



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 08:12 pm GMT

PDB ID : 1C14
Title : CRYSTAL STRUCTURE OF E COLI ENOYL REDUCTASE-NAD⁺-TRIC
LOSAN COMPLEX
Authors : Qiu, X.; Janson, C.; Court, R.; Smyth, M.; Payne, D.; Abdel-Meguid, S.
Deposited on : 1999-07-20
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

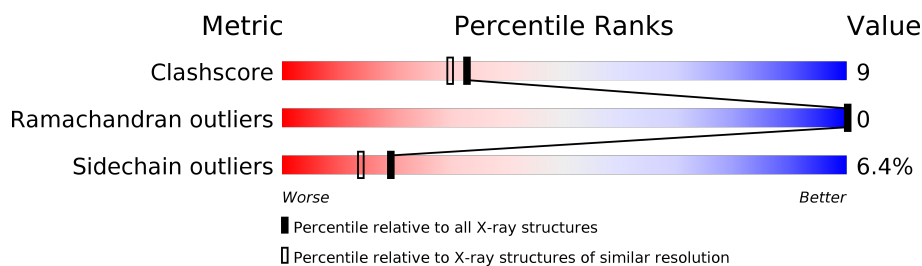
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	122078	8264 (2.00-2.00)
Ramachandran outliers	120005	8163 (2.00-2.00)
Sidechain outliers	119972	8162 (2.00-2.00)

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	262	
1	B	262	

2 Entry composition [i](#)

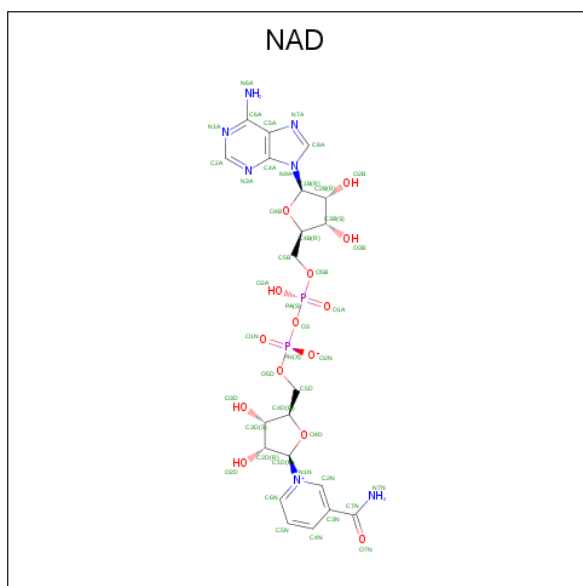
There are 4 unique types of molecules in this entry. The entry contains 4161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 REDUCTASE.

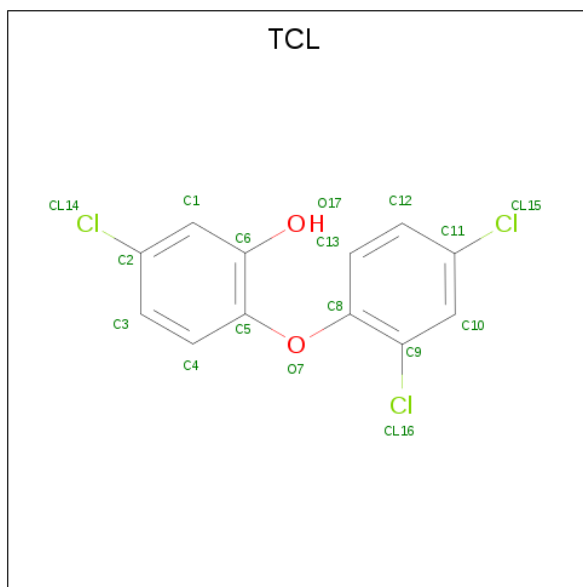
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1901	1198	329	361	13			
1	B	256	Total	C	N	O	S	0	0	0
			1901	1198	329	361	13			

- 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		

- Molecule 3 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
3	B	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 4 is water.

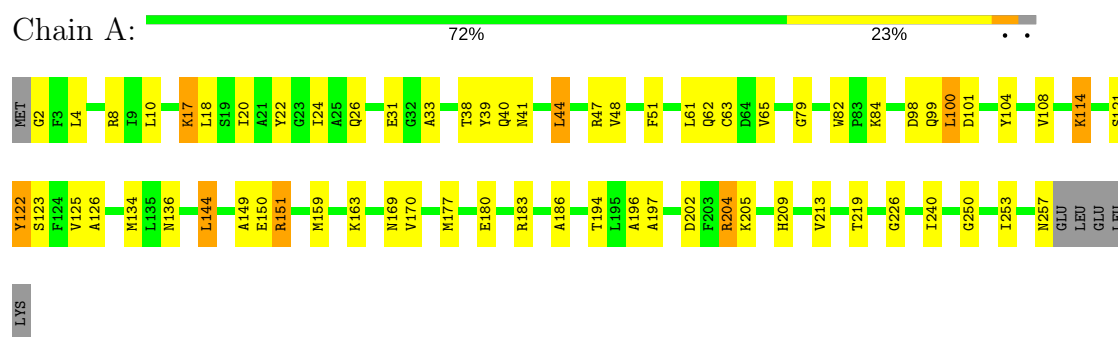
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	98	Total	O	0	0
			98	98		

3 Residue-property plots

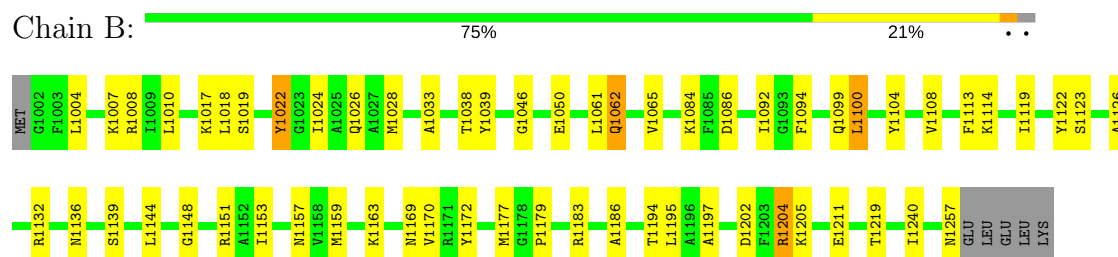
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: ENOYL REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.00 Å 79.00 Å 328.75 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	86.0 (7.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4161	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: TCL, 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	0.52	0/1933	0.74	1/2611 (0.0%)
1	B	0.55	0/1933	0.75	1/2611 (0.0%)
All	All	0.54	0/3866	0.75	2/5222 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	100	LEU	N-CA-C	5.67	126.30	111.00
1	B	1100	LEU	N-CA-C	5.43	125.66	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	TYR	Sidechain
1	B	1022	TYR	Sidechain

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	1901	0	1892	42	0
1	B	1901	0	1892	34	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
3	A	17	0	7	2	0
3	B	17	0	7	0	0
4	A	139	0	0	1	0
4	B	98	0	0	0	0
All	All	4161	0	3850	73	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 9.

All (73) 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:99:GLN:HE22	1:A:108:VAL:HA	1.46	0.79
1:A:98:ASP:HB2	4:A:2027:HOH:O	1.83	0.78
1:A:202:ASP:HB3	1:A:205:LYS:HE2	1.65	0.78
1:B:1211:GLU:HG3	1:B:1219:THR:HG23	1.66	0.78
1:A:47:ARG:HG3	1:A:51:PHE:CE1	2.27	0.69
1:A:4:LEU:HB3	1:A:33:ALA:HB2	1.77	0.67
1:B:1038:THR:HA	1:B:1061:LEU:O	1.95	0.66
1:A:10:LEU:HD11	1:A:38:THR:HG23	1.78	0.66
1:B:1004:LEU:HD23	1:B:1007:LYS:HG3	1.77	0.64
1:B:1122:TYR:CE2	1:B:1126:ALA:HB2	2.33	0.64
1:A:47:ARG:HG3	1:A:51:PHE:HE1	1.62	0.63
1:A:39:TYR:HD2	1:A:41:ASN:O	1.86	0.58
1:A:38:THR:HA	1:A:61:LEU:O	2.04	0.57
1:A:44:LEU:O	1:A:48:VAL:HG23	2.04	0.57
1:A:183:ARG:HD2	1:A:240:ILE:O	2.04	0.57
1:B:1065:VAL:HB	1:B:1123:SER:HB2	1.87	0.56
1:B:1017:LYS:HG2	1:B:1022:TYR:CE2	2.41	0.56
1:A:84:LYS:HD2	1:A:136:ASN:OD1	2.07	0.55
1:A:209:HIS:O	1:A:213:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1046:GLY:O	1:B:1050:GLU:HG3	2.07	0.53
1:A:170:VAL:HG21	1:A:186:ALA:HB2	1.89	0.53
1:A:177:MET:O	1:A:180:GLU:HG2	2.09	0.53
1:A:22:TYR:CE2	1:A:26:GLN:NE2	2.77	0.52
1:B:1211:GLU:CG	1:B:1219:THR:HG23	2.38	0.52
1:A:18:LEU:O	1:A:194:THR:HG22	2.10	0.52
1:B:1183:ARG:HD2	1:B:1240:ILE:O	2.11	0.51
1:B:1099:GLN:HE22	1:B:1108:VAL:HA	1.76	0.51
1:A:250:GLY:O	1:A:253:ILE:HG13	2.11	0.51
1:A:22:TYR:HE1	1:A:51:PHE:CD2	2.29	0.51
1:B:1194:THR:H	1:B:1197:ALA:HB3	1.76	0.51
1:B:1004:LEU:HB3	1:B:1033:ALA:HB2	1.93	0.50
1:B:1024:ILE:O	1:B:1028:MET:HG3	2.12	0.50
1:A:20:ILE:HG21	1:A:144:LEU:HD22	1.94	0.50
1:B:1004:LEU:O	1:B:1007:LYS:HB2	2.12	0.50
1:B:1092:ILE:HG23	2:B:1501:NAD:C4A	2.42	0.49
1:A:65:VAL:HB	1:A:123:SER:HB2	1.95	0.48
1:B:1010:LEU:HD11	1:B:1038:THR:HG23	1.94	0.48
1:A:196:ALA:HB1	3:A:502:TCL:C9	2.44	0.48
1:A:114:LYS:HD2	1:A:114:LYS:C	2.34	0.48
1:B:1086:ASP:HA	1:B:1139:SER:OG	2.13	0.48
1:B:1022:TYR:OH	1:B:1026:GLN:NE2	2.47	0.48
1:A:2:GLY:HA3	1:A:31:GLU:O	2.13	0.47
1:A:40:GLN:HA	1:A:63:CYS:O	2.14	0.47
1:B:1148:GLY:HA2	1:B:1153:ILE:HD12	1.96	0.47
1:B:1204:ARG:NH2	1:B:1204:ARG:HB2	2.29	0.47
1:A:202:ASP:CB	1:A:205:LYS:HE2	2.41	0.47
1:B:1205:LYS:HD3	1:B:1205:LYS:N	2.29	0.47
1:B:1094:PHE:HB3	1:B:1119:ILE:HG21	1.97	0.46
1:B:1039:TYR:CE2	1:B:1062:GLN:HB2	2.51	0.46
1:A:104:TYR:CD2	1:B:1172:TYR:HB3	2.51	0.46
1:B:1019:SER:O	1:B:1022:TYR:HB3	2.16	0.46
1:A:122:TYR:CE2	1:A:126:ALA:HB2	2.51	0.45
1:A:39:TYR:HB3	1:A:48:VAL:HG21	1.98	0.44
1:B:1202:ASP:HB3	1:B:1205:LYS:HG2	1.99	0.44
1:B:1132:ARG:HG3	1:B:1177:MET:CE	2.47	0.44
1:A:121:SER:HB3	1:B:1113:PHE:HZ	1.83	0.44
1:B:1084:LYS:HD2	1:B:1136:ASN:OD1	2.17	0.44
1:A:204:ARG:CD	1:A:204:ARG:H	2.30	0.43
1:A:159:MET:O	1:A:163:LYS:HG2	2.18	0.43
1:A:17:LYS:HD3	1:A:17:LYS:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:NE	1:A:51:PHE:CZ	2.88	0.42
1:B:1170:VAL:HG21	1:B:1186:ALA:HB2	2.02	0.42
1:A:159:MET:CE	1:A:163:LYS:HE2	2.50	0.42
1:A:149:ALA:HB2	1:A:163:LYS:HB3	2.01	0.42
1:A:24:ILE:HG12	1:A:226:GLY:HA2	2.01	0.42
1:A:84:LYS:HA	1:A:134:MET:O	2.19	0.42
1:A:79:GLY:HA2	1:A:82:TRP:O	2.21	0.41
1:B:1159:MET:O	1:B:1163:LYS:HG2	2.20	0.41
1:A:125:VAL:HG21	1:B:1108:VAL:HG11	2.02	0.41
1:B:1204:ARG:HB2	1:B:1204:ARG:HH21	1.84	0.41
1:A:150:GLU:C	1:A:151:ARG:HG2	2.41	0.41
1:A:197:ALA:HA	3:A:502:TCL:H41	2.03	0.41
1:B:1104:TYR:HD1	1:B:1157:ASN:HB3	1.86	0.41

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	254/262 (97%)	245 (96%)	9 (4%)	0	100	100
1	B	254/262 (97%)	241 (95%)	13 (5%)	0	100	100
All	All	508/524 (97%)	486 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	195/201 (97%)	182 (93%)	13 (7%)	18	12
1	B	195/201 (97%)	183 (94%)	12 (6%)	20	15
All	All	390/402 (97%)	365 (94%)	25 (6%)	19	14

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	17	LYS
1	A	44	LEU
1	A	62	GLN
1	A	100	LEU
1	A	101	ASP
1	A	114	LYS
1	A	144	LEU
1	A	151	ARG
1	A	169	ASN
1	A	204	ARG
1	A	219	THR
1	A	257	ASN
1	B	1008	ARG
1	B	1018	LEU
1	B	1062	GLN
1	B	1100	LEU
1	B	1114	LYS
1	B	1144	LEU
1	B	1151	ARG
1	B	1169	ASN
1	B	1179	PRO
1	B	1195	LEU
1	B	1204	ARG
1	B	1257	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	29	HIS

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Mol	Chain	Res	Type
1	A	40	GLN
1	A	54	GLN
1	A	99	GLN
1	A	169	ASN
1	A	257	ASN
1	B	1026	GLN
1	B	1040	GLN
1	B	1062	GLN
1	B	1099	GLN
1	B	1169	ASN
1	B	1257	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 ⓘ

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	-	40,48,48	0.99	2 (5%)	44,73,73	1.80	6 (13%)
3	TCL	A	502	-	18,18,18	1.42	3 (16%)	25,25,25	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	1501	-	40,48,48	1.16	5 (12%)	44,73,73	1.91	7 (15%)
3	TCL	B	1502	-	18,18,18	1.51	3 (16%)	25,25,25	0.81	1 (4%)

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
3	TCL	A	502	-	-	0/4/4/4	0/2/2/2
2	NAD	B	1501	-	-	0/22/62/62	0/5/5/5
3	TCL	B	1502	-	-	0/4/4/4	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	NAD	O4B-C4B	-2.25	1.40	1.45
2	B	1501	NAD	O4D-C1D	2.04	1.44	1.41
3	A	502	TCL	C1-C6	2.14	1.41	1.38
3	B	1502	TCL	C3-C4	2.18	1.42	1.38
2	B	1501	NAD	C2A-N3A	2.19	1.35	1.32
3	B	1502	TCL	C8-C9	2.25	1.43	1.39
3	A	502	TCL	C12-C11	2.27	1.42	1.38
3	B	1502	TCL	O17-C6	2.34	1.41	1.36
3	A	502	TCL	C10-C11	2.54	1.42	1.38
2	B	1501	NAD	O4B-C1B	2.58	1.44	1.41
2	A	501	NAD	C6N-N1N	2.72	1.42	1.35
2	B	1501	NAD	C3N-C7N	2.99	1.55	1.50
2	A	501	NAD	O4D-C1D	3.30	1.45	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	NAD	N3A-C2A-N1A	-8.00	122.02	128.86
2	A	501	NAD	N3A-C2A-N1A	-6.81	123.03	128.86
2	A	501	NAD	C1B-N9A-C4A	-4.45	118.95	126.64
2	A	501	NAD	C4B-O4B-C1B	-4.38	105.26	109.83
2	B	1501	NAD	C4B-O4B-C1B	-3.87	105.79	109.83
2	B	1501	NAD	O3D-C3D-C2D	-3.27	101.35	111.83
2	A	501	NAD	O2B-C2B-C3B	-3.06	102.02	111.83
2	B	1501	NAD	C1B-N9A-C4A	-3.02	121.42	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	O3D-C3D-C2D	-2.87	102.62	111.83
2	B	1501	NAD	O5B-C5B-C4B	-2.68	99.68	109.00
2	B	1501	NAD	C2B-C3B-C4B	2.19	106.82	102.62
3	B	1502	TCL	C8-C9-CL16	2.28	122.10	119.42
2	A	501	NAD	C4A-C5A-N7A	2.84	112.15	109.41
2	B	1501	NAD	C4A-C5A-N7A	2.86	112.18	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	TCL	2	0
2	B	1501	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.