



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2014 – 05:01 AM EDT

PDB ID : 4OXY
Title : Substrate-binding loop movement with inhibitor PT10 in the tetrameric Mycobacterium tuberculosis enoyl-ACP reductase InhA
Authors : Li, H.J.; Sullivan, T.J.; Pan, P.; Lai, C.T.; Liu, N.; Garcia-Diaz, M.; Simmerling, C.; Tonge, P.J.
Deposited on : 2014-02-10
Resolution : 2.35 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>

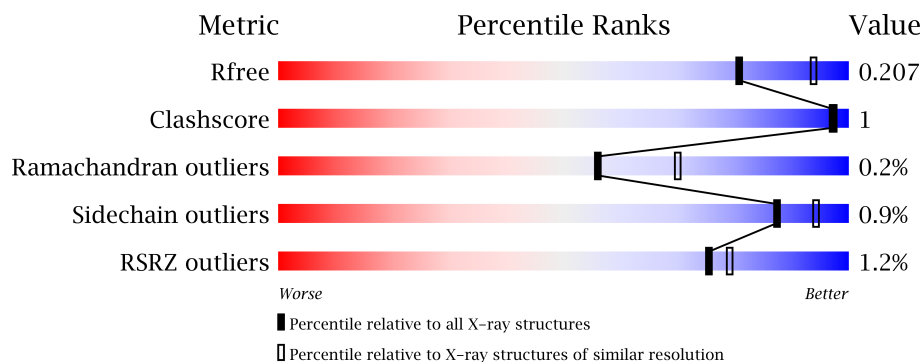
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.35 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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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.

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
1	C	289	
1	D	289	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8209 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-protein]reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	4	0
			1977	1261	339	367	10			
1	B	268	Total	C	N	O	S	0	3	0
			1972	1256	340	366	10			
1	C	261	Total	C	N	O	S	0	1	0
			1897	1208	332	347	10			
1	D	261	Total	C	N	O	S	0	2	0
			1892	1208	324	350	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P0A5Y6
A	-18	GLY	-	expression tag	UNP P0A5Y6
A	-17	SER	-	expression tag	UNP P0A5Y6
A	-16	SER	-	expression tag	UNP P0A5Y6
A	-15	HIS	-	expression tag	UNP P0A5Y6
A	-14	HIS	-	expression tag	UNP P0A5Y6
A	-13	HIS	-	expression tag	UNP P0A5Y6
A	-12	HIS	-	expression tag	UNP P0A5Y6
A	-11	HIS	-	expression tag	UNP P0A5Y6
A	-10	HIS	-	expression tag	UNP P0A5Y6
A	-9	SER	-	expression tag	UNP P0A5Y6
A	-8	SER	-	expression tag	UNP P0A5Y6
A	-7	GLY	-	expression tag	UNP P0A5Y6
A	-6	LEU	-	expression tag	UNP P0A5Y6
A	-5	VAL	-	expression tag	UNP P0A5Y6
A	-4	PRO	-	expression tag	UNP P0A5Y6
A	-3	ARG	-	expression tag	UNP P0A5Y6
A	-2	GLY	-	expression tag	UNP P0A5Y6
A	-1	SER	-	expression tag	UNP P0A5Y6
A	0	HIS	-	expression tag	UNP P0A5Y6
B	-19	MET	-	expression tag	UNP P0A5Y6

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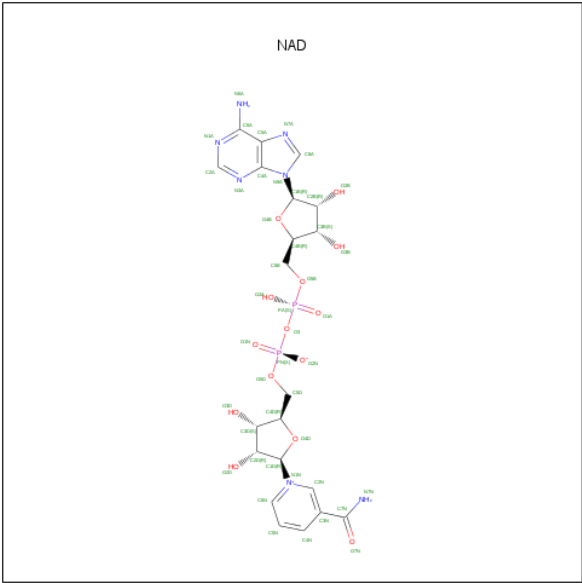
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P0A5Y6
B	-17	SER	-	expression tag	UNP P0A5Y6
B	-16	SER	-	expression tag	UNP P0A5Y6
B	-15	HIS	-	expression tag	UNP P0A5Y6
B	-14	HIS	-	expression tag	UNP P0A5Y6
B	-13	HIS	-	expression tag	UNP P0A5Y6
B	-12	HIS	-	expression tag	UNP P0A5Y6
B	-11	HIS	-	expression tag	UNP P0A5Y6
B	-10	HIS	-	expression tag	UNP P0A5Y6
B	-9	SER	-	expression tag	UNP P0A5Y6
B	-8	SER	-	expression tag	UNP P0A5Y6
B	-7	GLY	-	expression tag	UNP P0A5Y6
B	-6	LEU	-	expression tag	UNP P0A5Y6
B	-5	VAL	-	expression tag	UNP P0A5Y6
B	-4	PRO	-	expression tag	UNP P0A5Y6
B	-3	ARG	-	expression tag	UNP P0A5Y6
B	-2	GLY	-	expression tag	UNP P0A5Y6
B	-1	SER	-	expression tag	UNP P0A5Y6
B	0	HIS	-	expression tag	UNP P0A5Y6
C	-19	MET	-	expression tag	UNP P0A5Y6
C	-18	GLY	-	expression tag	UNP P0A5Y6
C	-17	SER	-	expression tag	UNP P0A5Y6
C	-16	SER	-	expression tag	UNP P0A5Y6
C	-15	HIS	-	expression tag	UNP P0A5Y6
C	-14	HIS	-	expression tag	UNP P0A5Y6
C	-13	HIS	-	expression tag	UNP P0A5Y6
C	-12	HIS	-	expression tag	UNP P0A5Y6
C	-11	HIS	-	expression tag	UNP P0A5Y6
C	-10	HIS	-	expression tag	UNP P0A5Y6
C	-9	SER	-	expression tag	UNP P0A5Y6
C	-8	SER	-	expression tag	UNP P0A5Y6
C	-7	GLY	-	expression tag	UNP P0A5Y6
C	-6	LEU	-	expression tag	UNP P0A5Y6
C	-5	VAL	-	expression tag	UNP P0A5Y6
C	-4	PRO	-	expression tag	UNP P0A5Y6
C	-3	ARG	-	expression tag	UNP P0A5Y6
C	-2	GLY	-	expression tag	UNP P0A5Y6
C	-1	SER	-	expression tag	UNP P0A5Y6
C	0	HIS	-	expression tag	UNP P0A5Y6
D	-19	MET	-	expression tag	UNP P0A5Y6
D	-18	GLY	-	expression tag	UNP P0A5Y6
D	-17	SER	-	expression tag	UNP P0A5Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P0A5Y6
D	-15	HIS	-	expression tag	UNP P0A5Y6
D	-14	HIS	-	expression tag	UNP P0A5Y6
D	-13	HIS	-	expression tag	UNP P0A5Y6
D	-12	HIS	-	expression tag	UNP P0A5Y6
D	-11	HIS	-	expression tag	UNP P0A5Y6
D	-10	HIS	-	expression tag	UNP P0A5Y6
D	-9	SER	-	expression tag	UNP P0A5Y6
D	-8	SER	-	expression tag	UNP P0A5Y6
D	-7	GLY	-	expression tag	UNP P0A5Y6
D	-6	LEU	-	expression tag	UNP P0A5Y6
D	-5	VAL	-	expression tag	UNP P0A5Y6
D	-4	PRO	-	expression tag	UNP P0A5Y6
D	-3	ARG	-	expression tag	UNP P0A5Y6
D	-2	GLY	-	expression tag	UNP P0A5Y6
D	-1	SER	-	expression tag	UNP P0A5Y6
D	0	HIS	-	expression tag	UNP P0A5Y6

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



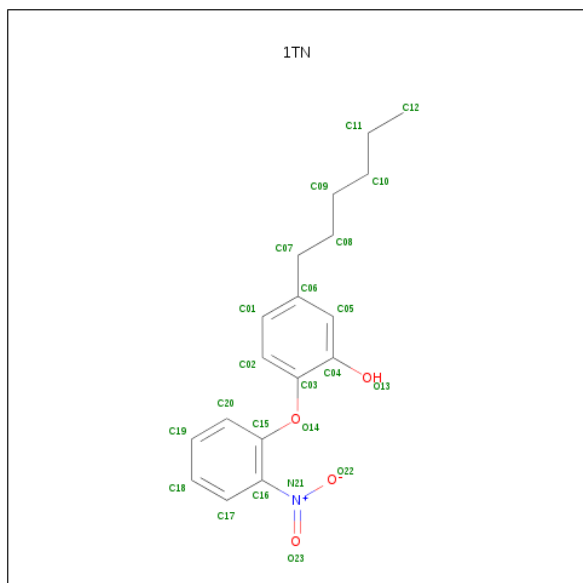
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

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

- Molecule 3 is 5-hexyl-2-(2-nitrophenoxy)phenol (three-letter code: 1TN) (formula: $C_{18}H_{21}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O		
			21	16	1	4		
3	B	1	Total	C	N	O		
			22	17	1	4		
3	C	1	Total	C	N	O		
			42	32	2	8		1
3	D	1	Total	C	N	O		
			21	16	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O		
			49	49	0	0
4	B	46	Total	O		
			46	46	0	0
4	C	48	Total	O		
			48	48	0	0

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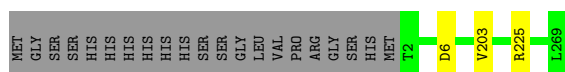
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	46	Total	O	0	0
			46	46		

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.

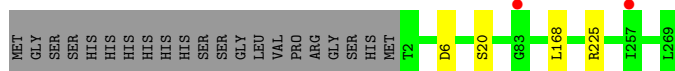
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH]

Chain A: 



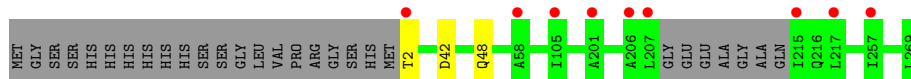
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH]

Chain B: 



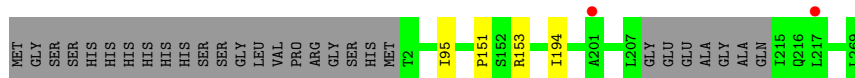
- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH]

Chain C: 



- Molecule 1: Enoyl-[acyl-carrier-protein]reductase [NADH]

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.83Å 91.08Å 148.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.55 – 2.35 48.35 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.55-2.35) 97.9 (48.35-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.166 , 0.220 0.155 , 0.207	Depositor DCC
R_{free} test set	2482 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.6	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 50989 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8209	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1TN, 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	0.38	0/2017	0.58	4/2743 (0.1%)
1	B	0.35	0/2010	0.53	0/2731
1	C	0.35	0/1934	0.50	0/2627
1	D	0.35	0/1932	0.71	4/2630 (0.2%)
All	All	0.36	0/7893	0.58	8/10731 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153[A]	ARG	NE-CZ-NH1	-12.40	114.10	120.30
1	D	153[B]	ARG	NE-CZ-NH1	-12.40	114.10	120.30
1	D	153[A]	ARG	NE-CZ-NH2	11.61	126.11	120.30
1	D	153[B]	ARG	NE-CZ-NH2	11.61	126.11	120.30
1	A	225[A]	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	A	225[B]	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	A	225[A]	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	A	225[B]	ARG	NE-CZ-NH2	5.30	122.95	120.30

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	1977	0	0	0	0
1	B	1972	0	0	2	0
1	C	1897	0	0	0	0
1	D	1892	0	0	1	0
2	A	44	0	0	1	0
2	B	44	0	0	3	0
2	C	44	0	0	1	0
2	D	44	0	0	1	0
3	A	21	0	0	0	0
3	B	22	0	0	1	0
3	C	42	0	0	0	0
3	D	21	0	0	0	0
4	A	49	0	0	0	0
4	B	46	0	0	1	0
4	C	48	0	0	0	0
4	D	46	0	0	0	0
All	All	8209	0	0	7	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 1.

All (7) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:301:NAD:O1N	2:C:301:NAD:N7N	2.30	0.65
1:B:225:ARG:NH2	4:B:426:HOH:O	2.40	0.55
2:A:301:NAD:N7N	2:A:301:NAD:O1N	2.42	0.52
2:B:301:NAD:O2D	3:B:302:1TN:O13	2.32	0.47
1:B:20:SER:OG	2:B:301:NAD:O1A	2.36	0.44
1:D:194:ILE:N	2:D:301:NAD:O7N	2.51	0.43
2:B:301:NAD:O1N	2:B:301:NAD:N7N	2.52	0.42

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	270/289 (93%)	259 (96%)	11 (4%)	0	100	100
1	B	269/289 (93%)	256 (95%)	13 (5%)	0	100	100
1	C	258/289 (89%)	246 (95%)	11 (4%)	1 (0%)	43	52
1	D	259/289 (90%)	244 (94%)	14 (5%)	1 (0%)	43	52
All	All	1056/1156 (91%)	1005 (95%)	49 (5%)	2 (0%)	56	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	ASP
1	D	151	PRO

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	194/222 (87%)	191 (98%)	3 (2%)	76	88
1	B	193/222 (87%)	190 (98%)	3 (2%)	75	87
1	C	181/222 (82%)	179 (99%)	2 (1%)	84	93
1	D	183/222 (82%)	181 (99%)	2 (1%)	84	93
All	All	751/888 (85%)	741 (99%)	10 (1%)	87	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	203[A]	VAL
1	A	203[B]	VAL
1	B	6	ASP
1	B	168[A]	LEU
1	B	168[B]	LEU
1	C	2	THR

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Mol	Chain	Res	Type
1	C	48	GLN
1	D	95[A]	ILE
1	D	95[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

9 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	301	-	48,48,48	3.02	20 (41%)	73,73,73	2.13	16 (21%)
3	1TN	A	302	-	22,22,24	1.53	3 (13%)	29,29,31	1.16	3 (10%)
2	NAD	B	301	-	48,48,48	3.03	21 (43%)	73,73,73	2.07	14 (19%)
3	1TN	B	302	-	23,23,24	1.74	4 (17%)	30,30,31	0.90	1 (3%)
2	NAD	C	301	-	48,48,48	3.03	21 (43%)	73,73,73	2.09	15 (20%)
3	1TN	C	302[B]	-	22,22,24	1.55	3 (13%)	29,29,31	1.06	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	1TN	C	302[C]	-	22,22,24	1.62	3 (13%)	29,29,31	1.20	3 (10%)
2	NAD	D	301	-	48,48,48	3.04	20 (41%)	73,73,73	2.10	16 (21%)
3	1TN	D	302	-	22,22,24	1.67	3 (13%)	29,29,31	1.14	2 (6%)

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	301	-	-	0/30/62/62	0/5/5/5
3	1TN	A	302	-	-	0/12/12/14	0/2/2/2
2	NAD	B	301	-	-	0/30/62/62	0/5/5/5
3	1TN	B	302	-	-	0/13/13/14	0/2/2/2
2	NAD	C	301	-	-	0/30/62/62	0/5/5/5
3	1TN	C	302[B]	-	-	0/12/12/14	0/2/2/2
3	1TN	C	302[C]	-	-	0/12/12/14	0/2/2/2
2	NAD	D	301	-	-	0/30/62/62	0/5/5/5
3	1TN	D	302	-	-	0/12/12/14	0/2/2/2

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAD	C2N-N1N	8.51	1.46	1.35
2	C	301	NAD	C2N-N1N	8.25	1.45	1.35
2	A	301	NAD	C2N-N1N	8.23	1.45	1.35
2	D	301	NAD	C2N-N1N	8.01	1.45	1.35
2	A	301	NAD	PN-O1N	6.73	1.65	1.48
2	D	301	NAD	PN-O1N	6.60	1.64	1.48
2	B	301	NAD	PN-O1N	6.36	1.64	1.48
2	A	301	NAD	C7N-N7N	6.36	1.46	1.33
2	C	301	NAD	PN-O1N	6.32	1.64	1.48
2	B	301	NAD	C7N-N7N	6.26	1.46	1.33
2	A	301	NAD	C4N-C3N	6.10	1.49	1.39
2	D	301	NAD	C7N-N7N	6.08	1.45	1.33
2	B	301	NAD	C4N-C3N	6.07	1.49	1.39
2	C	301	NAD	C7N-N7N	6.04	1.45	1.33
2	D	301	NAD	C4N-C3N	5.95	1.49	1.39
2	C	301	NAD	C4N-C3N	5.91	1.49	1.39
3	B	302	1TN	C11-C10	-5.80	1.52	1.55
2	A	301	NAD	C2A-N3A	5.28	1.41	1.32
2	C	301	NAD	C2A-N3A	5.23	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAD	C2A-N3A	5.23	1.41	1.32
2	B	301	NAD	C2A-N3A	5.18	1.41	1.32
3	D	302	1TN	C10-C09	-5.15	1.53	1.55
2	B	301	NAD	C6N-N1N	4.96	1.48	1.35
2	C	301	NAD	C8A-N7A	4.95	1.44	1.34
2	D	301	NAD	C8A-N7A	4.91	1.44	1.34
2	B	301	NAD	C8A-N7A	4.81	1.43	1.34
2	D	301	NAD	C6N-N1N	4.81	1.48	1.35
2	A	301	NAD	C6N-N1N	4.79	1.48	1.35
2	C	301	NAD	C6N-N1N	4.76	1.48	1.35
3	C	302[C]	1TN	C10-C09	-4.74	1.53	1.55
2	A	301	NAD	C8A-N7A	4.69	1.43	1.34
2	D	301	NAD	C2N-C3N	4.68	1.46	1.39
2	D	301	NAD	C4A-N9A	4.66	1.44	1.37
2	A	301	NAD	C2A-N1A	4.61	1.42	1.33
2	A	301	NAD	C2N-C3N	4.60	1.45	1.39
3	C	302[B]	1TN	C10-C09	-4.56	1.53	1.55
3	A	302	1TN	C10-C09	-4.50	1.53	1.55
2	C	301	NAD	C2N-C3N	4.42	1.45	1.39
2	C	301	NAD	C4A-N9A	4.35	1.44	1.37
2	D	301	NAD	C2A-N1A	4.35	1.42	1.33
2	B	301	NAD	C2N-C3N	4.29	1.45	1.39
3	B	302	1TN	O22-N21	-4.29	1.17	1.25
2	B	301	NAD	C2A-N1A	4.29	1.42	1.33
2	C	301	NAD	C2A-N1A	4.20	1.42	1.33
3	C	302[C]	1TN	O22-N21	-4.17	1.17	1.25
3	D	302	1TN	O22-N21	-4.09	1.17	1.25
3	C	302[B]	1TN	O22-N21	-4.05	1.17	1.25
2	C	301	NAD	C6A-N6A	3.98	1.47	1.34
2	D	301	NAD	PA-O3	3.94	1.66	1.59
2	B	301	NAD	C6A-N6A	3.89	1.47	1.34
2	C	301	NAD	PA-O3	3.87	1.66	1.59
3	A	302	1TN	O22-N21	-3.81	1.18	1.25
2	A	301	NAD	PA-O1A	3.80	1.65	1.51
2	C	301	NAD	PA-O1A	3.79	1.65	1.51
2	A	301	NAD	C6A-N6A	3.76	1.46	1.34
2	D	301	NAD	PA-O1A	3.74	1.65	1.51
2	B	301	NAD	PA-O1A	3.72	1.65	1.51
2	B	301	NAD	C4A-N9A	3.70	1.43	1.37
2	D	301	NAD	C6A-N6A	3.68	1.46	1.34
2	A	301	NAD	C4A-N9A	3.66	1.43	1.37
2	A	301	NAD	PA-O3	3.51	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAD	PA-O3	3.37	1.65	1.59
2	C	301	NAD	C6N-C5N	3.20	1.45	1.38
2	C	301	NAD	C3B-C4B	3.19	1.61	1.53
2	B	301	NAD	C3B-C4B	3.15	1.61	1.53
2	B	301	NAD	C6N-C5N	3.10	1.45	1.38
2	D	301	NAD	C6N-C5N	3.00	1.45	1.38
2	D	301	NAD	C3B-C4B	2.97	1.61	1.53
3	C	302[C]	1TN	O23-N21	-2.92	1.16	1.22
2	A	301	NAD	C2B-C1B	-2.92	1.49	1.53
2	A	301	NAD	C3B-C4B	2.91	1.61	1.53
2	D	301	NAD	C2B-C1B	-2.90	1.49	1.53
2	A	301	NAD	C6N-C5N	2.88	1.45	1.38
2	B	301	NAD	C2B-C1B	-2.75	1.49	1.53
2	D	301	NAD	PN-O3	2.72	1.66	1.60
3	D	302	1TN	O23-N21	-2.71	1.17	1.22
2	D	301	NAD	C5N-C4N	2.70	1.44	1.38
2	C	301	NAD	C5N-C4N	2.66	1.44	1.38
2	C	301	NAD	C2B-C1B	-2.64	1.49	1.53
2	B	301	NAD	C5N-C4N	2.61	1.44	1.38
3	A	302	1TN	O23-N21	-2.54	1.17	1.22
2	C	301	NAD	O7N-C7N	-2.47	1.18	1.24
2	C	301	NAD	PN-O3	2.43	1.65	1.60
3	C	302[B]	1TN	O23-N21	-2.42	1.17	1.22
2	B	301	NAD	PN-O3	2.42	1.65	1.60
2	A	301	NAD	O7N-C7N	-2.41	1.18	1.24
3	B	302	1TN	O23-N21	-2.40	1.17	1.22
2	D	301	NAD	O7N-C7N	-2.33	1.19	1.24
2	A	301	NAD	C5N-C4N	2.31	1.43	1.38
3	B	302	1TN	O13-C04	2.29	1.41	1.36
2	B	301	NAD	O7N-C7N	-2.28	1.19	1.24
2	A	301	NAD	C3D-C4D	2.27	1.59	1.53
2	D	301	NAD	C3D-C4D	2.22	1.59	1.53
2	A	301	NAD	PN-O3	2.19	1.64	1.60
2	B	301	NAD	C3N-C7N	2.16	1.54	1.50
2	B	301	NAD	C2D-C1D	-2.14	1.50	1.53
2	C	301	NAD	C3N-C7N	2.04	1.53	1.50
2	C	301	NAD	C3D-C4D	2.03	1.58	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAD	N3A-C2A-N1A	-11.05	119.17	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAD	N3A-C2A-N1A	-10.71	119.47	128.89
2	C	301	NAD	N3A-C2A-N1A	-10.56	119.60	128.89
2	A	301	NAD	N3A-C2A-N1A	-10.52	119.63	128.89
2	C	301	NAD	C4B-O4B-C1B	-7.16	101.85	109.72
2	A	301	NAD	C4B-O4B-C1B	-6.80	102.24	109.72
2	B	301	NAD	C4B-O4B-C1B	-6.76	102.29	109.72
2	D	301	NAD	C4B-O4B-C1B	-6.22	102.88	109.72
2	D	301	NAD	C5A-C4A-N3A	-5.32	120.79	125.98
2	C	301	NAD	C5A-C4A-N3A	-4.90	121.21	125.98
2	A	301	NAD	C5A-C4A-N3A	-4.56	121.53	125.98
2	B	301	NAD	C5A-C4A-N3A	-4.08	122.01	125.98
3	D	302	1TN	C07-C08-C09	3.71	120.34	113.20
2	D	301	NAD	N3A-C4A-N9A	3.61	131.59	125.39
3	C	302[C]	1TN	C07-C08-C09	3.61	120.13	113.20
2	A	301	NAD	C8A-N9A-C4A	3.60	109.89	106.96
2	B	301	NAD	C8A-N9A-C4A	3.58	109.87	106.96
2	A	301	NAD	N3A-C4A-N9A	3.57	131.51	125.39
2	A	301	NAD	C3D-C2D-C1D	-3.35	95.67	100.92
2	C	301	NAD	N3A-C4A-N9A	3.31	131.08	125.39
2	B	301	NAD	N3A-C4A-N9A	3.27	131.00	125.39
3	C	302[B]	1TN	C07-C08-C09	3.26	119.47	113.20
2	C	301	NAD	PN-O3-PA	-3.18	120.36	133.17
2	D	301	NAD	PN-O3-PA	-3.18	120.39	133.17
2	A	301	NAD	C2N-C3N-C4N	3.11	121.80	118.31
3	A	302	1TN	C07-C08-C09	3.06	119.09	113.20
3	A	302	1TN	C17-C16-N21	3.05	120.29	116.74
2	A	301	NAD	PN-O3-PA	-2.99	121.15	133.17
2	B	301	NAD	O2N-PN-O1N	-2.87	110.14	118.70
3	B	302	1TN	C17-C16-N21	2.78	119.97	116.74
2	D	301	NAD	C2N-C3N-C4N	2.73	121.38	118.31
3	C	302[C]	1TN	C17-C16-N21	2.71	119.90	116.74
2	D	301	NAD	C3N-C7N-N7N	2.63	120.71	117.78
2	B	301	NAD	C3D-C2D-C1D	-2.61	96.83	100.92
2	D	301	NAD	O2N-PN-O1N	-2.60	110.93	118.70
2	D	301	NAD	O4B-C4B-C5B	2.57	118.51	109.37
2	C	301	NAD	C2N-C3N-C4N	2.56	121.19	118.31
2	B	301	NAD	PN-O3-PA	-2.56	122.88	133.17
2	C	301	NAD	O2N-PN-O1N	-2.53	111.15	118.70
2	C	301	NAD	O4B-C1B-C2B	-2.52	103.03	106.69
2	B	301	NAD	N7A-C8A-N9A	-2.49	106.55	112.20
2	C	301	NAD	C8A-N9A-C4A	2.47	108.96	106.96
2	D	301	NAD	C3D-C2D-C1D	-2.47	97.05	100.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	1TN	C17-C16-N21	2.45	119.59	116.74
2	A	301	NAD	O2N-PN-O1N	-2.44	111.42	118.70
2	A	301	NAD	C3N-C7N-N7N	2.44	120.49	117.78
2	A	301	NAD	N7A-C8A-N9A	-2.42	106.70	112.20
2	A	301	NAD	O2D-C2D-C1D	2.41	119.10	111.49
2	C	301	NAD	O2B-C2B-C1B	2.38	119.03	111.49
2	A	301	NAD	C3N-C2N-N1N	-2.37	117.20	120.36
2	C	301	NAD	O3-PA-O5B	2.35	109.14	102.91
2	B	301	NAD	C2N-C3N-C4N	2.32	120.91	118.31
2	D	301	NAD	C2A-N3A-C4A	2.25	119.75	113.27
3	A	302	1TN	O14-C03-C04	2.24	120.78	116.23
2	B	301	NAD	C1B-N9A-C4A	-2.19	122.85	126.64
2	C	301	NAD	C3D-C2D-C1D	-2.18	97.50	100.92
2	D	301	NAD	C8A-N9A-C4A	2.14	108.70	106.96
3	C	302[B]	1TN	C17-C16-N21	2.14	119.23	116.74
2	D	301	NAD	O2D-C2D-C1D	2.14	118.26	111.49
2	A	301	NAD	O3D-C3D-C4D	2.13	117.33	111.07
2	C	301	NAD	N7A-C8A-N9A	-2.12	107.39	112.20
2	C	301	NAD	O2D-C2D-C1D	2.11	118.18	111.49
2	D	301	NAD	O3B-C3B-C4B	2.11	117.29	111.07
2	C	301	NAD	C2A-N3A-C4A	2.10	119.31	113.27
2	A	301	NAD	O3-PN-O5D	2.04	109.03	101.23
2	A	301	NAD	O7N-C7N-C3N	-2.04	117.31	119.59
2	D	301	NAD	N7A-C8A-N9A	-2.04	107.57	112.20
2	B	301	NAD	C3N-C7N-N7N	2.04	120.05	117.78
2	B	301	NAD	C3N-C2N-N1N	-2.03	117.65	120.36
2	D	301	NAD	C3N-C2N-N1N	-2.01	117.68	120.36
2	B	301	NAD	C2A-N3A-C4A	2.00	119.04	113.27
3	C	302[C]	1TN	O22-N21-O23	-2.00	117.46	121.86

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	268/289 (92%)	-0.46	0 100 100	17, 29, 53, 61	0
1	B	268/289 (92%)	-0.25	2 (0%) 84 88	19, 34, 50, 65	0
1	C	261/289 (90%)	-0.27	9 (3%) 43 47	17, 33, 57, 74	0
1	D	261/289 (90%)	-0.41	2 (0%) 83 86	20, 34, 54, 75	0
All	All	1058/1156 (91%)	-0.35	13 (1%) 75 79	17, 33, 54, 75	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	207	LEU	4.6
1	C	206	ALA	3.6
1	D	217	LEU	2.5
1	D	201	ALA	2.4
1	C	105	ILE	2.3
1	C	217	LEU	2.3
1	B	257	ILE	2.2
1	C	201	ALA	2.1
1	B	83	GLY	2.1
1	C	215	ILE	2.1
1	C	2	THR	2.1
1	C	257	ILE	2.1
1	C	58	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	1TN	B	302	22/23	0.11	0.22	21,31,41,49	0
2	NAD	A	301	44/44	0.10	0.08	17,22,30,34	0
3	1TN	C	302[B]	21/23	0.12	0.06	32,40,43,46	21
3	1TN	C	302[C]	21/23	0.12	0.06	32,39,44,47	21
2	NAD	C	301	44/44	0.10	-0.01	22,31,38,41	0
2	NAD	B	301	44/44	0.10	-0.21	20,30,37,43	0
3	1TN	D	302	21/23	0.11	-0.22	29,39,46,53	0
3	1TN	A	302	21/23	0.10	-0.23	17,26,36,40	0
2	NAD	D	301	44/44	0.09	-0.48	20,33,44,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.