



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:19 AM GMT

PDB ID : 1NHG
Title : CRYSTAL STRUCTURE ANALYSIS OF PLASMODIUM FALCIPARUM E
NOYL-ACYL-CARRIER-PROTEINREDUCTASE WITH TRICLOSAN
Authors : Perozzo, R.; Kuo, M.; Sidhu, A.S.; Valiyaveetil, J.T.; Bittman, R.; Jacobs
Jr., W.R.; Fidock, D.A.; Sacchettini, J.C.
Deposited on : 2002-12-19
Resolution : 2.43 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

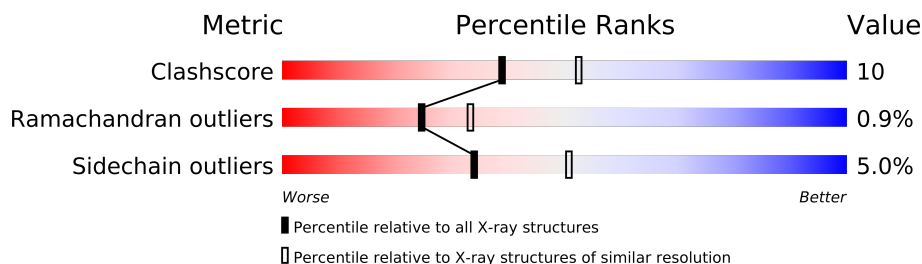
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.43 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	79885	3698 (2.48-2.40)
Ramachandran outliers	78287	3639 (2.48-2.40)
Sidechain outliers	78261	3640 (2.48-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	229	
1	B	229	
2	C	60	
2	D	60	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4700 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

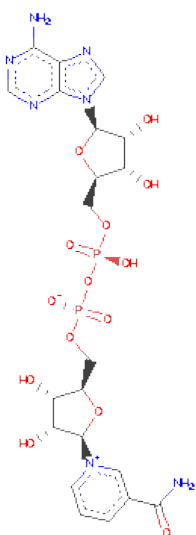
- Molecule 1 is a protein called enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1807	1148	309	340	10			
1	B	229	Total	C	N	O	S	0	0	0
			1807	1148	309	340	10			

- Molecule 2 is a protein called enoyl-acyl carrier reductase.

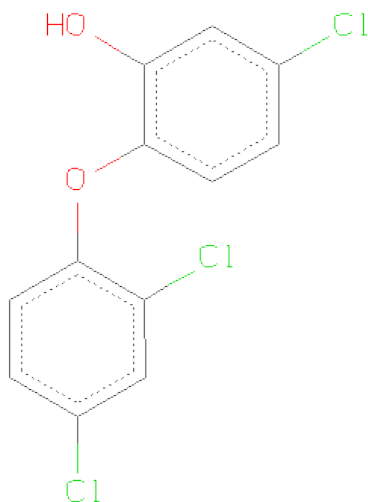
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	60	Total	C	N	O	S	0	0	0
			482	310	75	96	1			
2	D	60	Total	C	N	O	S	0	0	0
			482	310	75	96	1			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 4 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).



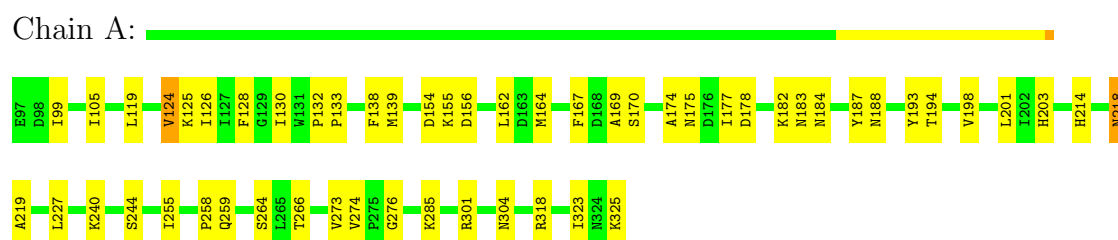
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	B	1	Total	C	Cl	O	0	0
			17	12	3	2		

3 Residue-property plots

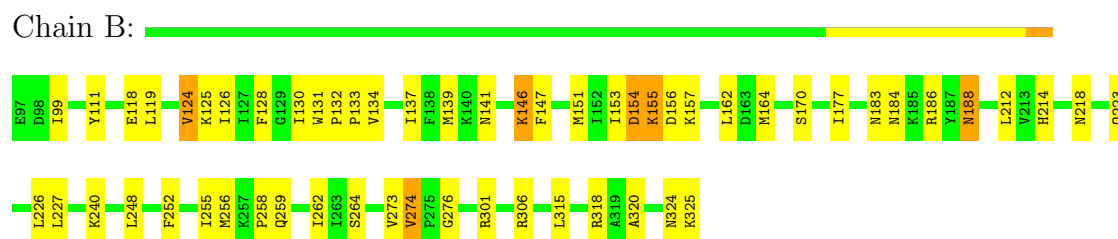
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



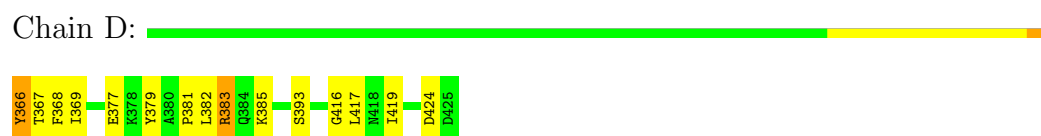
- Molecule 1: enoyl-acyl carrier reductase



- Molecule 2: enoyl-acyl carrier reductase



- Molecule 2: enoyl-acyl carrier 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 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.08Å 133.08Å 84.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.43	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.43)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.213	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4700	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	0.33	0/1840	0.57	0/2477
1	B	0.32	0/1840	0.56	0/2477
2	C	0.34	0/491	0.58	0/664
2	D	0.35	0/491	0.58	0/664
All	All	0.33	0/4662	0.57	0/6282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1807	0	1824	37	0
1	B	1807	0	1824	44	0
2	C	482	0	473	7	0
2	D	482	0	473	11	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
4	A	17	0	7	1	0
4	B	17	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4700	0	4660	91	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (91) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:153:ILE:HB	1:B:157:LYS:HB2	1.58	0.86
1:A:276:GLY:HA2	1:A:325:LYS:HG2	1.59	0.84
1:A:139:MET:SD	1:A:164:MET:HE2	2.28	0.73
2:C:379:TYR:OH	2:C:425:ASP:HB3	1.88	0.72
1:B:146:LYS:HA	1:B:146:LYS:HE3	1.71	0.71
1:A:183:ASN:HA	1:A:188:ASN:HD21	1.56	0.71
1:A:174:ALA:O	1:A:177:ILE:HG22	1.92	0.70
1:B:318:ARG:HH11	1:B:318:ARG:HG2	1.56	0.70
1:A:218:ASN:HD22	1:A:219:ALA:H	1.39	0.70
1:A:276:GLY:CA	1:A:325:LYS:HG2	2.23	0.69
1:B:139:MET:SD	1:B:164:MET:HE2	2.33	0.68
1:B:184:ASN:ND2	1:B:186:ARG:H	1.93	0.66
1:A:132:PRO:HB2	1:A:133:PRO:HD3	1.77	0.66
1:A:318:ARG:HH11	1:A:318:ARG:HG2	1.61	0.66
1:B:99:ILE:HD13	1:B:125:LYS:HB2	1.77	0.64
2:D:416:GLY:O	2:D:419:ILE:HG12	1.99	0.63
1:B:325:LYS:HG3	1:B:325:LYS:OXT	1.98	0.63
1:A:105:ILE:HD12	1:A:128:PHE:CD1	2.35	0.62
1:A:184:ASN:HD22	1:A:187:TYR:HD1	1.48	0.61
1:B:252:PHE:O	1:B:256:MET:HG3	2.00	0.61
1:B:155:LYS:HD3	1:B:157:LYS:NZ	2.17	0.60
1:B:318:ARG:NH1	1:B:318:ARG:HG2	2.19	0.58
1:B:320:ALA:HB1	2:D:369:ILE:HD13	1.87	0.57
1:B:154:ASP:O	1:B:156:ASP:N	2.32	0.56
1:B:223:GLN:HE21	1:B:324:ASN:HB3	1.71	0.56
1:A:167:PHE:HD1	1:A:198:VAL:HG11	1.72	0.54
2:D:366:TYR:N	2:D:366:TYR:CD2	2.76	0.54
1:B:128:PHE:HB3	1:B:130:ILE:HD11	1.88	0.54
1:A:119:LEU:O	1:A:124:VAL:HG13	2.07	0.54
2:C:366:TYR:CD2	2:C:366:TYR:N	2.76	0.53
2:D:366:TYR:HD2	2:D:366:TYR:N	2.06	0.52
1:A:318:ARG:HG2	1:A:318:ARG:NH1	2.25	0.52
1:A:194:THR:O	1:A:198:VAL:HG13	2.09	0.52
1:A:128:PHE:HB3	1:A:130:ILE:HD11	1.92	0.52
1:A:154:ASP:C	1:A:156:ASP:H	2.13	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:ILE:HD13	1:A:125:LYS:HB2	1.92	0.52
1:B:276:GLY:CA	1:B:325:LYS:HG2	2.41	0.51
1:A:218:ASN:HD22	1:A:219:ALA:N	2.05	0.51
1:B:155:LYS:HB2	1:B:157:LYS:NZ	2.25	0.51
1:A:177:ILE:HD12	1:A:193:TYR:OH	2.11	0.50
2:C:366:TYR:HD2	2:C:366:TYR:N	2.08	0.50
1:A:177:ILE:HD11	1:A:182:LYS:HA	1.94	0.50
1:B:252:PHE:CD1	1:B:255:ILE:HD11	2.47	0.49
1:A:301:ARG:NH2	2:D:379:TYR:HA	2.28	0.49
1:B:212:LEU:HB3	1:B:262:ILE:HG12	1.94	0.48
1:A:301:ARG:HH21	2:D:379:TYR:C	2.17	0.48
1:B:147:PHE:O	1:B:151:MET:HG3	2.13	0.48
1:B:274:VAL:HG22	1:B:274:VAL:O	2.12	0.48
1:B:301:ARG:HH21	2:C:379:TYR:C	2.17	0.48
2:C:416:GLY:O	2:C:419:ILE:HG12	2.13	0.47
1:B:170:SER:HB3	1:B:240:LYS:HE2	1.96	0.47
1:A:124:VAL:HG22	1:A:126:ILE:HD11	1.96	0.47
1:B:325:LYS:HB3	2:D:368:PHE:HB2	1.97	0.47
1:B:126:ILE:HG21	1:B:128:PHE:HE1	1.80	0.47
1:B:276:GLY:HA3	1:B:325:LYS:HG2	1.97	0.47
2:D:377:GLU:O	2:D:383:ARG:HG3	2.15	0.46
1:A:178:ASP:O	1:A:182:LYS:HB2	2.16	0.46
1:A:170:SER:HB3	1:A:240:LYS:HE2	1.97	0.46
1:B:118:GLU:HG3	2:D:393:SER:N	2.30	0.46
1:B:155:LYS:HB2	1:B:157:LYS:HZ1	1.82	0.45
1:B:134:VAL:O	1:B:137:ILE:HG23	2.16	0.45
1:B:248:LEU:O	1:B:252:PHE:HB2	2.17	0.45
1:B:188:ASN:HA	1:B:188:ASN:HD22	1.55	0.45
1:B:153:ILE:O	1:B:155:LYS:N	2.50	0.44
1:B:258:PRO:O	1:B:259:GLN:HB2	2.17	0.44
1:B:137:ILE:HD11	1:B:141:ASN:HD21	1.83	0.43
1:A:154:ASP:O	1:A:156:ASP:N	2.52	0.43
1:A:258:PRO:O	1:A:259:GLN:HB2	2.18	0.43
1:A:266:THR:HA	1:A:285:LYS:HD2	2.00	0.43
1:A:138:PHE:HE2	1:A:164:MET:CE	2.32	0.43
1:B:183:ASN:HA	1:B:188:ASN:ND2	2.34	0.42
1:B:155:LYS:HD3	1:B:157:LYS:HZ1	1.82	0.42
1:A:323:ILE:HD11	4:A:500:TCL:H131	1.99	0.42
1:B:131:TRP:CG	1:B:133:PRO:HD2	2.55	0.42
1:B:214:HIS:O	1:B:264:SER:HA	2.19	0.42
2:D:377:GLU:OE1	2:D:385:LYS:HG2	2.20	0.42
1:A:259:GLN:HG2	1:A:304:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:132:PRO:HB2	1:B:133:PRO:HD3	2.00	0.42
1:B:154:ASP:C	1:B:156:ASP:H	2.21	0.42
1:A:177:ILE:HG23	1:A:177:ILE:O	2.20	0.41
1:B:119:LEU:O	1:B:124:VAL:HG13	2.20	0.41
1:A:214:HIS:O	1:A:264:SER:HA	2.21	0.41
1:B:301:ARG:NH2	2:C:379:TYR:HA	2.35	0.41
1:A:203:HIS:HB2	1:A:255:ILE:HG21	2.01	0.41
1:B:155:LYS:CD	1:B:157:LYS:HZ1	2.34	0.41
2:D:381:PRO:HG2	2:D:419:ILE:HD11	2.03	0.41
1:A:138:PHE:CE2	1:A:164:MET:HE1	2.56	0.40
1:B:111:TYR:CE1	1:B:315:LEU:HD22	2.57	0.40
1:A:156:ASP:O	1:A:156:ASP:OD1	2.39	0.40
1:B:306:ARG:HG2	2:C:382:LEU:HD21	2.03	0.40
1:A:169:ALA:HB1	1:A:244:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

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	227/229 (99%)	216 (95%)	10 (4%)	1 (0%)	43	59
1	B	227/229 (99%)	216 (95%)	9 (4%)	2 (1%)	25	33
2	C	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
2	D	58/60 (97%)	54 (93%)	2 (3%)	2 (3%)	6	4
All	All	570/578 (99%)	540 (95%)	25 (4%)	5 (1%)	25	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	ASP
1	B	155	LYS
2	D	424	ASP
1	A	155	LYS

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Mol	Chain	Res	Type
2	D	367	THR

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	197/197 (100%)	189 (96%)	8 (4%)	41	61
1	B	197/197 (100%)	187 (95%)	10 (5%)	33	49
2	C	53/53 (100%)	50 (94%)	3 (6%)	29	43
2	D	53/53 (100%)	49 (92%)	4 (8%)	19	28
All	All	500/500 (100%)	475 (95%)	25 (5%)	34	51

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

Mol	Chain	Res	Type
1	A	124	VAL
1	A	162	LEU
1	A	175	ASN
1	A	201	LEU
1	A	218	ASN
1	A	227	LEU
1	A	273	VAL
1	A	274	VAL
1	B	124	VAL
1	B	146	LYS
1	B	162	LEU
1	B	177	ILE
1	B	188	ASN
1	B	218	ASN
1	B	226	LEU
1	B	227	LEU
1	B	273	VAL
1	B	274	VAL
2	C	366	TYR
2	C	383	ARG
2	C	417	LEU

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Mol	Chain	Res	Type
2	D	366	TYR
2	D	382	LEU
2	D	383	ARG
2	D	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	188	ASN
1	A	200	ASN
1	A	218	ASN
1	A	223	GLN
1	A	228	ASN
1	A	254	ASN
1	A	302	ASN
1	A	304	ASN
1	B	141	ASN
1	B	160	ASN
1	B	184	ASN
1	B	188	ASN
1	B	200	ASN
1	B	218	ASN
1	B	223	GLN
1	B	254	ASN
1	B	259	GLN
1	B	302	ASN
2	C	384	GLN
2	D	384	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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$
3	NAD	A	450	-	48,48,48	1.66	7 (14%)	73,73,73	2.61	16 (21%)
4	TCL	A	500	-	18,18,18	4.19	13 (72%)	25,25,25	1.80	6 (24%)
3	NAD	B	550	-	48,48,48	1.70	7 (14%)	73,73,73	2.56	16 (21%)
4	TCL	B	600	-	18,18,18	4.10	14 (77%)	25,25,25	1.75	5 (20%)

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	NAD	A	450	-	-	0/30/62/62	0/3/5/5
4	TCL	A	500	-	-	0/4/4/4	0/2/2/2
3	NAD	B	550	-	-	0/30/62/62	0/3/5/5
4	TCL	B	600	-	-	0/4/4/4	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	TCL	C8-C9	8.33	1.55	1.39
4	A	500	TCL	C8-C9	8.26	1.55	1.39
4	B	600	TCL	C10-C11	7.60	1.51	1.38
4	A	500	TCL	C10-C11	7.50	1.51	1.38
4	A	500	TCL	C6-C5	5.84	1.50	1.40
3	B	550	NAD	C2N-N1N	5.63	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	TCL	C1-C6	5.55	1.46	1.38
4	B	600	TCL	C1-C6	5.53	1.46	1.38
3	A	450	NAD	C2N-N1N	5.40	1.42	1.35
3	B	550	NAD	PN-O3	-5.06	1.50	1.60
4	B	600	TCL	C6-C5	4.95	1.48	1.40
3	A	450	NAD	PN-O3	-4.79	1.50	1.60
4	A	500	TCL	C13-C8	4.53	1.49	1.39
3	A	450	NAD	O7N-C7N	4.34	1.34	1.24
4	B	600	TCL	C3-C2	4.27	1.46	1.38
3	B	550	NAD	O7N-C7N	4.26	1.34	1.24
4	B	600	TCL	C13-C8	4.22	1.48	1.39
4	A	500	TCL	C3-C2	4.22	1.46	1.38
3	B	550	NAD	PA-O3	-4.12	1.52	1.59
4	B	600	TCL	C10-C9	4.09	1.45	1.38
4	A	500	TCL	C2-CL14	-4.05	1.65	1.74
4	A	500	TCL	C3-C4	3.96	1.46	1.38
4	B	600	TCL	C1-C2	3.90	1.45	1.38
4	A	500	TCL	C1-C2	3.77	1.45	1.38
4	B	600	TCL	C3-C4	3.76	1.46	1.38
3	A	450	NAD	PA-O3	-3.74	1.53	1.59
4	A	500	TCL	C10-C9	3.66	1.44	1.38
4	B	600	TCL	C2-CL14	-3.27	1.66	1.74
4	A	500	TCL	C11-CL15	-2.75	1.68	1.74
3	B	550	NAD	C6N-C5N	2.61	1.44	1.38
4	A	500	TCL	C9-CL16	-2.48	1.67	1.73
3	A	450	NAD	C6N-C5N	2.47	1.44	1.38
4	B	600	TCL	C11-CL15	-2.44	1.68	1.74
3	A	450	NAD	C2D-C1D	-2.43	1.50	1.53
4	B	600	TCL	C9-CL16	-2.35	1.67	1.73
4	B	600	TCL	C4-C5	2.31	1.44	1.39
4	B	600	TCL	O7-C8	2.26	1.44	1.39
4	A	500	TCL	C4-C5	2.24	1.44	1.39
3	A	450	NAD	C5N-C4N	2.20	1.44	1.39
3	B	550	NAD	C5N-C4N	2.12	1.43	1.39
3	B	550	NAD	C2D-C1D	-2.07	1.50	1.53

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	NAD	C8A-N9A-C1B	8.61	143.35	126.38
3	A	450	NAD	C2N-C3N-C4N	-8.41	108.79	118.31
3	B	550	NAD	C2N-C3N-C4N	-8.34	108.86	118.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	C8A-N9A-C1B	8.33	142.80	126.38
3	A	450	NAD	C1B-N9A-C4A	-7.76	113.22	126.64
3	B	550	NAD	C1B-N9A-C4A	-7.59	113.52	126.64
3	B	550	NAD	O7N-C7N-N7N	-7.41	111.88	122.59
3	A	450	NAD	O7N-C7N-N7N	-7.35	111.97	122.59
3	A	450	NAD	C3N-C7N-N7N	6.45	125.11	117.77
3	A	450	NAD	C5N-C4N-C3N	6.45	128.69	120.32
3	B	550	NAD	C3N-C7N-N7N	6.32	124.96	117.77
3	B	550	NAD	C5N-C4N-C3N	6.30	128.51	120.32
4	B	600	TCL	C13-C12-C11	5.47	125.32	119.22
4	A	500	TCL	C13-C12-C11	5.22	125.04	119.22
3	A	450	NAD	C4D-O4D-C1D	-4.62	104.73	109.75
3	A	450	NAD	C8A-N9A-C4A	-4.55	103.43	106.90
3	A	450	NAD	C3N-C2N-N1N	4.38	127.74	120.36
3	B	550	NAD	C3N-C2N-N1N	4.35	127.69	120.36
3	B	550	NAD	C8A-N9A-C4A	-4.22	103.68	106.90
3	B	550	NAD	C4D-O4D-C1D	-4.05	105.35	109.75
4	A	500	TCL	O7-C5-C6	3.63	123.74	116.33
4	B	600	TCL	O7-C5-C6	3.26	122.97	116.33
3	B	550	NAD	O7N-C7N-C3N	3.15	123.13	119.58
3	A	450	NAD	C2N-C3N-C7N	3.14	128.68	119.35
3	B	550	NAD	C2N-C3N-C7N	3.05	128.43	119.35
3	A	450	NAD	O7N-C7N-C3N	2.91	122.85	119.58
4	A	500	TCL	C10-C11-CL15	-2.54	116.01	119.14
4	A	500	TCL	C12-C11-CL15	2.53	123.52	119.34
3	A	450	NAD	O3-PN-O1N	2.46	114.69	108.83
4	B	600	TCL	C12-C11-CL15	2.36	123.23	119.34
3	B	550	NAD	O2N-PN-O5D	-2.28	98.76	108.19
3	A	450	NAD	C5N-C6N-N1N	-2.20	116.73	120.43
3	A	450	NAD	C3B-C2B-C1B	2.19	104.34	100.91
3	B	550	NAD	C5N-C6N-N1N	-2.18	116.75	120.43
4	A	500	TCL	O7-C8-C13	2.16	126.42	120.69
4	B	600	TCL	C10-C11-CL15	-2.12	116.53	119.14
3	A	450	NAD	O2N-PN-O5D	-2.12	99.44	108.19
4	A	500	TCL	C8-O7-C5	2.11	123.12	117.93
4	B	600	TCL	O7-C8-C13	2.09	126.24	120.69
3	B	550	NAD	O3-PN-O1N	2.06	113.75	108.83
3	B	550	NAD	C3B-C2B-C1B	2.06	104.12	100.91
3	B	550	NAD	O3B-C3B-C4B	-2.03	105.10	111.08
3	A	450	NAD	O4D-C1D-N1N	2.02	110.02	107.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.