Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2017 – 06:48 PM EST

PDB ID	:	5MTQ
Title	:	Crystal structure of M. tuberculosis InhA inhibited by PT511
Authors	:	Eltschkner, S.; Pschibul, A.; Spagnuolo, L.A.; Yu, W.; Tonge, P.J.; Kisker, C.
Deposited on	:	2017-01-10
Resolution	:	2.60 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
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:

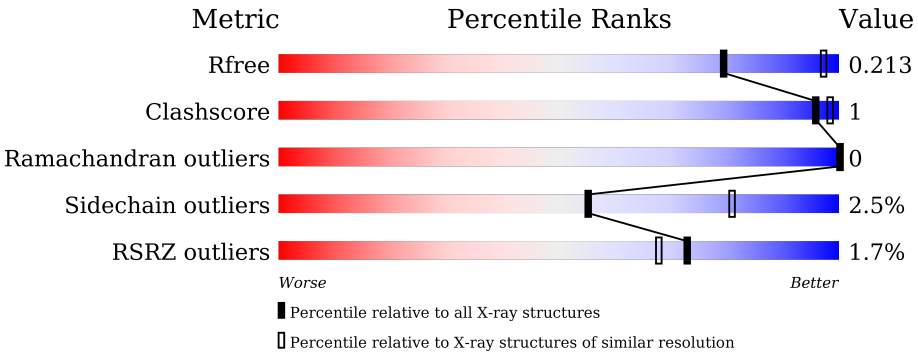
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	289	85% 6% • 7%
1	B	289	2% 90% • 7%
1	C	289	% 88% 5% 7%
1	D	289	% 90% • 7%
1	E	289	% 88% • 7%
1	F	289	2% 87% 5% • 7%

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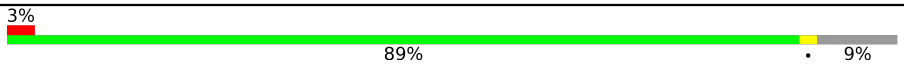
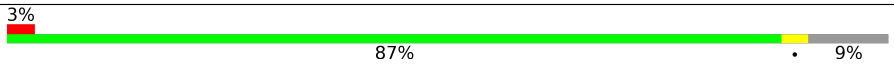
Mol	Chain	Length	Quality of chain
1	G	289	
1	H	289	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16844 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 [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	3	0
			2009	1273	348	377	11			
1	B	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			
1	E	268	Total	C	N	O	S	0	1	0
			1999	1266	348	375	10			
1	G	264	Total	C	N	O	S	0	2	0
			1978	1254	344	369	11			
1	C	268	Total	C	N	O	S	0	1	0
			1999	1266	348	375	10			
1	D	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			
1	F	268	Total	C	N	O	S	0	1	0
			2001	1268	348	374	11			
1	H	263	Total	C	N	O	S	0	0	0
			1966	1246	343	367	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WGR1
A	-18	GLY	-	expression tag	UNP P9WGR1
A	-17	SER	-	expression tag	UNP P9WGR1
A	-16	SER	-	expression tag	UNP P9WGR1
A	-15	HIS	-	expression tag	UNP P9WGR1
A	-14	HIS	-	expression tag	UNP P9WGR1
A	-13	HIS	-	expression tag	UNP P9WGR1
A	-12	HIS	-	expression tag	UNP P9WGR1
A	-11	HIS	-	expression tag	UNP P9WGR1
A	-10	HIS	-	expression tag	UNP P9WGR1
A	-9	SER	-	expression tag	UNP P9WGR1
A	-8	SER	-	expression tag	UNP P9WGR1
A	-7	GLY	-	expression tag	UNP P9WGR1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP P9WGR1
A	-5	VAL	-	expression tag	UNP P9WGR1
A	-4	PRO	-	expression tag	UNP P9WGR1
A	-3	ARG	-	expression tag	UNP P9WGR1
A	-2	GLY	-	expression tag	UNP P9WGR1
A	-1	SER	-	expression tag	UNP P9WGR1
A	0	HIS	-	expression tag	UNP P9WGR1
B	-19	MET	-	initiating methionine	UNP P9WGR1
B	-18	GLY	-	expression tag	UNP P9WGR1
B	-17	SER	-	expression tag	UNP P9WGR1
B	-16	SER	-	expression tag	UNP P9WGR1
B	-15	HIS	-	expression tag	UNP P9WGR1
B	-14	HIS	-	expression tag	UNP P9WGR1
B	-13	HIS	-	expression tag	UNP P9WGR1
B	-12	HIS	-	expression tag	UNP P9WGR1
B	-11	HIS	-	expression tag	UNP P9WGR1
B	-10	HIS	-	expression tag	UNP P9WGR1
B	-9	SER	-	expression tag	UNP P9WGR1
B	-8	SER	-	expression tag	UNP P9WGR1
B	-7	GLY	-	expression tag	UNP P9WGR1
B	-6	LEU	-	expression tag	UNP P9WGR1
B	-5	VAL	-	expression tag	UNP P9WGR1
B	-4	PRO	-	expression tag	UNP P9WGR1
B	-3	ARG	-	expression tag	UNP P9WGR1
B	-2	GLY	-	expression tag	UNP P9WGR1
B	-1	SER	-	expression tag	UNP P9WGR1
B	0	HIS	-	expression tag	UNP P9WGR1
E	-19	MET	-	initiating methionine	UNP P9WGR1
E	-18	GLY	-	expression tag	UNP P9WGR1
E	-17	SER	-	expression tag	UNP P9WGR1
E	-16	SER	-	expression tag	UNP P9WGR1
E	-15	HIS	-	expression tag	UNP P9WGR1
E	-14	HIS	-	expression tag	UNP P9WGR1
E	-13	HIS	-	expression tag	UNP P9WGR1
E	-12	HIS	-	expression tag	UNP P9WGR1
E	-11	HIS	-	expression tag	UNP P9WGR1
E	-10	HIS	-	expression tag	UNP P9WGR1
E	-9	SER	-	expression tag	UNP P9WGR1
E	-8	SER	-	expression tag	UNP P9WGR1
E	-7	GLY	-	expression tag	UNP P9WGR1
E	-6	LEU	-	expression tag	UNP P9WGR1
E	-5	VAL	-	expression tag	UNP P9WGR1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	PRO	-	expression tag	UNP P9WGR1
E	-3	ARG	-	expression tag	UNP P9WGR1
E	-2	GLY	-	expression tag	UNP P9WGR1
E	-1	SER	-	expression tag	UNP P9WGR1
E	0	HIS	-	expression tag	UNP P9WGR1
G	-19	MET	-	initiating methionine	UNP P9WGR1
G	-18	GLY	-	expression tag	UNP P9WGR1
G	-17	SER	-	expression tag	UNP P9WGR1
G	-16	SER	-	expression tag	UNP P9WGR1
G	-15	HIS	-	expression tag	UNP P9WGR1
G	-14	HIS	-	expression tag	UNP P9WGR1
G	-13	HIS	-	expression tag	UNP P9WGR1
G	-12	HIS	-	expression tag	UNP P9WGR1
G	-11	HIS	-	expression tag	UNP P9WGR1
G	-10	HIS	-	expression tag	UNP P9WGR1
G	-9	SER	-	expression tag	UNP P9WGR1
G	-8	SER	-	expression tag	UNP P9WGR1
G	-7	GLY	-	expression tag	UNP P9WGR1
G	-6	LEU	-	expression tag	UNP P9WGR1
G	-5	VAL	-	expression tag	UNP P9WGR1
G	-4	PRO	-	expression tag	UNP P9WGR1
G	-3	ARG	-	expression tag	UNP P9WGR1
G	-2	GLY	-	expression tag	UNP P9WGR1
G	-1	SER	-	expression tag	UNP P9WGR1
G	0	HIS	-	expression tag	UNP P9WGR1
C	-19	MET	-	initiating methionine	UNP P9WGR1
C	-18	GLY	-	expression tag	UNP P9WGR1
C	-17	SER	-	expression tag	UNP P9WGR1
C	-16	SER	-	expression tag	UNP P9WGR1
C	-15	HIS	-	expression tag	UNP P9WGR1
C	-14	HIS	-	expression tag	UNP P9WGR1
C	-13	HIS	-	expression tag	UNP P9WGR1
C	-12	HIS	-	expression tag	UNP P9WGR1
C	-11	HIS	-	expression tag	UNP P9WGR1
C	-10	HIS	-	expression tag	UNP P9WGR1
C	-9	SER	-	expression tag	UNP P9WGR1
C	-8	SER	-	expression tag	UNP P9WGR1
C	-7	GLY	-	expression tag	UNP P9WGR1
C	-6	LEU	-	expression tag	UNP P9WGR1
C	-5	VAL	-	expression tag	UNP P9WGR1
C	-4	PRO	-	expression tag	UNP P9WGR1
C	-3	ARG	-	expression tag	UNP P9WGR1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P9WGR1
C	-1	SER	-	expression tag	UNP P9WGR1
C	0	HIS	-	expression tag	UNP P9WGR1
D	-19	MET	-	initiating methionine	UNP P9WGR1
D	-18	GLY	-	expression tag	UNP P9WGR1
D	-17	SER	-	expression tag	UNP P9WGR1
D	-16	SER	-	expression tag	UNP P9WGR1
D	-15	HIS	-	expression tag	UNP P9WGR1
D	-14	HIS	-	expression tag	UNP P9WGR1
D	-13	HIS	-	expression tag	UNP P9WGR1
D	-12	HIS	-	expression tag	UNP P9WGR1
D	-11	HIS	-	expression tag	UNP P9WGR1
D	-10	HIS	-	expression tag	UNP P9WGR1
D	-9	SER	-	expression tag	UNP P9WGR1
D	-8	SER	-	expression tag	UNP P9WGR1
D	-7	GLY	-	expression tag	UNP P9WGR1
D	-6	LEU	-	expression tag	UNP P9WGR1
D	-5	VAL	-	expression tag	UNP P9WGR1
D	-4	PRO	-	expression tag	UNP P9WGR1
D	-3	ARG	-	expression tag	UNP P9WGR1
D	-2	GLY	-	expression tag	UNP P9WGR1
D	-1	SER	-	expression tag	UNP P9WGR1
D	0	HIS	-	expression tag	UNP P9WGR1
F	-19	MET	-	initiating methionine	UNP P9WGR1
F	-18	GLY	-	expression tag	UNP P9WGR1
F	-17	SER	-	expression tag	UNP P9WGR1
F	-16	SER	-	expression tag	UNP P9WGR1
F	-15	HIS	-	expression tag	UNP P9WGR1
F	-14	HIS	-	expression tag	UNP P9WGR1
F	-13	HIS	-	expression tag	UNP P9WGR1
F	-12	HIS	-	expression tag	UNP P9WGR1
F	-11	HIS	-	expression tag	UNP P9WGR1
F	-10	HIS	-	expression tag	UNP P9WGR1
F	-9	SER	-	expression tag	UNP P9WGR1
F	-8	SER	-	expression tag	UNP P9WGR1
F	-7	GLY	-	expression tag	UNP P9WGR1
F	-6	LEU	-	expression tag	UNP P9WGR1
F	-5	VAL	-	expression tag	UNP P9WGR1
F	-4	PRO	-	expression tag	UNP P9WGR1
F	-3	ARG	-	expression tag	UNP P9WGR1
F	-2	GLY	-	expression tag	UNP P9WGR1
F	-1	SER	-	expression tag	UNP P9WGR1

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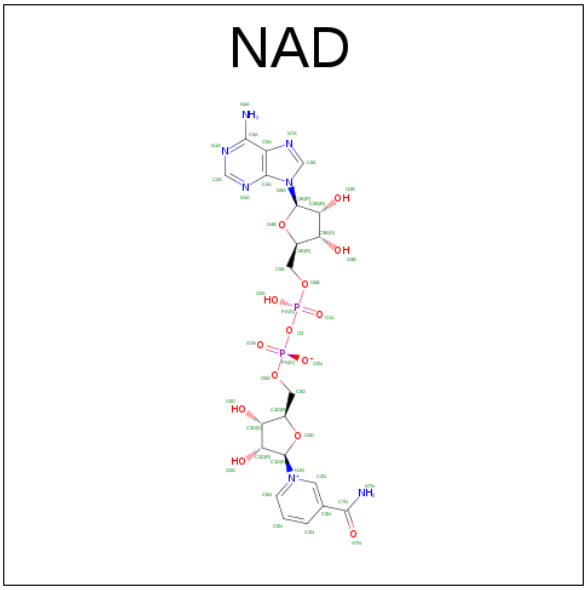
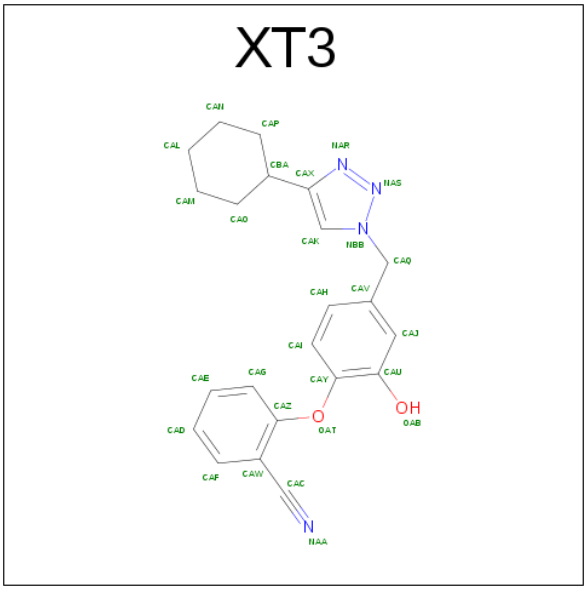
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P9WGR1
H	-19	MET	-	initiating methionine	UNP P9WGR1
H	-18	GLY	-	expression tag	UNP P9WGR1
H	-17	SER	-	expression tag	UNP P9WGR1
H	-16	SER	-	expression tag	UNP P9WGR1
H	-15	HIS	-	expression tag	UNP P9WGR1
H	-14	HIS	-	expression tag	UNP P9WGR1
H	-13	HIS	-	expression tag	UNP P9WGR1
H	-12	HIS	-	expression tag	UNP P9WGR1
H	-11	HIS	-	expression tag	UNP P9WGR1
H	-10	HIS	-	expression tag	UNP P9WGR1
H	-9	SER	-	expression tag	UNP P9WGR1
H	-8	SER	-	expression tag	UNP P9WGR1
H	-7	GLY	-	expression tag	UNP P9WGR1
H	-6	LEU	-	expression tag	UNP P9WGR1
H	-5	VAL	-	expression tag	UNP P9WGR1
H	-4	PRO	-	expression tag	UNP P9WGR1
H	-3	ARG	-	expression tag	UNP P9WGR1
H	-2	GLY	-	expression tag	UNP P9WGR1
H	-1	SER	-	expression tag	UNP P9WGR1
H	0	HIS	-	expression tag	UNP P9WGR1

- 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		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2-[4-[(4-cyclohexyl-1,2,3-triazol-1-yl)methyl]-2-oxidanyl-phenoxy]benzenecarbonitrile (three-letter code: XT3) (formula: $C_{22}H_{22}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	4	2		
3	B	1	Total	C	N	O	0	0
			28	22	4	2		
3	E	1	Total	C	N	O	0	0
			28	22	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			28	22	4	2		
3	C	1	Total	C	N	O	0	0
			28	22	4	2		
3	D	1	Total	C	N	O	0	0
			28	22	4	2		
3	F	1	Total	C	N	O	0	0
			28	22	4	2		
3	H	1	Total	C	N	O	0	0
			28	22	4	2		

- Molecule 4 is water.

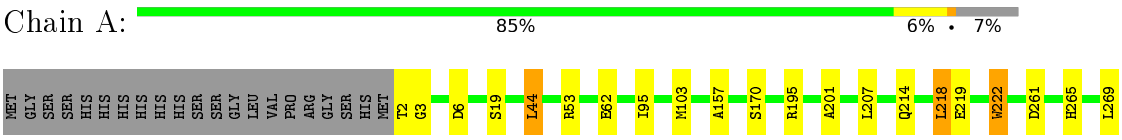
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	34	Total	O	0	0
			34	34		
4	E	30	Total	O	0	0
			30	30		
4	G	30	Total	O	0	0
			30	30		
4	C	50	Total	O	0	0
			50	50		
4	D	50	Total	O	0	0
			50	50		
4	F	40	Total	O	0	0
			40	40		
4	H	25	Total	O	0	0
			25	25		

3 Residue-property plots (i)

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.

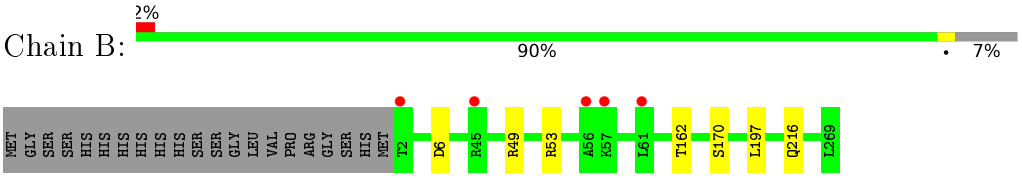
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



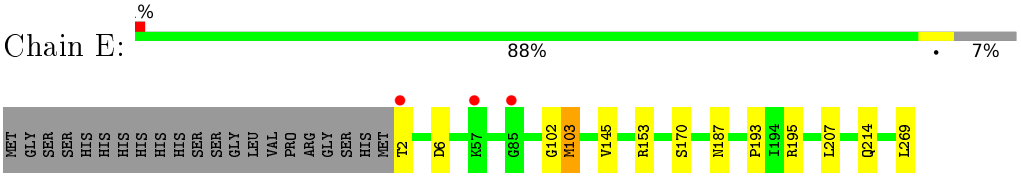
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain B:



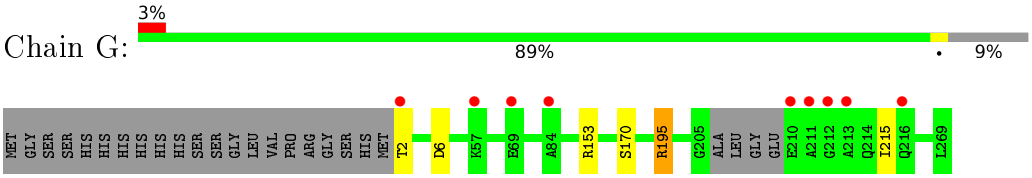
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain E:



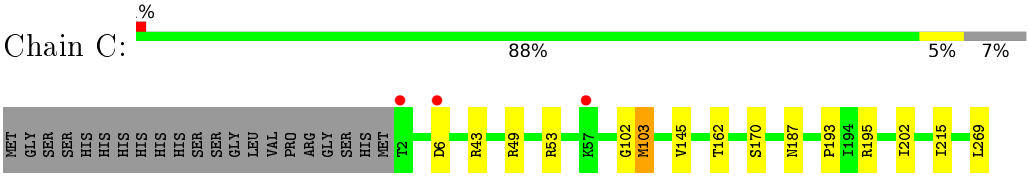
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain G:



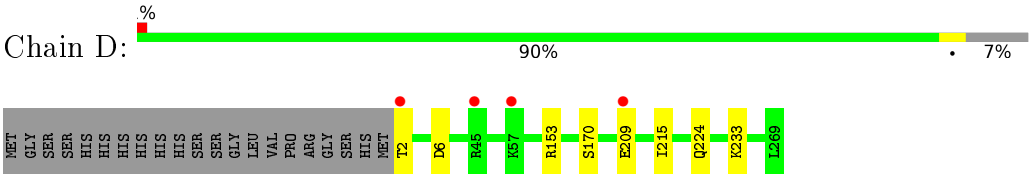
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain C:



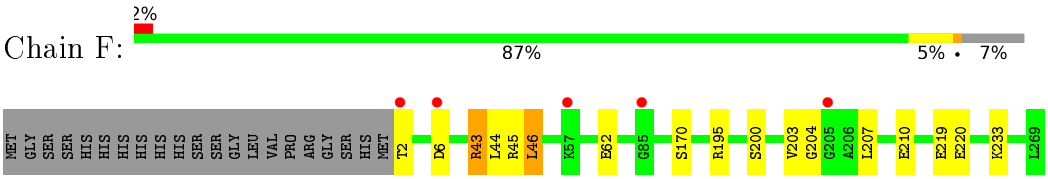
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:



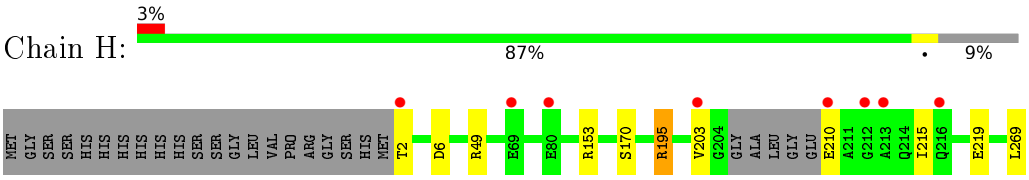
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain F:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.22Å 92.45Å 181.20Å 90.00° 96.46° 90.00°	Depositor
Resolution (Å)	45.00 – 2.60 45.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.00-2.60) 100.0 (45.01-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.191 , 0.213 0.191 , 0.213	Depositor DCC
R_{free} test set	4462 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16844	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4321e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XT3, 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	0.67	0/2056	0.83	4/2790 (0.1%)
1	B	0.64	0/2034	0.74	1/2761 (0.0%)
1	C	0.70	0/2040	0.81	5/2769 (0.2%)
1	D	0.67	0/2034	0.83	2/2761 (0.1%)
1	E	0.63	0/2040	0.73	1/2769 (0.0%)
1	F	0.78	3/2042 (0.1%)	0.82	3/2771 (0.1%)
1	G	0.61	0/2021	0.72	1/2741 (0.0%)
1	H	0.62	0/2003	0.74	1/2718 (0.0%)
All	All	0.67	3/16270 (0.0%)	0.78	18/22080 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	220	GLU	CG-CD	11.51	1.69	1.51
1	F	219	GLU	CD-OE2	6.76	1.33	1.25
1	F	220	GLU	CD-OE2	5.64	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	153	ARG	NE-CZ-NH1	14.13	127.36	120.30
1	A	103	MET	CA-CB-CG	10.88	131.79	113.30
1	F	220	GLU	OE1-CD-OE2	-10.41	110.81	123.30
1	C	53	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	D	153	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	A	53	ARG	NE-CZ-NH1	9.73	125.17	120.30
1	A	53	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	53	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	H	153	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	103	MET	CG-SD-CE	-5.80	90.91	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	46	LEU	CB-CG-CD1	5.60	120.52	111.00
1	A	53	ARG	CD-NE-CZ	5.58	131.42	123.60
1	G	153	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	E	103	MET	CG-SD-CE	5.53	109.05	100.20
1	C	53	ARG	CD-NE-CZ	5.50	131.31	123.60
1	C	43	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	F	43	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	53	ARG	CG-CD-NE	5.03	122.36	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2009	0	2031	10	0
1	B	1996	0	2013	1	1
1	C	1999	0	2018	11	0
1	D	1996	0	2013	6	0
1	E	1999	0	2018	6	0
1	F	2001	0	2022	13	0
1	G	1978	0	2001	3	0
1	H	1966	0	1984	4	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	2	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	28	0	0	1	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
3	E	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	0	0	0
3	G	28	0	0	0	0
3	H	28	0	0	0	0
4	A	65	0	0	0	0
4	B	34	0	0	0	0
4	C	50	0	0	1	0
4	D	50	0	0	0	0
4	E	30	0	0	0	0
4	F	40	0	0	3	0
4	G	30	0	0	1	0
4	H	25	0	0	1	0
All	All	16844	0	16308	49	1

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 1.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:MET:CE	1:C:202:ILE:HG22	1.80	1.11
1:C:103:MET:HE1	1:C:202:ILE:HG22	1.17	1.10
1:D:2:THR:HG23	4:F:436:HOH:O	1.54	1.06
1:D:2:THR:CG2	4:F:436:HOH:O	2.04	1.01
1:C:103:MET:CE	1:C:202:ILE:CG2	2.42	0.97
1:F:44:LEU:HD11	1:F:62:GLU:HG3	1.51	0.92
1:C:103:MET:HE2	1:C:202:ILE:CG2	2.03	0.89
1:C:103:MET:HE1	1:C:202:ILE:CG2	2.05	0.79
1:A:2:THR:HG23	1:A:3:GLY:H	1.51	0.75
1:A:19:SER:OG	1:F:233:LYS:HE3	1.89	0.71
1:E:207:LEU:CD1	1:E:214:GLN:HB2	2.26	0.66
1:H:49:ARG:NH1	4:H:401:HOH:O	2.28	0.65
1:A:201:ALA:HA	1:F:207:LEU:HD13	1.82	0.61
1:D:2:THR:HA	1:F:2:THR:HG21	1.83	0.60
1:F:204:GLY:O	1:F:207:LEU:HB2	2.03	0.58
1:C:103:MET:HE2	1:C:202:ILE:HG21	1.83	0.58
1:H:203:VAL:HG12	1:H:203:VAL:O	2.03	0.57
1:E:2:THR:HG23	1:E:2:THR:O	2.05	0.56
1:A:2:THR:HG23	1:A:3:GLY:N	2.18	0.55
1:F:203:VAL:HG11	1:F:210:GLU:HB2	1.89	0.55
1:C:195:ARG:HD2	4:C:425:HOH:O	2.07	0.54
1:H:203:VAL:HG11	1:H:210:GLU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:LEU:CD1	1:F:62:GLU:HG3	2.33	0.52
1:F:45:ARG:HB2	4:F:421:HOH:O	2.11	0.51
1:E:193:PRO:HA	2:E:301:NAD:O7N	2.13	0.49
1:E:102:GLY:O	1:E:103:MET:HG2	2.14	0.48
1:F:46:LEU:N	1:F:46:LEU:HD23	2.27	0.48
1:A:44:LEU:HD21	1:A:62:GLU:HG3	1.98	0.46
1:A:265:HIS:O	1:E:153:ARG:HD3	2.16	0.45
1:D:2:THR:HA	1:F:2:THR:CG2	2.46	0.45
1:F:203:VAL:HB	1:F:207:LEU:HG	1.99	0.45
1:A:218:LEU:HD13	3:A:302:XT3:CAN	2.47	0.45
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.82	0.45
1:C:102:GLY:O	1:C:103:MET:HG2	2.17	0.44
1:F:200:SER:O	1:F:207:LEU:HD11	2.18	0.43
2:E:301:NAD:C7N	3:E:302:XT3:CAH	2.97	0.43
1:G:195:ARG:NH2	1:G:215:ILE:HD12	2.34	0.43
1:G:195:ARG:HG2	4:G:421:HOH:O	2.19	0.42
1:D:215:ILE:HG21	1:D:215:ILE:HD13	1.80	0.42
1:B:197:LEU:HA	1:B:197:LEU:HD12	1.79	0.41
1:D:2:THR:CA	1:F:2:THR:HG21	2.48	0.41
1:G:195:ARG:HH22	1:G:215:ILE:HD12	1.85	0.41
1:A:95:ILE:HG21	1:A:95:ILE:HD13	1.90	0.41
1:C:145:VAL:HA	1:C:187:ASN:O	2.21	0.41
1:E:145:VAL:HA	1:E:187:ASN:O	2.21	0.41
1:A:157:ALA:HB2	1:A:207:LEU:HD21	2.03	0.40
1:C:193:PRO:HA	2:C:301:NAD:O7N	2.21	0.40
1:C:215:ILE:HD13	1:C:215:ILE:HG21	1.81	0.40
1:H:195:ARG:NH2	1:H:215:ILE:HD12	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:NH1	1:B:216:GLN:OE1[2_556]	2.00	0.20

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	269/289 (93%)	257 (96%)	12 (4%)	0	100	100
1	B	266/289 (92%)	253 (95%)	13 (5%)	0	100	100
1	C	267/289 (92%)	253 (95%)	14 (5%)	0	100	100
1	D	266/289 (92%)	255 (96%)	11 (4%)	0	100	100
1	E	267/289 (92%)	254 (95%)	13 (5%)	0	100	100
1	F	267/289 (92%)	253 (95%)	14 (5%)	0	100	100
1	G	262/289 (91%)	249 (95%)	13 (5%)	0	100	100
1	H	259/289 (90%)	246 (95%)	13 (5%)	0	100	100
All	All	2123/2312 (92%)	2020 (95%)	103 (5%)	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	207/222 (93%)	197 (95%)	10 (5%)	31	58
1	B	204/222 (92%)	201 (98%)	3 (2%)	72	90
1	C	205/222 (92%)	200 (98%)	5 (2%)	57	82
1	D	204/222 (92%)	199 (98%)	5 (2%)	55	81
1	E	205/222 (92%)	201 (98%)	4 (2%)	63	85
1	F	205/222 (92%)	201 (98%)	4 (2%)	63	85
1	G	204/222 (92%)	200 (98%)	4 (2%)	63	85
1	H	202/222 (91%)	196 (97%)	6 (3%)	48	76
All	All	1636/1776 (92%)	1595 (98%)	41 (2%)	55	81

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

Mol	Chain	Res	Type
1	A	6[A]	ASP
1	A	6[B]	ASP
1	A	44	LEU
1	A	170	SER
1	A	195	ARG
1	A	214	GLN
1	A	218	LEU
1	A	219	GLU
1	A	222	TRP
1	A	269	LEU
1	B	6	ASP
1	B	162	THR
1	B	170	SER
1	E	6	ASP
1	E	170	SER
1	E	195	ARG
1	E	269	LEU
1	G	2	THR
1	G	6	ASP
1	G	170	SER
1	G	195	ARG
1	C	6	ASP
1	C	49	ARG
1	C	162	THR
1	C	170	SER
1	C	269	LEU
1	D	6	ASP
1	D	170	SER
1	D	209	GLU
1	D	224	GLN
1	D	233	LYS
1	F	6	ASP
1	F	43	ARG
1	F	170	SER
1	F	195	ARG
1	H	2	THR
1	H	6	ASP
1	H	170	SER
1	H	195	ARG
1	H	219	GLU
1	H	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	224	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

16 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	-	42,48,48	0.81	1 (2%)	46,73,73	1.21	5 (10%)
3	XT3	A	302	-	30,31,31	2.77	8 (26%)	39,42,42	1.90	5 (12%)
2	NAD	B	301	-	42,48,48	0.96	2 (4%)	46,73,73	1.23	4 (8%)
3	XT3	B	302	-	30,31,31	2.23	9 (30%)	39,42,42	2.40	7 (17%)
2	NAD	C	301	-	42,48,48	1.03	2 (4%)	46,73,73	1.69	8 (17%)
3	XT3	C	302	-	30,31,31	2.09	7 (23%)	39,42,42	1.99	9 (23%)
2	NAD	D	301	-	42,48,48	0.77	2 (4%)	46,73,73	1.13	4 (8%)
3	XT3	D	302	-	30,31,31	2.20	4 (13%)	39,42,42	1.63	7 (17%)
2	NAD	E	301	-	42,48,48	0.94	2 (4%)	46,73,73	1.56	10 (21%)
3	XT3	E	302	-	30,31,31	2.44	7 (23%)	39,42,42	1.56	5 (12%)
2	NAD	F	301	-	42,48,48	0.85	1 (2%)	46,73,73	1.39	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	XT3	F	302	-	30,31,31	2.19	7 (23%)	39,42,42	1.80	5 (12%)
2	NAD	G	301	-	42,48,48	0.79	1 (2%)	46,73,73	1.15	2 (4%)
3	XT3	G	302	-	30,31,31	2.21	6 (20%)	39,42,42	1.36	3 (7%)
2	NAD	H	301	-	42,48,48	0.82	2 (4%)	46,73,73	1.41	4 (8%)
3	XT3	H	302	-	30,31,31	2.59	6 (20%)	39,42,42	2.24	7 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	301	-	-	0/22/62/62	0/5/5/5
3	XT3	A	302	-	-	0/14/22/22	0/4/4/4
2	NAD	B	301	-	-	0/22/62/62	0/5/5/5
3	XT3	B	302	-	-	1/14/22/22	0/4/4/4
2	NAD	C	301	-	-	0/22/62/62	0/5/5/5
3	XT3	C	302	-	-	0/14/22/22	0/4/4/4
2	NAD	D	301	-	-	0/22/62/62	0/5/5/5
3	XT3	D	302	-	-	0/14/22/22	0/4/4/4
2	NAD	E	301	-	-	0/22/62/62	0/5/5/5
3	XT3	E	302	-	-	0/14/22/22	0/4/4/4
2	NAD	F	301	-	-	0/22/62/62	0/5/5/5
3	XT3	F	302	-	-	0/14/22/22	0/4/4/4
2	NAD	G	301	-	-	0/22/62/62	0/5/5/5
3	XT3	G	302	-	-	0/14/22/22	0/4/4/4
2	NAD	H	301	-	-	0/22/62/62	0/5/5/5
3	XT3	H	302	-	-	1/14/22/22	0/4/4/4

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	XT3	NAR-NAS	-10.18	1.19	1.34
3	H	302	XT3	CAW-CAC	-9.93	1.29	1.44
3	E	302	XT3	NAR-NAS	-8.97	1.21	1.34
3	F	302	XT3	NAR-NAS	-7.55	1.23	1.34
3	D	302	XT3	CAW-CAC	-7.13	1.33	1.44
3	A	302	XT3	NAS-NBB	-6.85	1.21	1.34
3	G	302	XT3	CAW-CAC	-6.24	1.35	1.44
3	B	302	XT3	CAQ-CAV	-6.16	1.36	1.51
3	G	302	XT3	NAS-NBB	-6.12	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	XT3	CAW-CAC	-5.53	1.36	1.44
3	D	302	XT3	NAS-NBB	-5.48	1.23	1.34
3	G	302	XT3	CAQ-CAV	-5.39	1.38	1.51
3	C	302	XT3	CAQ-CAV	-5.35	1.38	1.51
3	A	302	XT3	CAQ-CAV	-5.30	1.38	1.51
3	E	302	XT3	CAQ-CAV	-5.24	1.39	1.51
3	H	302	XT3	CAQ-CAV	-5.11	1.39	1.51
3	B	302	XT3	CAW-CAC	-5.02	1.36	1.44
3	D	302	XT3	CAQ-CAV	-4.89	1.39	1.51
2	C	301	NAD	O4D-C1D	-4.78	1.34	1.41
3	B	302	XT3	NAS-NBB	-4.76	1.25	1.34
3	D	302	XT3	NAR-NAS	-4.60	1.27	1.34
2	B	301	NAD	O4D-C1D	-4.21	1.35	1.41
3	H	302	XT3	NAR-NAS	-4.15	1.28	1.34
3	A	302	XT3	CAW-CAC	-4.01	1.38	1.44
3	F	302	XT3	CAQ-CAV	-3.76	1.42	1.51
3	C	302	XT3	CAC-NAA	-3.76	1.05	1.14
3	F	302	XT3	NAS-NBB	-3.67	1.27	1.34
3	C	302	XT3	OAT-CAZ	-3.53	1.31	1.39
2	A	301	NAD	O4D-C1D	-3.42	1.36	1.41
3	G	302	XT3	NAR-NAS	-3.24	1.29	1.34
3	H	302	XT3	CAK-NBB	-3.03	1.32	1.35
3	B	302	XT3	CAK-NBB	-3.02	1.32	1.35
3	A	302	XT3	CAM-CAO	-3.00	1.45	1.53
3	G	302	XT3	CAM-CAO	-2.68	1.46	1.53
3	A	302	XT3	CAK-NBB	-2.58	1.32	1.35
3	B	302	XT3	CAN-CAP	-2.57	1.46	1.53
3	B	302	XT3	CAM-CAO	-2.49	1.46	1.53
2	D	301	NAD	O4D-C1D	-2.48	1.37	1.41
3	B	302	XT3	CAX-NAR	-2.37	1.31	1.34
2	H	301	NAD	C3N-C7N	-2.31	1.46	1.50
3	F	302	XT3	CAX-NAR	-2.21	1.31	1.34
2	C	301	NAD	C6N-C5N	-2.13	1.33	1.38
3	C	302	XT3	CAG-CAZ	-2.13	1.35	1.39
3	A	302	XT3	CAF-CAW	-2.13	1.36	1.40
2	E	301	NAD	C2D-C1D	-2.09	1.50	1.53
3	A	302	XT3	CAX-NAR	-2.07	1.31	1.34
3	H	302	XT3	CAW-CAZ	-2.05	1.36	1.40
3	E	302	XT3	OAT-CAZ	-2.03	1.34	1.39
2	H	301	NAD	C7N-N7N	-2.02	1.28	1.33
3	C	302	XT3	CAX-CBA	2.01	1.56	1.50
2	D	301	NAD	C2N-N1N	2.06	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	302	XT3	CAC-NAA	2.25	1.19	1.14
3	E	302	XT3	CAP-CBA	2.26	1.59	1.53
3	B	302	XT3	CAQ-NBB	2.55	1.51	1.47
3	E	302	XT3	CAC-NAA	2.58	1.20	1.14
2	B	301	NAD	O7N-C7N	2.65	1.29	1.24
3	G	302	XT3	CAC-NAA	2.92	1.21	1.14
2	G	301	NAD	C2N-N1N	3.17	1.39	1.35
3	F	302	XT3	CAW-CAC	3.25	1.49	1.44
3	E	302	XT3	CAW-CAC	3.38	1.49	1.44
2	F	301	NAD	C2N-N1N	3.55	1.40	1.35
2	E	301	NAD	C2N-N1N	3.68	1.40	1.35
3	B	302	XT3	CAC-NAA	3.74	1.23	1.14
3	C	302	XT3	CAQ-NBB	4.19	1.54	1.47
3	H	302	XT3	CAC-NAA	4.82	1.25	1.14
3	F	302	XT3	CAQ-NBB	4.82	1.55	1.47
3	E	302	XT3	CAQ-NBB	4.84	1.55	1.47

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	302	XT3	CAQ-NBB-CAK	-7.60	119.50	129.19
2	C	301	NAD	O4D-C1D-N1N	-7.01	100.54	108.10
3	B	302	XT3	CAQ-NBB-CAK	-6.67	120.69	129.19
2	H	301	NAD	C4B-O4B-C1B	-6.43	102.83	109.64
3	C	302	XT3	CAQ-NBB-CAK	-5.84	121.74	129.19
2	F	301	NAD	C4B-O4B-C1B	-5.33	103.99	109.64
3	H	302	XT3	CAK-CAX-CBA	-5.19	121.93	129.43
3	B	302	XT3	CAK-CAX-CBA	-4.81	122.48	129.43
2	C	301	NAD	C4B-O4B-C1B	-4.62	104.75	109.64
2	E	301	NAD	C4D-O4D-C1D	-4.53	104.84	109.64
2	B	301	NAD	C4B-O4B-C1B	-4.49	104.88	109.64
2	G	301	NAD	C4B-O4B-C1B	-4.35	105.03	109.64
2	E	301	NAD	C4B-O4B-C1B	-4.28	105.10	109.64
2	A	301	NAD	C4B-O4B-C1B	-4.12	105.28	109.64
2	F	301	NAD	C4D-O4D-C1D	-3.87	105.54	109.64
3	D	302	XT3	CAQ-NBB-CAK	-3.82	124.31	129.19
3	C	302	XT3	CAK-CAX-CBA	-3.81	123.93	129.43
3	H	302	XT3	CAP-CBA-CAX	-3.62	105.32	111.51
2	D	301	NAD	C4B-O4B-C1B	-3.57	105.86	109.64
3	H	302	XT3	CAV-CAQ-NBB	-3.46	107.08	112.17
3	A	302	XT3	CAO-CBA-CAX	-3.46	105.59	111.51
2	B	301	NAD	O4D-C1D-N1N	-3.40	104.43	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	NAD	O4D-C1D-N1N	-3.39	104.44	108.10
3	E	302	XT3	CAV-CAQ-NBB	-3.29	107.33	112.17
2	E	301	NAD	O2A-PA-O3	-3.21	91.51	105.27
3	G	302	XT3	CAO-CBA-CAX	-3.10	106.21	111.51
3	A	302	XT3	CAV-CAQ-NBB	-3.08	107.64	112.17
2	B	301	NAD	O2A-PA-O5B	-3.06	93.64	108.24
3	B	302	XT3	CAP-CBA-CAX	-3.05	106.28	111.51
2	D	301	NAD	O4D-C1D-N1N	-2.98	104.89	108.10
2	E	301	NAD	C1B-N9A-C4A	-2.95	123.51	126.81
3	F	302	XT3	CAL-CAM-CAO	-2.93	105.38	111.44
3	D	302	XT3	CAY-OAT-CAZ	-2.85	110.72	117.84
3	C	302	XT3	CAL-CAN-CAP	-2.82	105.62	111.44
3	F	302	XT3	CAV-CAQ-NBB	-2.78	108.08	112.17
2	A	301	NAD	O2A-PA-O5B	-2.66	95.56	108.24
2	H	301	NAD	C1B-N9A-C4A	-2.59	123.91	126.81
2	E	301	NAD	O2D-C2D-C1D	-2.59	103.52	111.61
2	C	301	NAD	C1B-N9A-C4A	-2.53	123.98	126.81
3	C	302	XT3	CAQ-CAV-CAH	-2.51	115.40	120.41
2	A	301	NAD	O4D-C1D-N1N	-2.50	105.40	108.10
3	B	302	XT3	CAV-CAQ-NBB	-2.47	108.53	112.17
2	D	301	NAD	C1B-N9A-C4A	-2.42	124.10	126.81
3	D	302	XT3	CAL-CAM-CAO	-2.41	106.47	111.44
2	H	301	NAD	C4D-O4D-C1D	-2.35	107.15	109.64
2	C	301	NAD	O2A-PA-O5B	-2.31	97.22	108.24
3	A	302	XT3	CAX-CAK-NBB	-2.30	103.18	106.97
2	D	301	NAD	O2A-PA-O3	-2.21	95.80	105.27
2	H	301	NAD	O2A-PA-O3	-2.19	95.89	105.27
2	G	301	NAD	O2D-C2D-C1D	-2.18	104.79	111.61
3	E	302	XT3	CAK-NBB-NAS	-2.16	105.19	109.15
2	E	301	NAD	O5B-C5B-C4B	-2.15	101.34	109.09
2	C	301	NAD	C4N-C3N-C7N	-2.07	115.61	121.11
2	B	301	NAD	O4B-C1B-N9A	2.07	112.01	108.11
2	F	301	NAD	O2A-PA-O1A	2.17	123.84	112.56
2	E	301	NAD	O5D-C5D-C4D	2.19	116.99	109.09
2	E	301	NAD	O2N-PN-O5D	2.24	118.91	108.24
2	A	301	NAD	O2A-PA-O1A	2.25	124.26	112.56
2	E	301	NAD	O2B-C2B-C3B	2.30	119.28	111.86
2	C	301	NAD	O4B-C1B-N9A	2.34	112.53	108.11
2	C	301	NAD	C2N-C3N-C7N	2.38	126.08	119.24
2	E	301	NAD	O2A-PA-O1A	2.41	125.09	112.56
3	H	302	XT3	CAZ-CAW-CAC	2.44	121.47	119.45
3	D	302	XT3	OAT-CAY-CAU	2.45	120.93	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	302	XT3	CBA-CAX-NAR	2.50	124.44	120.09
2	A	301	NAD	C2D-C1D-N1N	2.60	118.63	113.53
3	C	302	XT3	OAT-CAY-CAU	2.62	121.26	116.12
3	C	302	XT3	NAR-NAS-NBB	2.62	109.29	107.31
2	C	301	NAD	O2A-PA-O1A	2.66	126.38	112.56
3	C	302	XT3	CAQ-CAV-CAJ	2.93	125.06	120.26
3	D	302	XT3	CAZ-CAW-CAC	3.01	121.94	119.45
3	E	302	XT3	OAT-CAY-CAU	3.03	122.07	116.12
3	G	302	XT3	CAZ-CAW-CAC	3.27	122.15	119.45
3	F	302	XT3	CAZ-CAW-CAC	3.67	122.49	119.45
3	F	302	XT3	CAQ-NBB-CAK	3.69	133.89	129.19
3	D	302	XT3	CBA-CAX-NAR	3.73	126.58	120.09
3	B	302	XT3	CAZ-CAW-CAC	3.85	122.63	119.45
3	C	302	XT3	CBA-CAX-NAR	4.17	127.36	120.09
3	E	302	XT3	NAR-NAS-NBB	4.51	110.71	107.31
3	G	302	XT3	NAR-NAS-NBB	4.52	110.72	107.31
3	B	302	XT3	CBA-CAX-NAR	4.58	128.07	120.09
3	C	302	XT3	CAZ-CAW-CAC	4.71	123.34	119.45
3	D	302	XT3	NAR-NAS-NBB	4.97	111.06	107.31
3	H	302	XT3	CBA-CAX-NAR	5.18	129.11	120.09
3	H	302	XT3	NAR-NAS-NBB	5.29	111.30	107.31
3	A	302	XT3	CAZ-CAW-CAC	6.15	124.53	119.45
3	A	302	XT3	NAR-NAS-NBB	7.07	112.64	107.31
3	F	302	XT3	NAR-NAS-NBB	7.61	113.05	107.31
3	B	302	XT3	NAR-NAS-NBB	8.17	113.47	107.31

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	302	XT3	CAO-CBA-CAX-CAK
3	B	302	XT3	CAO-CBA-CAX-CAK

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	XT3	1	0
2	C	301	NAD	1	0
2	E	301	NAD	2	0
3	E	302	XT3	1	0

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, 95^{th} 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%)	-0.55	0 100 100	25, 40, 66, 89	0
1	B	268/289 (92%)	-0.22	5 (1%) 70 64	26, 49, 83, 107	0
1	C	268/289 (92%)	-0.52	3 (1%) 82 79	24, 40, 68, 108	0
1	D	268/289 (92%)	-0.28	4 (1%) 76 71	24, 44, 74, 97	0
1	E	268/289 (92%)	-0.03	3 (1%) 82 79	32, 56, 83, 96	0
1	F	268/289 (92%)	-0.25	5 (1%) 70 64	25, 46, 77, 102	0
1	G	264/289 (91%)	-0.18	9 (3%) 49 41	33, 58, 86, 101	0
1	H	263/289 (91%)	-0.21	8 (3%) 54 47	31, 52, 80, 98	0
All	All	2135/2312 (92%)	-0.28	37 (1%) 73 68	24, 48, 80, 108	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	210	GLU	4.1
1	F	2	THR	3.8
1	B	57	LYS	3.5
1	G	210	GLU	3.4
1	H	213	ALA	3.4
1	B	2	THR	3.3
1	G	84	ALA	3.3
1	B	45	ARG	3.1
1	D	2	THR	2.9
1	D	45	ARG	2.9
1	D	57	LYS	2.8
1	G	216	GLN	2.8
1	E	85	GLY	2.8
1	E	57	LYS	2.8
1	G	211	ALA	2.7
1	C	2	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	216	GLN	2.6
1	D	209	GLU	2.4
1	F	85	GLY	2.4
1	H	212	GLY	2.4
1	G	2	THR	2.3
1	G	213	ALA	2.3
1	G	212	GLY	2.3
1	E	2	THR	2.3
1	G	57	LYS	2.2
1	G	69	GLU	2.2
1	F	6	ASP	2.2
1	H	2	THR	2.1
1	H	80	GLU	2.1
1	C	6	ASP	2.1
1	H	69	GLU	2.1
1	F	57	LYS	2.1
1	B	56	ALA	2.1
1	B	61	LEU	2.0
1	F	205	GLY	2.0
1	C	57	LYS	2.0
1	H	203	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	XT3	F	302	28/28	0.97	0.13	0.36	29,36,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	XT3	G	302	28/28	0.97	0.16	-0.00	38,46,51,54	0
3	XT3	H	302	28/28	0.97	0.15	-0.12	34,43,46,47	0
3	XT3	E	302	28/28	0.97	0.13	-0.49	30,47,50,51	0
2	NAD	C	301	44/44	0.98	0.11	-0.66	24,30,33,34	0
2	NAD	A	301	44/44	0.98	0.11	-0.73	24,29,36,37	0
3	XT3	A	302	28/28	0.98	0.11	-0.85	25,33,50,54	0
3	XT3	D	302	28/28	0.98	0.10	-0.92	26,34,39,41	0
2	NAD	G	301	44/44	0.97	0.11	-0.93	42,53,57,68	0
2	NAD	B	301	44/44	0.97	0.12	-0.97	28,36,41,43	0
3	XT3	B	302	28/28	0.98	0.11	-0.99	28,39,45,46	0
3	XT3	C	302	28/28	0.98	0.11	-1.16	28,36,41,42	0
2	NAD	F	301	44/44	0.98	0.10	-1.17	27,37,42,43	0
2	NAD	D	301	44/44	0.98	0.11	-1.17	28,34,44,48	0
2	NAD	H	301	44/44	0.97	0.10	-1.54	36,44,52,67	0
2	NAD	E	301	44/44	0.98	0.10	-1.95	35,43,50,53	0

6.5 Other polymers (i)

There are no such residues in this entry.