:O	1:C:50:GLU:HB3	2.19	0.42
1:B:84:LYS:HA	1:B:84:LYS:HD3	1.78	0.42
1:C:114:LYS:HG2	1:D:114:LYS:HE3	2.01	0.42
1:D:99:GLN:O	1:D:100:LEU:HD23	2.20	0.42
1:C:81:VAL:HG23	1:C:82:TRP:N	2.35	0.42
1:D:77:GLU:HA	1:D:80:LYS:CD	2.50	0.42
1:C:47:ARG:HB2	1:C:47:ARG:HE	1.51	0.42
1:C:108:VAL:O	1:D:129:LYS:CE	2.58	0.42
1:C:4:LEU:HA	1:C:4:LEU:HD23	1.65	0.42
1:A:163:LYS:O	1:A:167:GLU:HG3	2.20	0.41
1:C:44:LEU:HD22	1:C:44:LEU:N	2.35	0.41
2:B:501:NAD:C5D	2:B:501:NAD:O5B	2.69	0.41
1:C:117:HIS:CD2	1:D:117:HIS:CD2	3.08	0.41
1:D:65:VAL:HG22	2:D:501:NAD:N1A	2.36	0.41
1:A:105:VAL:O	1:B:129:LYS:HE2	2.19	0.41
1:A:8:ARG:HD3	1:A:82:TRP:CD1	2.56	0.41
1:A:4:LEU:HA	1:A:4:LEU:HD12	1.88	0.41
1:A:189:ALA:HB3	2:A:501:NAD:C5N	2.51	0.41
1:C:47:ARG:HG2	1:C:51:PHE:CE2	2.56	0.41
1:C:8:ARG:HG2	1:C:82:TRP:CZ2	2.56	0.41
1:A:81:VAL:HG23	1:A:82:TRP:N	2.36	0.41
1:D:12:THR:CG2	1:D:92:ILE:CD1	2.98	0.40
1:D:209:HIS:O	1:D:213:VAL:HG22	2.21	0.40
1:C:4:LEU:HB3	1:C:33:ALA:HB2	2.03	0.40
1:B:16:SER:OG	1:B:17:LYS:N	2.54	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ILE:HD11	1:D:81:VAL:HG11	2.03	0.40
1:B:90:HIS:O	1:B:143:THR:HA	2.21	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	243/261 (93%)	235 (97%)	8 (3%)	0	100	100
1	B	243/261 (93%)	236 (97%)	7 (3%)	0	100	100
1	C	243/261 (93%)	233 (96%)	6 (2%)	4 (2%)	12	6
1	D	243/261 (93%)	237 (98%)	6 (2%)	0	100	100
All	All	972/1044 (93%)	941 (97%)	27 (3%)	4 (0%)	39	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	45	LYS
1	C	194	THR
1	C	257	ASN
1	C	193	ARG

### 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	189/200 (94%)	182 (96%)	7 (4%)	41	41
1	B	189/200 (94%)	177 (94%)	12 (6%)	22	18
1	C	189/200 (94%)	182 (96%)	7 (4%)	41	41
1	D	189/200 (94%)	174 (92%)	15 (8%)	15	11
All	All	756/800 (94%)	715 (95%)	41 (5%)	27	24

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	111	GLU
1	A	151	ARG
1	A	195	LEU
1	A	206	MET
1	A	210	CYS
1	A	257	ASN
1	B	4	LEU
1	B	16	SER
1	B	18	LEU
1	B	44	LEU
1	B	86	ASP
1	B	100	LEU
1	B	111	GLU
1	B	114	LYS
1	B	120	SER
1	B	180	GLU
1	B	193	ARG
1	B	218	ARG
1	C	18	LEU
1	C	47	ARG
1	C	61	LEU
1	C	144	LEU
1	C	166	LEU
1	C	206	MET
1	C	218	ARG
1	D	12	THR
1	D	17	LYS
1	D	41	ASN
1	D	47	ARG
1	D	58	ASP
1	D	62	GLN
1	D	110	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	114	LYS
1	D	144	LEU
1	D	151	ARG
1	D	166	LEU
1	D	193	ARG
1	D	195	LEU
1	D	207	LEU
1	D	218	ARG

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	26	GLN
1	A	209	HIS
1	B	26	GLN
1	B	175	ASN

### 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](#)

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	NAD	A	501	-	38,48,48	2.55	14 (36%)	47,73,73	2.28	14 (29%)
2	NAD	B	501	-	38,48,48	2.24	11 (28%)	47,73,73	2.80	12 (25%)
2	NAD	C	501	-	38,48,48	2.50	15 (39%)	47,73,73	2.82	11 (23%)
2	NAD	D	501	-	38,48,48	2.33	13 (34%)	47,73,73	2.58	15 (31%)

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	501	-	-	0/22/62/62	0/5/5/5
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	O2B-C2B	-3.96	1.33	1.43
2	C	501	NAD	O4B-C1B	-3.91	1.36	1.41
2	D	501	NAD	O4B-C1B	-3.55	1.36	1.41
2	A	501	NAD	O2B-C2B	-3.32	1.35	1.43
2	C	501	NAD	O2D-C2D	-3.23	1.35	1.43
2	D	501	NAD	O2D-C2D	-2.78	1.36	1.43
2	C	501	NAD	O2B-C2B	-2.76	1.36	1.43
2	D	501	NAD	O2B-C2B	-2.71	1.36	1.43
2	A	501	NAD	O3D-C3D	-2.48	1.37	1.43
2	A	501	NAD	O2D-C2D	-2.39	1.37	1.43
2	D	501	NAD	O3D-C3D	-2.15	1.37	1.43
2	D	501	NAD	C5B-C4B	-2.07	1.44	1.51
2	B	501	NAD	O4B-C1B	-2.00	1.38	1.41
2	A	501	NAD	C3D-C4D	2.09	1.58	1.53
2	D	501	NAD	C2N-C3N	2.10	1.42	1.39
2	A	501	NAD	C2N-C3N	2.13	1.42	1.39
2	C	501	NAD	C3D-C4D	2.15	1.58	1.53
2	B	501	NAD	O3B-C3B	2.18	1.48	1.43
2	C	501	NAD	C5N-C4N	2.19	1.43	1.38
2	C	501	NAD	C7N-N7N	2.21	1.37	1.33
2	B	501	NAD	C3B-C4B	2.26	1.59	1.53
2	D	501	NAD	C3D-C4D	2.34	1.59	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C3D-C4D	2.43	1.59	1.53
2	B	501	NAD	PA-O1A	2.46	1.60	1.51
2	D	501	NAD	C3B-C4B	2.50	1.59	1.53
2	A	501	NAD	O4B-C4B	2.54	1.50	1.45
2	C	501	NAD	C3B-C4B	2.54	1.59	1.53
2	B	501	NAD	O4B-C4B	2.58	1.51	1.45
2	C	501	NAD	O3B-C3B	2.59	1.49	1.43
2	C	501	NAD	O4D-C1D	2.91	1.44	1.41
2	D	501	NAD	C2A-N3A	2.99	1.37	1.32
2	D	501	NAD	O3B-C3B	2.99	1.50	1.43
2	A	501	NAD	C4A-N3A	3.15	1.40	1.35
2	A	501	NAD	C5N-C4N	3.22	1.45	1.38
2	C	501	NAD	C2N-C3N	3.45	1.44	1.39
2	C	501	NAD	O7N-C7N	3.55	1.31	1.24
2	A	501	NAD	C3B-C4B	3.61	1.62	1.53
2	A	501	NAD	O3B-C3B	3.69	1.51	1.43
2	C	501	NAD	C2A-N3A	3.90	1.39	1.32
2	A	501	NAD	O4D-C1D	4.11	1.46	1.41
2	C	501	NAD	C4A-N3A	4.36	1.42	1.35
2	B	501	NAD	C2A-N3A	4.41	1.40	1.32
2	B	501	NAD	C4A-N3A	4.50	1.42	1.35
2	B	501	NAD	O4D-C4D	4.54	1.55	1.45
2	A	501	NAD	C2A-N3A	4.84	1.40	1.32
2	D	501	NAD	O4D-C1D	5.29	1.47	1.41
2	A	501	NAD	O4D-C4D	5.51	1.57	1.45
2	D	501	NAD	C3N-C7N	5.86	1.59	1.50
2	C	501	NAD	O4D-C4D	5.98	1.58	1.45
2	D	501	NAD	O4D-C4D	6.33	1.59	1.45
2	C	501	NAD	C3N-C7N	6.81	1.61	1.50
2	B	501	NAD	C3N-C7N	7.20	1.61	1.50
2	A	501	NAD	C3N-C7N	7.64	1.62	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	C3N-C2N-N1N	-8.08	111.05	120.36
2	C	501	NAD	N3A-C2A-N1A	-7.44	123.20	128.89
2	B	501	NAD	N3A-C2A-N1A	-6.58	123.86	128.89
2	B	501	NAD	C5N-C4N-C3N	-6.19	112.55	120.33
2	C	501	NAD	C3N-C2N-N1N	-6.12	113.31	120.36
2	D	501	NAD	N3A-C2A-N1A	-5.99	124.31	128.89
2	D	501	NAD	C5N-C4N-C3N	-5.84	112.99	120.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	C3N-C2N-N1N	-5.82	113.65	120.36
2	C	501	NAD	C5N-C4N-C3N	-5.35	113.61	120.33
2	A	501	NAD	C3N-C2N-N1N	-5.31	114.24	120.36
2	A	501	NAD	C5N-C4N-C3N	-5.05	113.99	120.33
2	A	501	NAD	N3A-C2A-N1A	-4.92	125.13	128.89
2	C	501	NAD	O7N-C7N-C3N	-3.98	115.24	119.59
2	D	501	NAD	O7N-C7N-C3N	-3.25	116.04	119.59
2	D	501	NAD	O4D-C4D-C3D	-2.57	99.98	105.15
2	C	501	NAD	O4D-C4D-C3D	-2.53	100.05	105.15
2	C	501	NAD	O3D-C3D-C4D	-2.46	103.67	111.05
2	A	501	NAD	O4D-C4D-C3D	-2.40	100.31	105.15
2	D	501	NAD	O3D-C3D-C4D	-2.38	103.91	111.05
2	B	501	NAD	O7N-C7N-C3N	-2.37	117.00	119.59
2	A	501	NAD	O7N-C7N-C3N	-2.34	117.03	119.59
2	A	501	NAD	C2N-C3N-C7N	-2.33	112.55	119.31
2	B	501	NAD	O4D-C4D-C3D	-2.18	100.75	105.15
2	D	501	NAD	C2N-C3N-C7N	-2.17	113.02	119.31
2	A	501	NAD	C2B-C1B-N9A	-2.12	111.05	114.29
2	D	501	NAD	C4A-C5A-N7A	-2.07	107.58	109.48
2	D	501	NAD	C4B-O4B-C1B	-2.05	107.46	109.72
2	B	501	NAD	C2N-C3N-C7N	-2.03	113.42	119.31
2	A	501	NAD	O3D-C3D-C4D	-2.01	105.01	111.05
2	A	501	NAD	O2N-PN-O1N	2.04	123.57	112.53
2	C	501	NAD	C2B-C3B-C4B	2.10	106.94	102.61
2	D	501	NAD	O2B-C2B-C3B	2.20	118.97	111.83
2	D	501	NAD	O7N-C7N-N7N	2.42	126.00	122.59
2	B	501	NAD	O2B-C2B-C3B	2.45	119.80	111.83
2	A	501	NAD	C6N-C5N-C4N	2.48	123.19	119.44
2	D	501	NAD	C6N-C5N-C4N	2.63	123.42	119.44
2	A	501	NAD	O2B-C2B-C3B	2.69	120.58	111.83
2	B	501	NAD	C6N-C5N-C4N	2.80	123.67	119.44
2	C	501	NAD	O3D-C3D-C2D	2.80	120.93	111.83
2	B	501	NAD	O7N-C7N-N7N	3.30	127.25	122.59
2	A	501	NAD	C2A-N1A-C6A	3.42	124.87	118.77
2	C	501	NAD	C2A-N1A-C6A	3.75	125.47	118.77
2	B	501	NAD	C2A-N1A-C6A	3.88	125.71	118.77
2	D	501	NAD	C2A-N1A-C6A	4.09	126.08	118.77
2	A	501	NAD	O4D-C1D-N1N	4.20	112.74	108.13
2	B	501	NAD	O4D-C1D-N1N	6.43	115.20	108.13
2	D	501	NAD	O4D-C1D-N1N	6.84	115.65	108.13
2	A	501	NAD	C2N-C3N-C4N	7.49	126.63	118.29
2	D	501	NAD	C2N-C3N-C4N	8.11	127.32	118.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C2N-C3N-C4N	8.43	127.68	118.29
2	B	501	NAD	C2N-C3N-C4N	9.23	128.57	118.29
2	C	501	NAD	O4D-C1D-N1N	9.25	118.30	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	6	0
2	B	501	NAD	10	0
2	C	501	NAD	7	0
2	D	501	NAD	4	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 ⓘ

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.