



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:44 PM GMT

PDB ID : 3UIC  
Title : Crystal Structure of FabI, an Enoyl Reductase from *F. tularensis*, in complex with a Novel and Potent Inhibitor  
Authors : Mehboob, S.; Santarsiero, B.D.; Truong, K.; Johnson, M.E.  
Deposited on : 2011-11-04  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

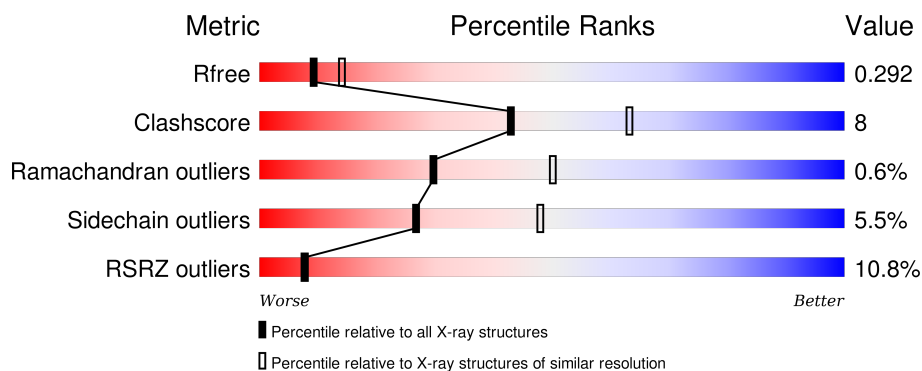
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	
1	B	280	
1	C	280	
1	D	280	
1	E	280	

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Mol	Chain	Length	Quality of chain
1	F	280	
1	G	280	
1	H	280	
1	I	280	
1	J	280	
1	K	280	
1	L	280	
1	M	280	
1	N	280	
1	O	280	
1	P	280	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	09T	B	262	-	-	X	X
3	09T	M	262	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32732 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	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	B	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	C	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	D	256	Total	C	N	O	S	0	0	0
			1913	1215	320	362	16			
1	E	258	Total	C	N	O	S	0	0	0
			1928	1224	323	365	16			
1	F	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	G	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	H	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	I	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	J	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	K	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	L	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	M	257	Total	C	N	O	S	0	0	0
			1921	1219	322	364	16			
1	N	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			
1	O	256	Total	C	N	O	S	0	0	0
			1913	1215	320	362	16			
1	P	259	Total	C	N	O	S	0	0	0
			1936	1230	324	366	16			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
A	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
A	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
A	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
A	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
A	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
A	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
A	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
A	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
A	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
A	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
A	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
A	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
A	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
A	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
A	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
A	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
A	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
A	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
A	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
B	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
B	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
B	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
B	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
B	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
B	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
B	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
B	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
B	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
B	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
B	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
B	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
B	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
B	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
B	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
B	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
B	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
B	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
B	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
B	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
C	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
C	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
C	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
C	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
C	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
C	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
C	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
C	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
C	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
C	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
C	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
C	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
C	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
C	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
C	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
C	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
C	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
C	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
C	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
D	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
D	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
D	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
D	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
D	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
D	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
D	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
D	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
D	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
D	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
D	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
D	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
D	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
D	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
D	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
D	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
D	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
D	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
D	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
D	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
E	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
E	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
E	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
E	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
E	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
E	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
E	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
E	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
E	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
E	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
E	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
E	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
E	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
E	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
E	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
E	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
E	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
E	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
E	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
F	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
F	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
F	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
F	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
F	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
F	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
F	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
F	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
F	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
F	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
F	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
F	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
F	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
F	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
F	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
F	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
F	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
F	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
F	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
F	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
G	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
G	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
G	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
G	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
G	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
G	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
G	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
G	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
G	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
G	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
G	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
G	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
G	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
G	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
G	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
G	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
G	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
G	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
G	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
H	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
H	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
H	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
H	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
H	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
H	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
H	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
H	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
H	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
H	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
H	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
H	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
H	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
H	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
H	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
H	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
H	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
H	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
H	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
H	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
I	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
I	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
I	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
I	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
I	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
I	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
I	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
I	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
I	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
I	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
I	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
I	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
I	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
I	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
I	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
I	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
I	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
I	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
I	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
J	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
J	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
J	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
J	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
J	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
J	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
J	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
J	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
J	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
J	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
J	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
J	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
J	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
J	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
J	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
J	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
J	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
J	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
J	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
J	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
K	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
K	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
K	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
K	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
K	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
K	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
K	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
K	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
K	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
K	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
K	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
K	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
K	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
K	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
K	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
K	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
K	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
K	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
K	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
L	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
L	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
L	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
L	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
L	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
L	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
L	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
L	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
L	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
L	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
L	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
L	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
L	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
L	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
L	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
L	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
L	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
L	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
L	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
L	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
M	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
M	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
M	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
M	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
M	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
M	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
M	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
M	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
M	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
M	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
M	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
M	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
M	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
M	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
M	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
M	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
M	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
M	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
M	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
N	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
N	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
N	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
N	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
N	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
N	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
N	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
N	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
N	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
N	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
N	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
N	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
N	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
N	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
N	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
N	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
N	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
N	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
N	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
N	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
O	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
O	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
O	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
O	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
O	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
O	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
O	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
O	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
O	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
O	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
O	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
O	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
O	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
O	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
O	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
O	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
O	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
O	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
O	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
P	-19	MET	-	EXPRESSION TAG	UNP Q5NGQ3
P	-18	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
P	-17	SER	-	EXPRESSION TAG	UNP Q5NGQ3
P	-16	SER	-	EXPRESSION TAG	UNP Q5NGQ3
P	-15	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
P	-14	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
P	-13	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
P	-12	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
P	-11	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
P	-10	HIS	-	EXPRESSION TAG	UNP Q5NGQ3
P	-9	SER	-	EXPRESSION TAG	UNP Q5NGQ3
P	-8	SER	-	EXPRESSION TAG	UNP Q5NGQ3
P	-7	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
P	-6	LEU	-	EXPRESSION TAG	UNP Q5NGQ3
P	-5	VAL	-	EXPRESSION TAG	UNP Q5NGQ3
P	-4	PRO	-	EXPRESSION TAG	UNP Q5NGQ3
P	-3	ARG	-	EXPRESSION TAG	UNP Q5NGQ3
P	-2	GLY	-	EXPRESSION TAG	UNP Q5NGQ3
P	-1	SER	-	EXPRESSION TAG	UNP Q5NGQ3
P	0	HIS	-	EXPRESSION TAG	UNP Q5NGQ3

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



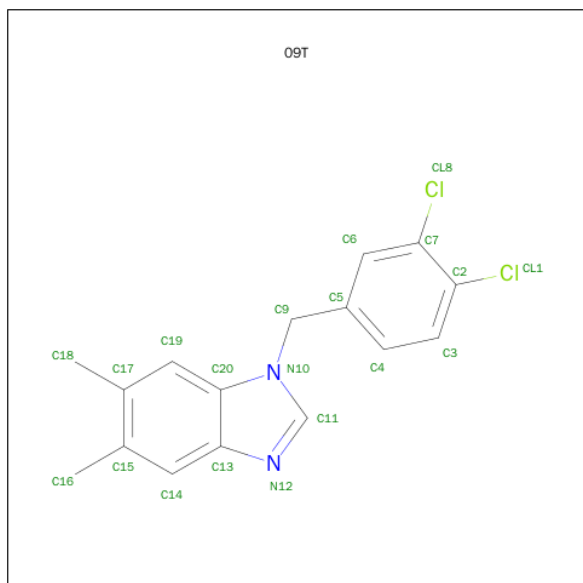
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	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		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	M	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	N	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is 1-(3,4-DICHLOROBENZYL)-5,6-DIMETHYL-1H-BENZIMIDAZOLE (three-letter code: 09T) (formula:  $\text{C}_{16}\text{H}_{14}\text{Cl}_2\text{N}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 20	C 16	Cl 2	N 2	0	0
3	B	1	Total 20	C 16	Cl 2	N 2	0	0
3	C	1	Total 20	C 16	Cl 2	N 2	0	0
3	D	1	Total 20	C 16	Cl 2	N 2	0	0
3	E	1	Total 20	C 16	Cl 2	N 2	0	0
3	F	1	Total 20	C 16	Cl 2	N 2	0	0
3	G	1	Total 20	C 16	Cl 2	N 2	0	0
3	H	1	Total 20	C 16	Cl 2	N 2	0	0
3	I	1	Total 20	C 16	Cl 2	N 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	K	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	L	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	M	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	N	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	O	1	Total	C	Cl	N	0	0
			20	16	2	2		
3	P	1	Total	C	Cl	N	0	0
			20	16	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	55	Total	O	0	0
			55	55		
4	C	71	Total	O	0	0
			71	71		
4	D	77	Total	O	0	0
			77	77		
4	E	48	Total	O	0	0
			48	48		
4	F	48	Total	O	0	0
			48	48		
4	G	35	Total	O	0	0
			35	35		
4	H	33	Total	O	0	0
			33	33		
4	I	77	Total	O	0	0
			77	77		
4	J	63	Total	O	0	0
			63	63		
4	K	79	Total	O	0	0
			79	79		
4	L	56	Total	O	0	0
			56	56		

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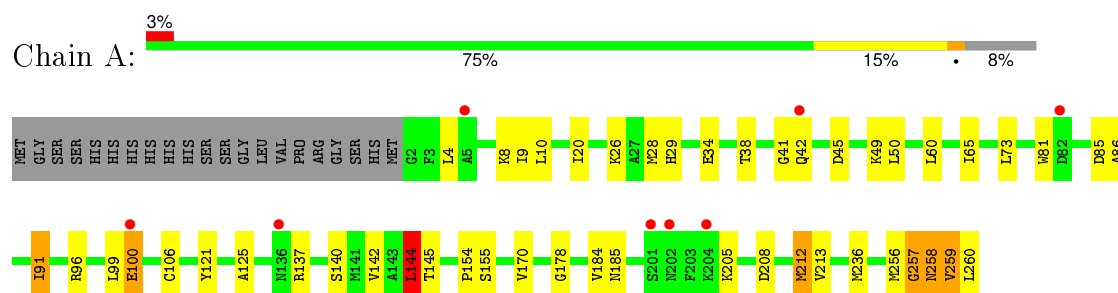
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	35	Total 35	O 35	0	0
4	N	34	Total 34	O 34	0	0
4	O	38	Total 38	O 38	0	0
4	P	41	Total 41	O 41	0	0



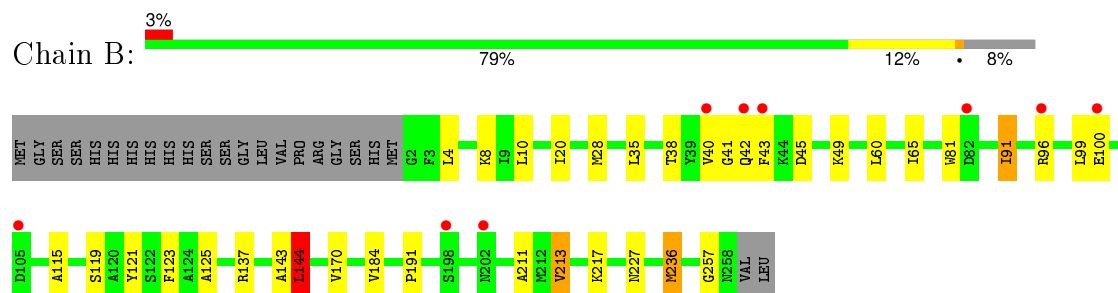
### 3 Residue-property plots [i](#)

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.

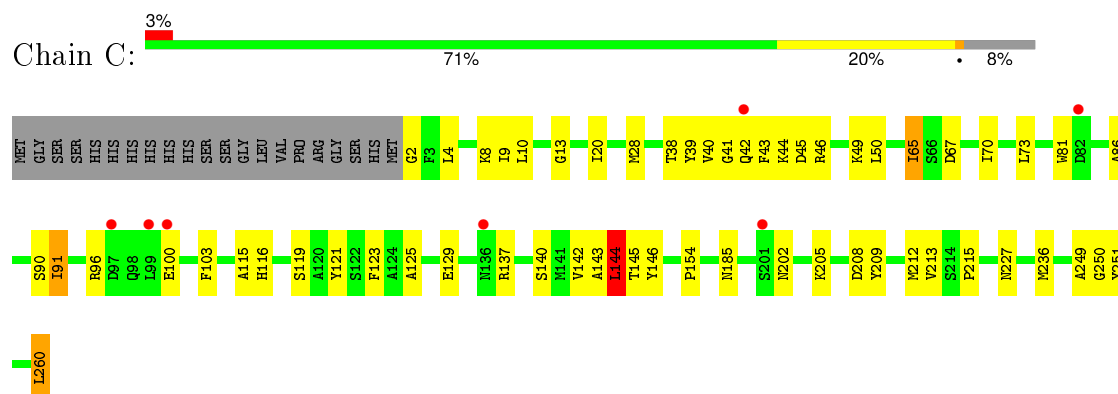
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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

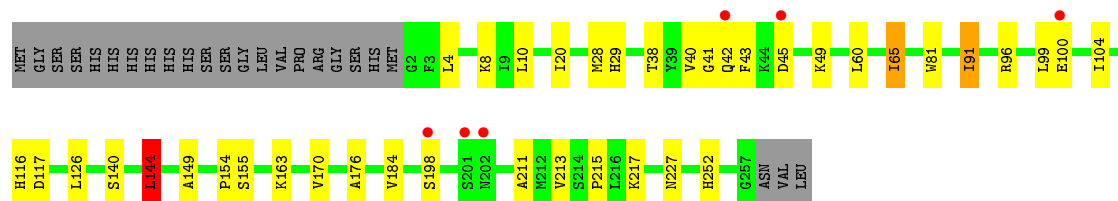


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

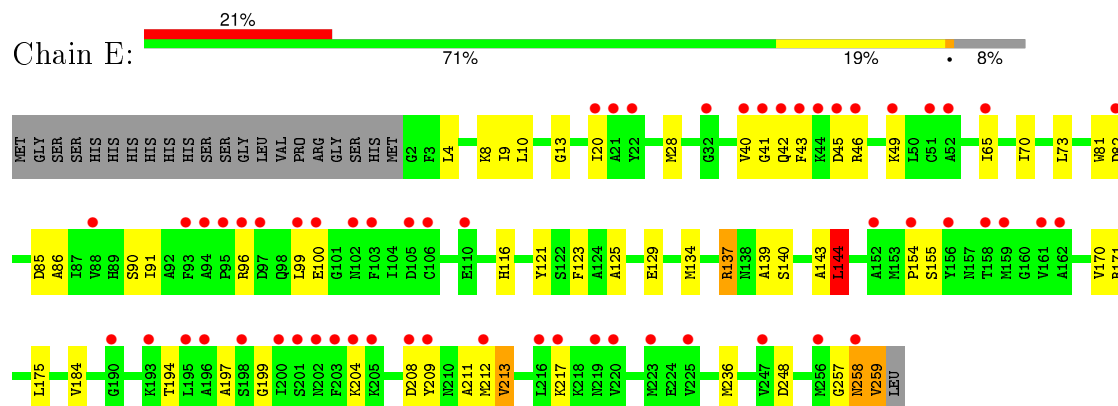


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

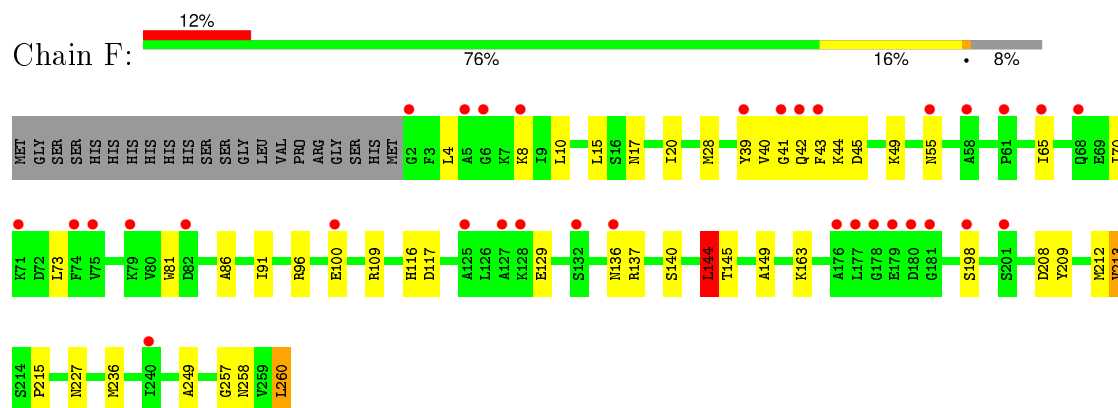




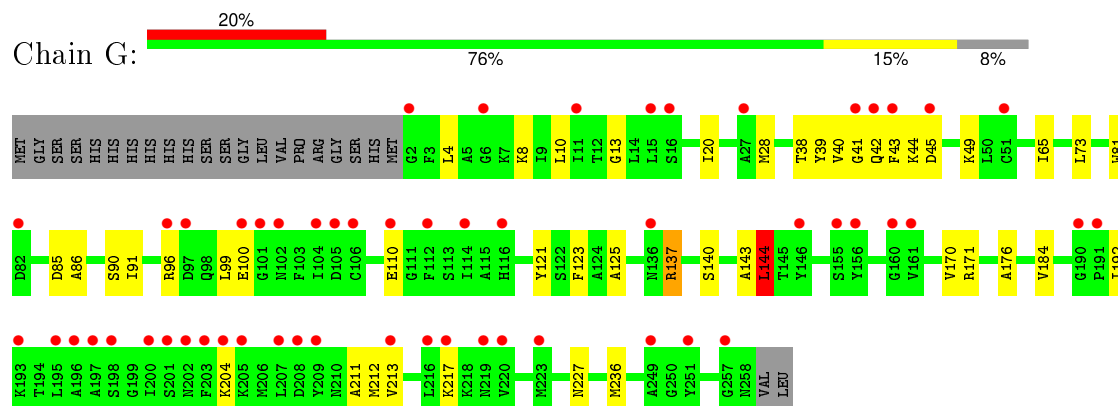
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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



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

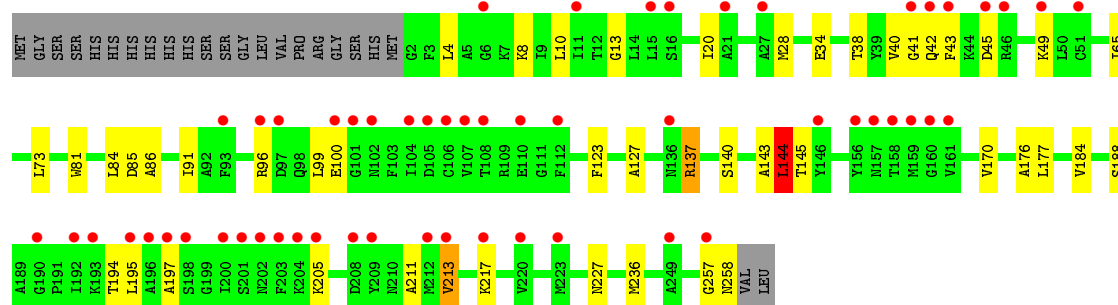
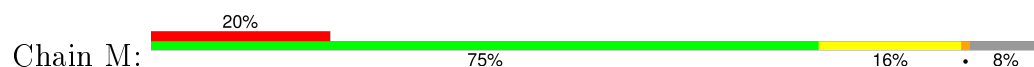


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

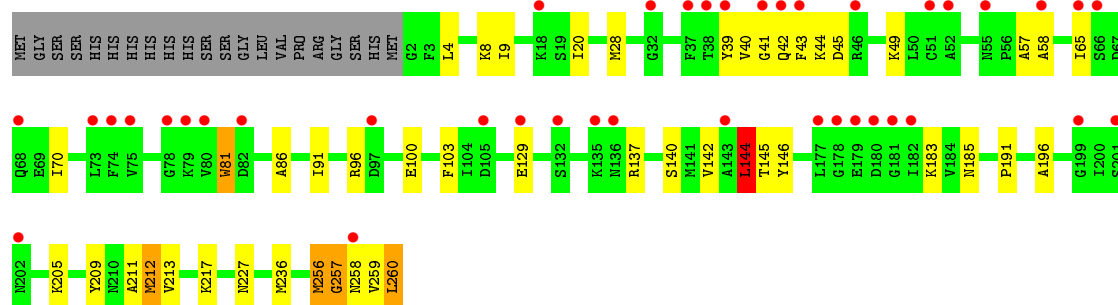
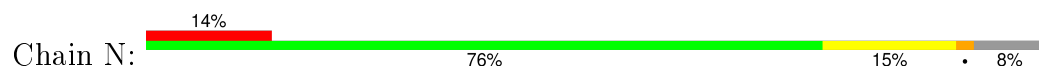




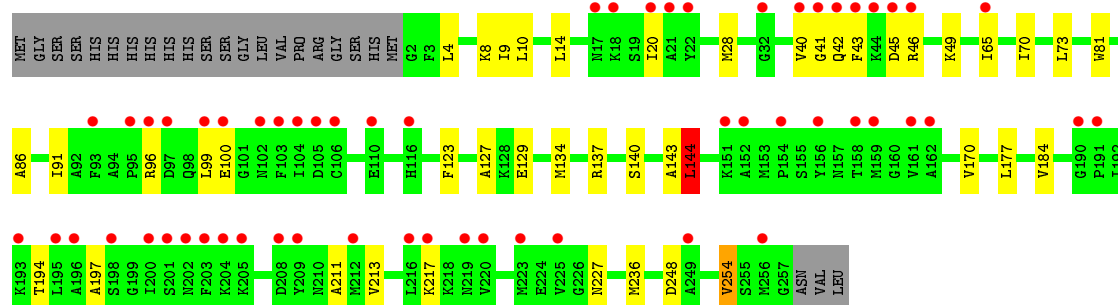
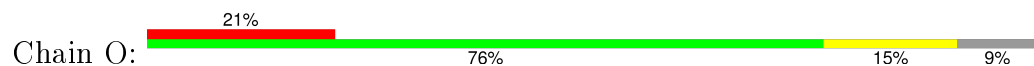
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



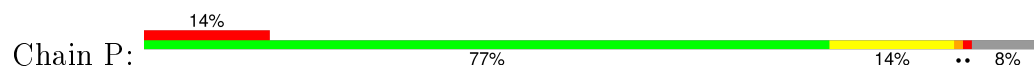
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

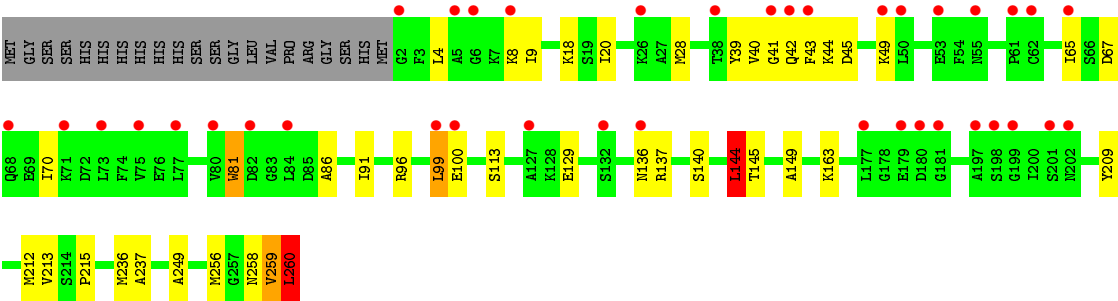


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.41Å 123.46Å 203.33Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-2.50) 99.8 (19.99-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.241 , 0.292 0.241 , 0.292	Depositor DCC
$R_{free}$ test set	7281 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.5	EDS
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	11 of 145213 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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 64.84 % 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 7.7847e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 09T, 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	0.97	0/1967	0.95	3/2655 (0.1%)
1	B	0.92	0/1952	0.88	2/2634 (0.1%)
1	C	0.95	0/1967	0.92	3/2655 (0.1%)
1	D	0.96	0/1944	0.91	2/2623 (0.1%)
1	E	0.73	0/1959	0.79	2/2644 (0.1%)
1	F	0.71	0/1967	0.79	1/2655 (0.0%)
1	G	0.70	0/1952	0.77	1/2634 (0.0%)
1	H	0.70	1/1967 (0.1%)	0.80	3/2655 (0.1%)
1	I	0.97	2/1967 (0.1%)	0.92	2/2655 (0.1%)
1	J	0.96	1/1952 (0.1%)	0.90	4/2634 (0.2%)
1	K	1.01	1/1967 (0.1%)	0.94	2/2655 (0.1%)
1	L	0.91	0/1952	0.88	1/2634 (0.0%)
1	M	0.71	0/1952	0.79	1/2634 (0.0%)
1	N	0.70	1/1967 (0.1%)	0.79	1/2655 (0.0%)
1	O	0.72	0/1944	0.80	3/2623 (0.1%)
1	P	0.70	1/1967 (0.1%)	0.82	5/2655 (0.2%)
All	All	0.84	7/31343 (0.0%)	0.86	36/42300 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	243	GLU	CD-OE1	5.36	1.31	1.25
1	I	2	GLY	N-CA	5.32	1.54	1.46
1	I	81	TRP	CD2-CE2	5.09	1.47	1.41
1	K	81	TRP	CD2-CE2	5.09	1.47	1.41
1	N	81	TRP	CD2-CE2	5.06	1.47	1.41
1	H	81	TRP	CD2-CE2	5.05	1.47	1.41
1	P	81	TRP	CD2-CE2	5.00	1.47	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	144	LEU	CA-CB-CG	-9.26	94.00	115.30
1	M	144	LEU	CA-CB-CG	-9.19	94.17	115.30
1	G	144	LEU	CA-CB-CG	-9.08	94.42	115.30
1	K	144	LEU	CA-CB-CG	-8.87	94.89	115.30
1	C	144	LEU	CA-CB-CG	-8.86	94.92	115.30
1	N	144	LEU	CA-CB-CG	-8.82	95.00	115.30
1	A	144	LEU	CA-CB-CG	-8.65	95.40	115.30
1	H	144	LEU	CA-CB-CG	-8.44	95.88	115.30
1	D	144	LEU	CA-CB-CG	-8.33	96.14	115.30
1	J	144	LEU	CA-CB-CG	-8.17	96.50	115.30
1	L	144	LEU	CA-CB-CG	-8.12	96.62	115.30
1	F	144	LEU	CA-CB-CG	-8.09	96.69	115.30
1	B	144	LEU	CA-CB-CG	-8.04	96.80	115.30
1	O	254	VAL	CG1-CB-CG2	7.56	123.00	110.90
1	P	144	LEU	CA-CB-CG	-7.46	98.14	115.30
1	E	144	LEU	CA-CB-CG	-7.29	98.54	115.30
1	H	260	LEU	CA-CB-CG	7.24	131.95	115.30
1	H	97	ASP	CB-CG-OD1	6.85	124.47	118.30
1	O	144	LEU	CA-CB-CG	-6.78	99.71	115.30
1	E	248	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	D	117	ASP	CB-CG-OD1	6.07	123.77	118.30
1	J	67	ASP	CB-CG-OD1	6.07	123.76	118.30
1	P	99	LEU	CB-CG-CD1	6.06	121.30	111.00
1	P	67	ASP	CB-CG-OD1	6.03	123.72	118.30
1	C	67	ASP	CB-CG-OD1	5.99	123.69	118.30
1	P	260	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	208	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	P	99	LEU	CA-CB-CG	5.73	128.48	115.30
1	I	50	LEU	CB-CG-CD2	-5.60	101.49	111.00
1	A	50	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	C	50	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	B	236	MET	CG-SD-CE	5.37	108.80	100.20
1	K	50	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	O	248	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	J	117	ASP	CB-CG-OD1	5.19	122.97	118.30
1	J	126	LEU	CB-CG-CD2	-5.08	102.37	111.00

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	1936	0	1956	65	0
1	B	1921	0	1936	19	0
1	C	1936	0	1956	45	0
1	D	1913	0	1930	27	0
1	E	1928	0	1945	46	0
1	F	1936	0	1956	38	0
1	G	1921	0	1936	26	0
1	H	1936	0	1956	54	0
1	I	1936	0	1956	35	0
1	J	1921	0	1936	22	0
1	K	1936	0	1956	54	0
1	L	1921	0	1936	25	0
1	M	1921	0	1936	28	0
1	N	1936	0	1956	53	0
1	O	1913	0	1930	22	0
1	P	1936	0	1956	37	0
2	A	44	0	26	2	0
2	B	44	0	26	6	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	6	0
2	F	44	0	26	2	0
2	G	44	0	26	4	0
2	H	44	0	26	3	0
2	I	44	0	26	2	0
2	J	44	0	26	1	0
2	K	44	0	26	3	0
2	L	44	0	26	3	0
2	M	44	0	26	10	0
2	N	44	0	26	3	0
2	O	44	0	26	3	0
2	P	44	0	26	1	0
3	A	20	0	14	1	0
3	B	20	0	14	7	0
3	C	20	0	14	1	0
3	D	20	0	14	2	0
3	E	20	0	14	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	20	0	14	0	0
3	G	20	0	14	3	0
3	H	20	0	14	0	0
3	I	20	0	14	1	0
3	J	20	0	14	2	0
3	K	20	0	14	1	0
3	L	20	0	14	2	0
3	M	20	0	14	12	0
3	N	20	0	14	1	0
3	O	20	0	14	5	0
3	P	20	0	14	0	0
4	A	71	0	0	7	0
4	B	55	0	0	1	0
4	C	71	0	0	2	0
4	D	77	0	0	8	0
4	E	48	0	0	8	0
4	F	48	0	0	7	0
4	G	35	0	0	3	0
4	H	33	0	0	1	0
4	I	77	0	0	4	0
4	J	63	0	0	3	0
4	K	79	0	0	3	0
4	L	56	0	0	4	0
4	M	35	0	0	5	0
4	N	34	0	0	5	0
4	O	38	0	0	3	0
4	P	41	0	0	8	0
All	All	32732	0	31773	520	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 8.

All (520) 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:E:70:ILE:HA	4:E:653:HOH:O	1.39	1.19
1:F:55:ASN:HB2	4:F:600:HOH:O	1.42	1.19
1:N:212:MET:CE	1:N:259:VAL:HG11	1.73	1.17
1:M:34:GLU:HG2	4:M:840:HOH:O	1.43	1.14
1:F:109:ARG:HA	4:F:613:HOH:O	1.45	1.13
1:N:212:MET:HE2	1:N:259:VAL:HG11	1.13	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:261:NAD:H2D	4:L:835:HOH:O	1.53	1.06
1:K:212:MET:HE2	1:K:259:VAL:HG11	1.36	1.05
2:E:261:NAD:O7N	3:E:262:09T:H4	1.64	0.97
1:K:212:MET:CE	1:K:259:VAL:HG11	1.96	0.95
1:E:73:LEU:HB3	4:E:653:HOH:O	1.66	0.94
2:M:261:NAD:H71N	3:M:262:09T:H4	1.32	0.94
1:N:260:LEU:HD12	1:N:260:LEU:H	1.36	0.90
1:G:204:LYS:HB3	4:G:803:HOH:O	1.72	0.90
1:E:199:GLY:HA3	4:E:854:HOH:O	1.72	0.90
1:A:258:ASN:HD22	1:C:154:PRO:HB3	1.36	0.89
1:A:212:MET:HE2	1:A:259:VAL:HG21	1.55	0.88
2:M:261:NAD:N7N	3:M:262:09T:H4	1.88	0.88
1:A:212:MET:CE	1:A:259:VAL:HG21	2.03	0.87
1:A:205:LYS:HZ3	1:H:258:ASN:CB	1.89	0.85
1:H:259:VAL:CG2	1:H:260:LEU:H	1.90	0.85
1:N:212:MET:HE2	1:N:259:VAL:CG1	2.05	0.84
1:K:205:LYS:HD3	1:N:258:ASN:OD1	1.79	0.83
1:N:260:LEU:H	1:N:260:LEU:CD1	1.91	0.83
1:A:258:ASN:ND2	1:C:154:PRO:HB3	1.94	0.82
1:A:258:ASN:CB	1:H:205:LYS:HD3	2.11	0.81
1:A:205:LYS:HD3	1:H:258:ASN:HB3	1.64	0.80
1:H:212:MET:CE	1:H:259:VAL:HG21	2.12	0.80
2:G:261:NAD:O7N	3:G:262:09T:H4	1.81	0.79
1:N:260:LEU:HD12	1:N:260:LEU:N	1.97	0.79
2:B:261:NAD:C7N	3:B:262:09T:H4	2.14	0.78
1:C:202:ASN:HB2	1:F:260:LEU:HD12	1.65	0.77
1:N:212:MET:CE	1:N:259:VAL:CG1	2.59	0.77
1:A:205:LYS:HZ3	1:H:258:ASN:HB2	1.50	0.77
1:E:204:LYS:HB3	4:E:798:HOH:O	1.84	0.77
1:H:259:VAL:HG23	1:H:260:LEU:N	1.99	0.77
2:O:261:NAD:O7N	3:O:262:09T:H4	1.85	0.77
1:N:57:ALA:C	4:N:575:HOH:O	2.23	0.76
1:E:208:ASP:HB3	1:L:212:MET:HG3	1.68	0.75
1:M:99:LEU:HD13	3:M:262:09T:H9	1.67	0.75
2:B:261:NAD:C2N	3:B:262:09T:H6	2.17	0.75
1:H:259:VAL:CG2	1:H:260:LEU:N	2.48	0.74
1:M:99:LEU:CD1	3:M:262:09T:H9	2.18	0.74
1:A:258:ASN:ND2	1:C:154:PRO:CB	2.51	0.73
1:A:260:LEU:HD23	1:F:212:MET:HE2	1.70	0.72
1:G:212:MET:HG3	1:J:208:ASP:HB3	1.70	0.72
1:D:154:PRO:HA	4:D:827:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:HIS:HD2	4:A:630:HOH:O	1.74	0.71
1:A:9:ILE:HG12	1:A:86:ALA:HB3	1.74	0.70
1:E:257:GLY:O	1:E:258:ASN:HB2	1.90	0.70
1:B:213:VAL:HG22	1:B:257:GLY:HA3	1.74	0.69
1:H:259:VAL:HG23	1:H:260:LEU:H	1.52	0.69
1:E:13:GLY:HA2	2:E:261:NAD:O3B	1.92	0.69
1:K:258:ASN:CB	1:N:205:LYS:HD3	2.23	0.69
1:K:212:MET:SD	1:N:212:MET:CE	2.82	0.68
2:B:261:NAD:C3N	3:B:262:09T:H6	2.23	0.68
1:H:212:MET:HE2	1:H:259:VAL:HG11	1.74	0.68
1:N:212:MET:HE1	1:N:259:VAL:HG11	1.74	0.68
1:O:4:LEU:CD1	1:O:28:MET:HG2	2.24	0.68
1:L:213:VAL:HG22	1:L:257:GLY:HA3	1.75	0.68
1:K:212:MET:CE	1:N:212:MET:SD	2.84	0.66
1:A:212:MET:CE	1:H:212:MET:SD	2.84	0.66
1:C:209:TYR:HB2	1:F:212:MET:HE1	1.78	0.65
1:I:260:LEU:HB3	1:N:258:ASN:HB2	1.78	0.65
1:H:259:VAL:O	1:H:260:LEU:HD22	1.96	0.65
1:K:9:ILE:HG12	1:K:86:ALA:HB3	1.79	0.65
1:E:4:LEU:CD1	1:E:28:MET:HG2	2.26	0.65
1:P:237:ALA:HA	4:P:814:HOH:O	1.97	0.65
1:K:204:LYS:NZ	4:K:705:HOH:O	2.29	0.65
1:K:205:LYS:CD	1:N:258:ASN:OD1	2.44	0.64
1:A:212:MET:CE	1:A:259:VAL:CG2	2.76	0.64
1:A:212:MET:SD	1:H:212:MET:CE	2.86	0.64
1:I:260:LEU:HD12	1:N:260:LEU:HD11	1.79	0.64
1:N:58:ALA:HA	4:N:575:HOH:O	1.96	0.64
1:C:212:MET:HE1	1:F:209:TYR:HB2	1.80	0.64
2:O:261:NAD:C7N	3:O:262:09T:H4	2.28	0.64
1:J:257:GLY:O	1:J:258:ASN:ND2	2.31	0.63
1:A:258:ASN:ND2	1:H:205:LYS:NZ	2.47	0.63
1:K:80:VAL:HG23	4:K:841:HOH:O	1.99	0.63
1:C:212:MET:CE	1:F:209:TYR:HB2	2.29	0.62
1:I:212:MET:CE	1:P:209:TYR:HB2	2.29	0.62
1:I:209:TYR:HB2	1:P:212:MET:HE1	1.82	0.62
1:D:252:HIS:HB2	4:D:781:HOH:O	1.99	0.62
1:N:58:ALA:N	4:N:575:HOH:O	2.32	0.62
1:P:256:MET:CG	1:P:259:VAL:HG13	2.29	0.62
2:B:261:NAD:C2N	3:B:262:09T:C11	2.78	0.62
1:G:40:VAL:HG23	1:G:43:PHE:HD1	1.66	0.61
1:P:256:MET:HG3	1:P:259:VAL:CG1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:256:MET:HG2	1:P:259:VAL:HG13	1.81	0.61
1:C:40:VAL:HG23	1:C:43:PHE:HD1	1.66	0.61
1:A:258:ASN:ND2	1:H:205:LYS:HZ3	1.99	0.61
2:M:261:NAD:H71N	3:M:262:09T:H1	1.65	0.61
1:A:258:ASN:HB3	1:H:205:LYS:HD3	1.83	0.60
1:H:259:VAL:HG22	1:H:260:LEU:H	1.63	0.60
1:K:212:MET:HE3	1:N:212:MET:SD	2.41	0.60
1:M:40:VAL:HG23	1:M:43:PHE:HD1	1.65	0.60
1:A:34:GLU:HG2	4:A:770:HOH:O	2.00	0.60
1:K:212:MET:CE	1:K:259:VAL:CG1	2.78	0.60
1:K:205:LYS:CE	1:N:258:ASN:OD1	2.50	0.59
1:P:113:SER:HA	4:P:379:HOH:O	2.02	0.59
1:A:260:LEU:HD11	1:F:260:LEU:CD2	2.32	0.59
1:I:212:MET:HE2	1:N:260:LEU:HD23	1.85	0.59
1:P:256:MET:CG	1:P:259:VAL:CG1	2.81	0.59
1:I:209:TYR:HB2	1:P:212:MET:CE	2.33	0.58
1:D:29:HIS:HD2	4:D:535:HOH:O	1.86	0.58
1:O:46:ARG:NH1	4:O:876:HOH:O	2.36	0.58
1:K:205:LYS:HZ3	1:N:258:ASN:CG	2.07	0.58
1:A:212:MET:SD	1:H:212:MET:HE1	2.43	0.58
1:M:4:LEU:CD1	1:M:28:MET:HG2	2.34	0.58
1:D:198:SER:HB3	4:D:651:HOH:O	2.01	0.58
1:N:144:LEU:N	4:N:629:HOH:O	2.36	0.58
1:P:40:VAL:HG23	1:P:43:PHE:HD1	1.69	0.57
1:K:260:LEU:HD11	1:P:260:LEU:HD13	1.86	0.57
1:H:259:VAL:O	1:H:260:LEU:CD2	2.52	0.57
1:F:40:VAL:HG23	1:F:43:PHE:HD1	1.70	0.57
1:E:209:TYR:HA	1:L:212:MET:HE3	1.87	0.56
1:O:20:ILE:HG21	1:O:144:LEU:HD22	1.87	0.56
1:B:170:VAL:HG13	1:B:184:VAL:HG12	1.85	0.56
1:G:99:LEU:HD13	3:G:262:09T:H9	1.86	0.56
1:I:154:PRO:HB3	1:K:258:ASN:OD1	2.05	0.56
1:N:256:MET:O	1:N:257:GLY:O	2.23	0.56
1:E:40:VAL:HG23	1:E:43:PHE:HD1	1.69	0.56
1:I:8:LYS:HD2	1:I:81:TRP:CG	2.40	0.56
1:C:8:LYS:HD2	1:C:81:TRP:CG	2.41	0.56
1:A:258:ASN:CG	1:H:205:LYS:HD3	2.25	0.56
1:A:205:LYS:HZ3	1:H:258:ASN:CG	2.09	0.56
1:N:58:ALA:CA	4:N:575:HOH:O	2.52	0.56
1:N:40:VAL:HG23	1:N:43:PHE:HD1	1.71	0.56
1:K:212:MET:SD	1:N:212:MET:HE1	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:CD1	1:F:260:LEU:CD2	2.83	0.56
1:A:205:LYS:HZ3	1:H:258:ASN:ND2	2.03	0.56
2:M:261:NAD:H71N	3:M:262:09T:C9	2.12	0.55
1:A:212:MET:HE1	1:A:259:VAL:HG21	1.86	0.55
1:A:260:LEU:HD11	1:F:260:LEU:HD21	1.88	0.55
1:I:20:ILE:HG21	1:I:144:LEU:HD22	1.89	0.55
1:H:40:VAL:HG23	1:H:43:PHE:HD1	1.71	0.55
1:P:136:ASN:HA	4:P:578:HOH:O	2.06	0.55
1:O:99:LEU:HD13	3:O:262:09T:H9	1.88	0.55
1:I:212:MET:HE1	1:P:209:TYR:HB2	1.88	0.55
1:A:205:LYS:CD	1:H:258:ASN:HB3	2.35	0.55
1:P:237:ALA:C	4:P:814:HOH:O	2.45	0.54
1:F:8:LYS:HD2	1:F:81:TRP:CG	2.42	0.54
1:E:10:LEU:HD21	1:E:73:LEU:HD21	1.89	0.54
1:C:20:ILE:HG21	1:C:144:LEU:HD22	1.89	0.54
1:I:154:PRO:CB	1:K:258:ASN:OD1	2.54	0.54
1:J:128:LYS:HE3	4:J:735:HOH:O	2.07	0.54
1:O:10:LEU:HD21	1:O:73:LEU:HD21	1.89	0.54
1:J:40:VAL:HG23	1:J:43:PHE:HD1	1.73	0.54
1:B:99:LEU:HD13	3:B:262:09T:H9	1.89	0.54
1:I:2:GLY:HA2	4:I:688:HOH:O	2.08	0.54
1:D:40:VAL:HG23	1:D:43:PHE:HD1	1.73	0.54
1:L:170:VAL:HG13	1:L:184:VAL:HG12	1.89	0.53
1:E:13:GLY:C	2:E:261:NAD:HO3A	2.12	0.53
1:D:99:LEU:HD13	3:D:262:09T:H9	1.88	0.53
1:K:20:ILE:HG21	1:K:144:LEU:HD22	1.90	0.53
1:K:205:LYS:NZ	1:N:258:ASN:OD1	2.42	0.53
1:A:205:LYS:NZ	1:H:258:ASN:HB2	2.21	0.53
1:A:20:ILE:HG21	1:A:144:LEU:HD22	1.91	0.53
1:H:64:VAL:HG22	2:H:261:NAD:N1A	2.24	0.53
1:I:10:LEU:HD11	1:I:38:THR:HG23	1.91	0.53
1:K:258:ASN:HB3	1:N:205:LYS:HD3	1.90	0.53
1:A:205:LYS:NZ	1:H:258:ASN:ND2	2.57	0.53
2:M:261:NAD:C2N	3:M:262:09T:H6	2.39	0.52
1:N:196:ALA:O	3:N:262:09T:H8	2.09	0.52
1:D:20:ILE:HG21	1:D:144:LEU:HD22	1.90	0.52
1:D:154:PRO:CA	4:D:827:HOH:O	2.53	0.52
1:M:195:LEU:HB2	4:M:757:HOH:O	2.08	0.52
1:H:8:LYS:HD2	1:H:81:TRP:CG	2.44	0.52
1:A:212:MET:HE3	1:H:212:MET:SD	2.49	0.52
1:P:20:ILE:HG21	1:P:144:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:261:NAD:N7N	3:M:262:09T:H1	2.24	0.52
1:C:202:ASN:CB	1:F:260:LEU:HD12	2.38	0.52
1:F:117:ASP:HA	4:F:486:HOH:O	2.10	0.52
1:M:20:ILE:HG21	1:M:144:LEU:HD22	1.92	0.52
1:P:4:LEU:CD1	1:P:28:MET:HG2	2.39	0.52
1:A:145:THR:O	2:A:261:NAD:H6N	2.10	0.52
1:J:8:LYS:HD2	1:J:81:TRP:CG	2.45	0.52
1:E:213:VAL:HG22	1:E:257:GLY:HA3	1.90	0.52
1:H:39:TYR:CZ	1:H:44:LYS:HG3	2.45	0.52
1:A:205:LYS:NZ	1:H:258:ASN:HD22	2.08	0.52
1:G:4:LEU:CD1	1:G:28:MET:HG2	2.40	0.52
1:G:8:LYS:HD2	1:G:81:TRP:CG	2.45	0.52
1:O:40:VAL:HG23	1:O:43:PHE:HD1	1.75	0.52
1:I:29:HIS:HE1	4:I:299:HOH:O	1.92	0.52
1:C:10:LEU:HD11	1:C:38:THR:HG23	1.91	0.52
1:E:20:ILE:HG21	1:E:144:LEU:HD22	1.92	0.51
1:J:99:LEU:HD13	3:J:262:09T:H9	1.92	0.51
1:D:8:LYS:HD2	1:D:81:TRP:CG	2.45	0.51
1:B:40:VAL:HG23	1:B:43:PHE:HD1	1.75	0.51
1:A:258:ASN:HB2	1:H:205:LYS:CE	2.40	0.51
1:H:259:VAL:O	1:H:260:LEU:CB	2.58	0.51
1:P:8:LYS:HD2	1:P:81:TRP:CG	2.45	0.51
1:I:116:HIS:CD2	1:J:116:HIS:CD2	2.98	0.51
1:A:100:GLU:HB3	4:A:675:HOH:O	2.10	0.51
1:F:20:ILE:HG21	1:F:144:LEU:HD22	1.92	0.51
1:E:212:MET:CE	1:E:259:VAL:HG21	2.41	0.51
1:K:212:MET:SD	1:N:212:MET:HE3	2.50	0.51
1:J:99:LEU:CD1	3:J:262:09T:H9	2.41	0.51
1:C:4:LEU:CD1	1:C:28:MET:HG2	2.41	0.51
1:G:123:PHE:CE1	1:G:143:ALA:HB2	2.46	0.51
1:L:121:TYR:CE2	1:L:125:ALA:HB2	2.46	0.51
1:M:205:LYS:HE3	4:M:751:HOH:O	2.11	0.51
1:E:212:MET:HE1	1:E:259:VAL:HG21	1.93	0.50
1:G:171:ARG:HD3	4:G:359:HOH:O	2.11	0.50
1:L:8:LYS:HD2	1:L:81:TRP:CG	2.46	0.50
1:N:8:LYS:HD2	1:N:81:TRP:CG	2.46	0.50
2:M:261:NAD:C3N	3:M:262:09T:H6	2.41	0.50
1:A:212:MET:HE1	1:H:212:MET:SD	2.51	0.50
1:F:198:SER:HB3	4:F:644:HOH:O	2.12	0.50
1:J:227:ASN:HB3	1:K:236:MET:HB3	1.93	0.50
2:H:261:NAD:O1N	2:H:261:NAD:H2N	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:TYR:CZ	1:N:44:LYS:HG3	2.46	0.50
1:F:17:ASN:N	4:F:783:HOH:O	2.24	0.50
1:A:258:ASN:CB	1:H:205:LYS:CD	2.86	0.50
1:I:10:LEU:HD21	1:I:73:LEU:HD21	1.94	0.50
2:I:261:NAD:H52N	4:I:279:HOH:O	2.11	0.50
1:D:38:THR:HA	1:D:60:LEU:O	2.11	0.50
1:H:212:MET:HE2	1:H:259:VAL:HG21	1.94	0.50
1:F:70:ILE:HG22	1:F:129:GLU:HG3	1.94	0.50
1:L:217:LYS:NZ	4:L:523:HOH:O	2.43	0.50
1:M:236:MET:HA	4:M:397:HOH:O	2.12	0.50
1:K:260:LEU:CD1	1:P:212:MET:HE2	2.42	0.49
1:M:213:VAL:HG22	1:M:257:GLY:HA3	1.93	0.49
1:M:211:ALA:O	1:M:217:LYS:HA	2.12	0.49
1:F:136:ASN:HA	4:F:883:HOH:O	2.13	0.49
1:B:211:ALA:O	1:B:217:LYS:HA	2.13	0.49
1:E:8:LYS:HD2	1:E:81:TRP:CG	2.48	0.49
1:C:65:ILE:HG12	4:C:576:HOH:O	2.12	0.49
1:E:70:ILE:CA	4:E:653:HOH:O	2.22	0.49
2:E:261:NAD:O7N	3:E:262:O9T:C9	2.49	0.49
1:E:257:GLY:O	1:E:258:ASN:CB	2.59	0.49
1:I:208:ASP:HB2	1:P:212:MET:HG3	1.95	0.49
1:K:121:TYR:CE2	1:K:125:ALA:HB2	2.48	0.49
1:K:145:THR:O	2:K:261:NAD:H6N	2.12	0.49
1:J:211:ALA:O	1:J:217:LYS:HA	2.13	0.49
1:K:8:LYS:HD2	1:K:81:TRP:CG	2.48	0.49
1:N:227:ASN:HB3	1:O:236:MET:HB3	1.95	0.49
1:A:205:LYS:NZ	1:H:258:ASN:CB	2.69	0.49
2:O:261:NAD:C3N	3:O:262:O9T:H6	2.43	0.49
1:O:123:PHE:CE1	1:O:143:ALA:HB2	2.47	0.49
1:F:258:ASN:ND2	4:F:527:HOH:O	2.46	0.49
1:D:10:LEU:HD11	1:D:38:THR:HG23	1.94	0.49
1:K:99:LEU:HD13	3:K:262:O9T:H9	1.94	0.49
1:K:18:LYS:HG3	4:K:384:HOH:O	2.11	0.49
1:C:209:TYR:HB2	1:F:212:MET:CE	2.42	0.48
1:L:40:VAL:HG23	1:L:43:PHE:HD1	1.78	0.48
1:H:4:LEU:CD1	1:H:28:MET:HG2	2.43	0.48
1:M:145:THR:O	1:M:188:SER:HA	2.13	0.48
1:G:20:ILE:HG21	1:G:144:LEU:HD22	1.95	0.48
1:M:99:LEU:HD11	3:M:262:O9T:H9	1.94	0.48
1:E:212:MET:CE	1:E:259:VAL:CG2	2.91	0.48
1:G:10:LEU:HD11	1:G:38:THR:HG23	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:GLY:HA2	2:M:261:NAD:O3B	2.12	0.48
1:E:13:GLY:CA	2:E:261:NAD:O3B	2.59	0.48
1:H:212:MET:SD	1:H:259:VAL:HG21	2.53	0.48
1:G:99:LEU:CD1	3:G:262:09T:H9	2.43	0.48
1:B:99:LEU:CD1	3:B:262:09T:H9	2.43	0.48
1:H:20:ILE:HG21	1:H:144:LEU:HD22	1.95	0.48
1:G:110:GLU:HB2	4:G:869:HOH:O	2.12	0.48
1:H:212:MET:HE1	1:H:259:VAL:HG21	1.95	0.48
1:A:10:LEU:HD21	1:A:73:LEU:HD21	1.94	0.48
1:D:155:SER:HA	4:D:859:HOH:O	2.13	0.48
1:G:13:GLY:HA2	2:G:261:NAD:O3B	2.13	0.48
1:N:20:ILE:HG21	1:N:144:LEU:HD22	1.96	0.48
1:J:10:LEU:HD11	1:J:38:THR:HG23	1.96	0.48
1:B:8:LYS:HD2	1:B:81:TRP:CG	2.48	0.48
2:K:261:NAD:O1N	2:K:261:NAD:H2N	2.14	0.48
1:O:127:ALA:HB1	1:O:177:LEU:HD11	1.95	0.48
1:M:10:LEU:HD11	1:M:38:THR:HG23	1.95	0.48
1:A:236:MET:HB3	1:D:227:ASN:HB3	1.96	0.48
1:C:40:VAL:HG23	1:C:43:PHE:CD1	2.47	0.48
1:I:40:VAL:HG23	1:I:43:PHE:HD1	1.78	0.48
1:L:115:ALA:O	1:L:119:SER:HB2	2.14	0.48
1:L:191:PRO:HA	2:L:261:NAD:O7N	2.14	0.48
1:B:4:LEU:CD1	1:B:28:MET:HG2	2.44	0.48
1:I:4:LEU:CD1	1:I:28:MET:HG2	2.44	0.48
1:C:10:LEU:HD21	1:C:73:LEU:HD21	1.96	0.47
1:F:39:TYR:CZ	1:F:44:LYS:HG3	2.49	0.47
1:O:4:LEU:HD13	1:O:28:MET:HG2	1.95	0.47
1:B:123:PHE:CE1	1:B:143:ALA:HB2	2.49	0.47
1:C:2:GLY:HA2	4:C:668:HOH:O	2.13	0.47
1:M:10:LEU:HD21	1:M:73:LEU:HD21	1.96	0.47
1:B:38:THR:HA	1:B:60:LEU:O	2.14	0.47
1:H:86:ALA:HA	1:H:140:SER:O	2.15	0.47
1:A:258:ASN:ND2	1:C:154:PRO:HB2	2.29	0.47
1:C:260:LEU:HG	1:H:258:ASN:OD1	2.14	0.47
1:K:260:LEU:HD12	1:P:212:MET:HE2	1.97	0.47
1:I:115:ALA:O	1:I:119:SER:HB2	2.13	0.47
1:A:121:TYR:CE2	1:A:125:ALA:HB2	2.49	0.47
1:O:170:VAL:HG13	1:O:184:VAL:HG12	1.95	0.47
1:L:123:PHE:CE1	1:L:143:ALA:HB2	2.50	0.47
1:P:39:TYR:CZ	1:P:44:LYS:HG3	2.50	0.47
1:F:149:ALA:HB2	1:F:163:LYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HG13	1:A:184:VAL:HG12	1.97	0.47
1:L:85:ASP:CG	1:L:137:ARG:HH11	2.17	0.47
1:F:213:VAL:HG22	1:F:257:GLY:HA3	1.97	0.47
1:M:227:ASN:HB3	1:P:236:MET:HB3	1.96	0.47
1:M:123:PHE:CE1	1:M:143:ALA:HB2	2.49	0.47
1:K:212:MET:HE1	1:K:259:VAL:HG11	1.90	0.47
1:O:134:MET:HE1	1:O:140:SER:O	2.15	0.47
1:A:106:CYS:HB2	4:A:583:HOH:O	2.15	0.47
1:J:149:ALA:HB2	1:J:163:LYS:HB3	1.97	0.46
1:C:115:ALA:O	1:C:119:SER:HB2	2.16	0.46
1:K:258:ASN:OD1	1:N:205:LYS:NZ	2.47	0.46
1:H:256:MET:O	1:H:257:GLY:O	2.32	0.46
1:F:4:LEU:CD1	1:F:28:MET:HG2	2.45	0.46
1:E:99:LEU:HD13	3:E:262:09T:H9	1.97	0.46
1:A:86:ALA:HA	1:A:140:SER:O	2.14	0.46
1:C:86:ALA:HA	1:C:140:SER:O	2.15	0.46
1:N:70:ILE:HG22	1:N:129:GLU:HG3	1.98	0.46
2:M:261:NAD:C2N	3:M:262:09T:C11	2.94	0.46
1:O:8:LYS:HD2	1:O:81:TRP:CG	2.50	0.46
1:D:65:ILE:HG12	4:D:561:HOH:O	2.16	0.46
1:J:20:ILE:HG21	1:J:144:LEU:HD22	1.98	0.46
1:G:211:ALA:O	1:G:217:LYS:HA	2.16	0.46
1:P:86:ALA:HA	1:P:140:SER:O	2.16	0.46
4:B:592:HOH:O	1:D:154:PRO:HD3	2.16	0.46
1:I:209:TYR:N	1:P:212:MET:HE3	2.30	0.46
1:P:136:ASN:C	4:P:578:HOH:O	2.54	0.46
1:L:211:ALA:O	1:L:217:LYS:HA	2.15	0.46
1:I:86:ALA:HA	1:I:140:SER:O	2.14	0.46
1:I:146:TYR:CZ	3:I:262:09T:H3	2.50	0.46
2:A:261:NAD:O1N	2:A:261:NAD:H2N	2.16	0.46
1:K:85:ASP:CG	1:K:137:ARG:HH11	2.19	0.46
1:K:256:MET:O	1:K:257:GLY:O	2.33	0.45
1:B:121:TYR:CE2	1:B:125:ALA:HB2	2.51	0.45
1:F:145:THR:O	2:F:261:NAD:H6N	2.16	0.45
1:M:195:LEU:CB	4:M:757:HOH:O	2.64	0.45
1:B:227:ASN:HB3	1:C:236:MET:HB3	1.99	0.45
1:C:70:ILE:HG22	1:C:129:GLU:HG3	1.97	0.45
1:E:90:SER:OG	2:E:261:NAD:H52N	2.16	0.45
1:P:237:ALA:CA	4:P:814:HOH:O	2.61	0.45
1:A:34:GLU:CG	4:A:770:HOH:O	2.61	0.45
1:P:70:ILE:HG22	1:P:129:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:149:ALA:HB2	1:P:163:LYS:HB3	1.98	0.45
1:F:15:LEU:HB2	2:F:261:NAD:O3B	2.17	0.45
1:E:211:ALA:O	1:E:217:LYS:HA	2.17	0.45
1:E:123:PHE:CE1	1:E:143:ALA:HB2	2.51	0.45
1:E:86:ALA:HA	1:E:140:SER:O	2.16	0.45
1:K:10:LEU:HD11	1:K:38:THR:HG23	1.97	0.45
1:J:107:VAL:N	4:J:687:HOH:O	2.49	0.45
1:E:70:ILE:HG22	1:E:129:GLU:HG3	1.99	0.45
1:H:144:LEU:N	4:H:417:HOH:O	2.48	0.45
1:A:154:PRO:O	1:A:155:SER:HB2	2.17	0.45
1:A:99:LEU:HD13	3:A:262:O9T:H9	1.98	0.45
1:O:86:ALA:HA	1:O:140:SER:O	2.16	0.45
1:N:145:THR:O	2:N:261:NAD:H6N	2.16	0.45
1:B:20:ILE:HG21	1:B:144:LEU:HD22	1.99	0.45
1:N:191:PRO:HA	2:N:261:NAD:O7N	2.16	0.45
1:A:8:LYS:HD2	1:A:81:TRP:CG	2.51	0.45
1:B:191:PRO:HA	2:B:261:NAD:O7N	2.16	0.45
1:D:170:VAL:HG13	1:D:184:VAL:HG12	1.98	0.45
1:O:14:LEU:CB	4:O:733:HOH:O	2.65	0.45
1:K:4:LEU:CD1	1:K:28:MET:HG2	2.47	0.45
1:M:8:LYS:HD2	1:M:81:TRP:CG	2.52	0.45
1:E:170:VAL:HG13	1:E:184:VAL:HG12	1.99	0.45
1:G:192:ILE:O	2:G:261:NAD:N7N	2.48	0.45
1:E:259:VAL:O	1:E:259:VAL:HG23	2.17	0.45
1:F:236:MET:HB3	1:G:227:ASN:HB3	1.99	0.45
1:B:115:ALA:O	1:B:119:SER:HB2	2.17	0.45
1:G:86:ALA:HA	1:G:140:SER:O	2.17	0.45
1:I:85:ASP:CG	1:I:137:ARG:HH11	2.21	0.44
1:C:9:ILE:HG12	1:C:86:ALA:HB3	1.98	0.44
1:K:170:VAL:HG13	1:K:184:VAL:HG12	1.99	0.44
1:M:86:ALA:HA	1:M:140:SER:O	2.16	0.44
1:G:90:SER:HG	2:G:261:NAD:H52N	1.83	0.44
1:D:149:ALA:HB2	1:D:163:LYS:HB3	1.99	0.44
1:F:86:ALA:HA	1:F:140:SER:O	2.16	0.44
1:L:4:LEU:CD1	1:L:28:MET:HG2	2.47	0.44
1:K:260:LEU:HB3	1:P:212:MET:HE1	1.99	0.44
1:M:40:VAL:HG23	1:M:43:PHE:CD1	2.49	0.44
1:O:194:THR:H	1:O:197:ALA:HB3	1.82	0.44
1:A:4:LEU:CD1	1:A:28:MET:HG2	2.47	0.44
1:N:211:ALA:O	1:N:217:LYS:HA	2.18	0.44
1:E:134:MET:HE3	1:E:139:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:ILE:HG12	1:E:86:ALA:HB3	2.00	0.44
1:P:215:PRO:HD2	1:P:249:ALA:O	2.18	0.44
1:K:21:ALA:HA	1:K:24:ILE:HD12	2.00	0.44
1:K:123:PHE:CE1	1:K:143:ALA:HB2	2.52	0.44
1:I:39:TYR:CZ	1:I:44:LYS:HG3	2.53	0.44
1:J:170:VAL:HG13	1:J:184:VAL:HG12	1.99	0.44
1:J:139:ALA:HB3	1:J:182:ILE:HG12	1.99	0.44
1:N:4:LEU:CD1	1:N:28:MET:HG2	2.48	0.44
1:M:84:LEU:O	1:M:137:ARG:HD2	2.17	0.44
1:C:145:THR:O	2:C:261:NAD:H6N	2.18	0.44
1:D:4:LEU:CD1	1:D:28:MET:HG2	2.47	0.43
1:K:205:LYS:NZ	1:N:258:ASN:ND2	2.66	0.43
1:C:142:VAL:HA	1:C:185:ASN:O	2.18	0.43
1:A:85:ASP:CG	1:A:137:ARG:HH11	2.21	0.43
1:M:170:VAL:HG13	1:M:184:VAL:HG12	1.99	0.43
1:L:7:LYS:HE2	4:L:403:HOH:O	2.17	0.43
1:A:91:ILE:HD13	1:A:91:ILE:HG23	1.74	0.43
1:H:70:ILE:HG22	1:H:129:GLU:HG3	1.99	0.43
1:K:86:ALA:HA	1:K:140:SER:O	2.18	0.43
1:G:10:LEU:HD21	1:G:73:LEU:HD21	2.00	0.43
1:A:91:ILE:HD12	1:A:91:ILE:HG21	1.70	0.43
1:M:176:ALA:HB2	1:N:103:PHE:HB3	1.99	0.43
1:P:145:THR:O	2:P:261:NAD:H6N	2.18	0.43
1:I:116:HIS:CD2	1:J:116:HIS:HD2	2.34	0.43
1:C:123:PHE:CE1	1:C:143:ALA:HB2	2.52	0.43
1:H:142:VAL:HA	1:H:185:ASN:O	2.18	0.43
1:P:18:LYS:HD2	4:P:707:HOH:O	2.17	0.43
1:N:86:ALA:HA	1:N:140:SER:O	2.17	0.43
1:C:13:GLY:HA3	1:C:90:SER:O	2.18	0.43
1:E:236:MET:HB3	1:H:227:ASN:HB3	2.00	0.43
1:O:99:LEU:CD1	3:O:262:09T:H9	2.48	0.43
1:K:91:ILE:HG21	1:K:91:ILE:HD12	1.66	0.43
1:J:29:HIS:HD2	4:J:385:HOH:O	2.00	0.43
1:K:10:LEU:HD21	1:K:73:LEU:HD21	2.01	0.43
1:C:146:TYR:CZ	3:C:262:09T:H3	2.54	0.43
1:D:91:ILE:HD12	1:D:91:ILE:HG21	1.79	0.43
1:N:140:SER:OG	1:N:183:LYS:NZ	2.37	0.43
1:I:215:PRO:HD2	1:I:249:ALA:O	2.18	0.43
1:L:99:LEU:HD13	3:L:262:09T:H9	1.99	0.43
1:E:4:LEU:HD13	1:E:28:MET:HG2	1.99	0.43
1:N:142:VAL:HA	1:N:185:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:TYR:CE2	1:C:125:ALA:HB2	2.54	0.43
1:B:236:MET:HB3	1:C:227:ASN:HB3	2.01	0.43
1:C:39:TYR:CZ	1:C:44:LYS:HG3	2.54	0.43
1:B:91:ILE:HD12	1:B:91:ILE:HG21	1.73	0.43
1:J:91:ILE:HG21	1:J:91:ILE:HD12	1.77	0.43
1:N:9:ILE:HG12	1:N:86:ALA:HB3	2.01	0.42
1:D:211:ALA:O	1:D:217:LYS:HA	2.19	0.42
1:O:211:ALA:O	1:O:217:LYS:HA	2.19	0.42
1:C:202:ASN:CB	1:F:260:LEU:CD1	2.96	0.42
1:G:121:TYR:CE2	1:G:125:ALA:HB2	2.54	0.42
1:K:212:MET:HE1	1:N:212:MET:SD	2.59	0.42
1:P:40:VAL:HG23	1:P:43:PHE:CD1	2.51	0.42
1:A:8:LYS:CE	4:A:473:HOH:O	2.67	0.42
1:F:10:LEU:HD21	1:F:73:LEU:HD21	2.01	0.42
1:I:8:LYS:HB3	1:I:81:TRP:CE3	2.55	0.42
1:I:91:ILE:HD12	1:I:91:ILE:HG21	1.73	0.42
1:L:20:ILE:HG21	1:L:144:LEU:HD22	2.00	0.42
1:J:215:PRO:O	1:K:178:GLY:HA3	2.19	0.42
1:L:38:THR:HA	1:L:60:LEU:O	2.19	0.42
2:M:261:NAD:H71N	3:M:262:09T:C4	2.30	0.42
2:B:261:NAD:O7N	3:B:262:09T:H4	2.20	0.42
1:I:145:THR:O	2:I:261:NAD:H6N	2.19	0.42
1:C:212:MET:HG3	1:F:208:ASP:HB2	2.02	0.42
1:D:99:LEU:CD1	3:D:262:09T:H9	2.50	0.42
1:O:9:ILE:HG12	1:O:86:ALA:HB3	2.02	0.42
1:C:103:PHE:HB3	1:D:176:ALA:HB2	2.02	0.42
1:I:205:LYS:HG3	4:I:627:HOH:O	2.20	0.42
1:L:91:ILE:HD12	1:L:91:ILE:HG21	1.76	0.42
1:C:215:PRO:HD2	1:C:249:ALA:O	2.19	0.42
1:M:85:ASP:CG	1:M:137:ARG:HH11	2.23	0.42
1:M:194:THR:H	1:M:197:ALA:HB3	1.85	0.42
1:K:142:VAL:HA	1:K:185:ASN:O	2.19	0.42
1:A:258:ASN:HB2	1:H:205:LYS:HE2	2.02	0.41
1:K:40:VAL:HG23	1:K:43:PHE:HD1	1.84	0.41
1:K:116:HIS:CD2	1:L:116:HIS:CD2	3.08	0.41
1:A:38:THR:HA	1:A:60:LEU:O	2.20	0.41
1:K:205:LYS:HZ2	1:N:258:ASN:HD21	1.67	0.41
1:G:40:VAL:HG23	1:G:43:PHE:CD1	2.49	0.41
1:I:9:ILE:HG12	1:I:86:ALA:HB3	2.02	0.41
1:G:39:TYR:CZ	1:G:44:LYS:HG3	2.56	0.41
1:F:215:PRO:HD2	1:F:249:ALA:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASN:HD21	1:C:154:PRO:HB2	1.85	0.41
1:N:256:MET:O	1:N:257:GLY:C	2.59	0.41
1:I:123:PHE:CE1	1:I:143:ALA:HB2	2.54	0.41
1:N:236:MET:HB3	1:O:227:ASN:HB3	2.03	0.41
1:A:260:LEU:HD13	1:F:260:LEU:CD2	2.50	0.41
1:C:8:LYS:HB3	1:C:81:TRP:CE3	2.55	0.41
1:K:38:THR:HA	1:K:60:LEU:O	2.20	0.41
1:J:90:SER:OG	2:J:261:NAD:H52N	2.21	0.41
1:E:82:ASP:HB2	4:E:477:HOH:O	2.20	0.41
1:G:176:ALA:HB2	1:H:103:PHE:HB3	2.02	0.41
2:L:261:NAD:C7N	3:L:262:09T:H4	2.51	0.41
1:J:85:ASP:CG	1:J:137:ARG:HH11	2.23	0.41
1:D:104:ILE:HD13	1:D:104:ILE:HA	1.89	0.41
1:C:91:ILE:HG21	1:C:91:ILE:HD12	1.66	0.41
1:D:126:LEU:HA	1:D:126:LEU:HD23	1.87	0.41
1:D:154:PRO:HB3	4:D:827:HOH:O	2.20	0.41
1:P:113:SER:CB	4:P:379:HOH:O	2.68	0.41
1:A:256:MET:O	1:A:257:GLY:O	2.38	0.41
1:A:142:VAL:HA	1:A:185:ASN:O	2.21	0.41
1:N:209:TYR:CE1	1:P:258:ASN:OD1	2.74	0.41
1:E:154:PRO:O	1:E:155:SER:HB2	2.21	0.41
1:E:171:ARG:HD3	4:E:540:HOH:O	2.20	0.41
1:I:70:ILE:HG22	1:I:129:GLU:HG3	2.03	0.41
1:B:35:LEU:HD23	1:B:35:LEU:HA	1.83	0.41
1:E:209:TYR:HA	1:L:212:MET:CE	2.50	0.41
1:O:46:ARG:CZ	4:O:876:HOH:O	2.68	0.41
1:E:40:VAL:HG23	1:E:43:PHE:CD1	2.52	0.41
1:K:13:GLY:HA2	2:K:261:NAD:O3B	2.21	0.41
1:L:43:PHE:HD2	1:L:46:ARG:HH21	1.69	0.41
1:K:256:MET:HG2	1:K:256:MET:O	2.21	0.41
1:A:256:MET:O	1:A:256:MET:HG2	2.20	0.41
1:L:14:LEU:O	4:L:287:HOH:O	2.22	0.41
1:C:250:GLY:O	1:C:251:TYR:C	2.58	0.41
1:H:40:VAL:HG23	1:H:43:PHE:CD1	2.53	0.41
1:H:145:THR:O	2:H:261:NAD:H6N	2.21	0.41
1:B:10:LEU:HD11	1:B:38:THR:HG23	2.03	0.41
1:A:178:GLY:HA3	1:D:215:PRO:O	2.20	0.41
1:C:208:ASP:HB2	1:F:212:MET:HG3	2.03	0.40
1:C:43:PHE:HD2	1:C:46:ARG:HH21	1.69	0.40
1:F:40:VAL:HG23	1:F:43:PHE:CD1	2.52	0.40
1:L:85:ASP:OD1	1:L:137:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:LEU:O	1:K:137:ARG:HD2	2.22	0.40
1:E:116:HIS:CD2	1:F:116:HIS:CD2	3.09	0.40
1:L:126:LEU:HA	1:L:126:LEU:HD23	1.89	0.40
1:E:175:LEU:HA	1:H:215:PRO:HB3	2.03	0.40
1:F:227:ASN:HB3	1:G:236:MET:HB3	2.03	0.40
1:N:146:TYR:HB2	2:N:261:NAD:C5N	2.52	0.40
1:E:194:THR:H	1:E:197:ALA:HB3	1.86	0.40
1:E:121:TYR:CE2	1:E:125:ALA:HB2	2.57	0.40
1:E:85:ASP:CG	1:E:137:ARG:HH11	2.25	0.40
1:H:259:VAL:O	1:H:260:LEU:HB3	2.21	0.40
1:A:260:LEU:CD2	1:C:205:LYS:HB3	2.52	0.40
1:P:9:ILE:HG12	1:P:86:ALA:HB3	2.03	0.40
1:E:99:LEU:CD1	3:E:262:09T:H9	2.52	0.40
1:I:208:ASP:CB	1:P:212:MET:HG3	2.52	0.40
1:E:134:MET:HE1	1:E:140:SER:O	2.22	0.40
1:A:8:LYS:HE3	4:A:473:HOH:O	2.21	0.40
1:O:70:ILE:HG22	1:O:129:GLU:HG3	2.02	0.40
1:E:46:ARG:NH1	4:E:745:HOH:O	2.50	0.40
1:C:116:HIS:CD2	1:D:116:HIS:CD2	3.09	0.40
1:G:170:VAL:HG13	1:G:184:VAL:HG12	2.03	0.40
1:G:85:ASP:CG	1:G:137:ARG:HH11	2.25	0.40
1:M:127:ALA:HB1	1:M:177:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/280 (92%)	242 (94%)	13 (5%)	2 (1%)	24	41
1	B	255/280 (91%)	241 (94%)	13 (5%)	1 (0%)	39	61
1	C	257/280 (92%)	244 (95%)	12 (5%)	1 (0%)	39	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	254/280 (91%)	240 (94%)	13 (5%)	1 (0%)	39	61
1	E	256/280 (91%)	241 (94%)	13 (5%)	2 (1%)	24	41
1	F	257/280 (92%)	243 (95%)	13 (5%)	1 (0%)	39	61
1	G	255/280 (91%)	243 (95%)	11 (4%)	1 (0%)	39	61
1	H	257/280 (92%)	239 (93%)	14 (5%)	4 (2%)	12	21
1	I	257/280 (92%)	244 (95%)	12 (5%)	1 (0%)	39	61
1	J	255/280 (91%)	237 (93%)	17 (7%)	1 (0%)	39	61
1	K	257/280 (92%)	238 (93%)	17 (7%)	2 (1%)	24	41
1	L	255/280 (91%)	241 (94%)	13 (5%)	1 (0%)	39	61
1	M	255/280 (91%)	241 (94%)	13 (5%)	1 (0%)	39	61
1	N	257/280 (92%)	241 (94%)	13 (5%)	3 (1%)	16	29
1	O	254/280 (91%)	239 (94%)	14 (6%)	1 (0%)	39	61
1	P	257/280 (92%)	242 (94%)	14 (5%)	1 (0%)	39	61
All	All	4095/4480 (91%)	3856 (94%)	215 (5%)	24 (1%)	30	50

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	GLY
1	C	41	GLY
1	F	41	GLY
1	H	41	GLY
1	I	41	GLY
1	J	41	GLY
1	L	41	GLY
1	N	41	GLY
1	P	41	GLY
1	A	41	GLY
1	D	41	GLY
1	E	41	GLY
1	E	258	ASN
1	G	41	GLY
1	H	257	GLY
1	K	41	GLY
1	M	41	GLY
1	O	41	GLY
1	N	257	GLY

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Mol	Chain	Res	Type
1	A	257	GLY
1	H	256	MET
1	H	259	VAL
1	K	257	GLY
1	N	256	MET

### 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	203/221 (92%)	190 (94%)	13 (6%)	22	39
1	B	201/221 (91%)	191 (95%)	10 (5%)	30	53
1	C	203/221 (92%)	192 (95%)	11 (5%)	27	49
1	D	200/221 (90%)	190 (95%)	10 (5%)	30	53
1	E	202/221 (91%)	191 (95%)	11 (5%)	27	49
1	F	203/221 (92%)	192 (95%)	11 (5%)	27	49
1	G	201/221 (91%)	191 (95%)	10 (5%)	30	53
1	H	203/221 (92%)	190 (94%)	13 (6%)	22	39
1	I	203/221 (92%)	191 (94%)	12 (6%)	24	44
1	J	201/221 (91%)	192 (96%)	9 (4%)	34	59
1	K	203/221 (92%)	192 (95%)	11 (5%)	27	49
1	L	201/221 (91%)	191 (95%)	10 (5%)	30	53
1	M	201/221 (91%)	190 (94%)	11 (6%)	27	48
1	N	203/221 (92%)	191 (94%)	12 (6%)	24	44
1	O	200/221 (90%)	189 (94%)	11 (6%)	27	48
1	P	203/221 (92%)	190 (94%)	13 (6%)	22	39
All	All	3231/3536 (91%)	3053 (94%)	178 (6%)	27	48

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	42	GLN
1	A	45	ASP
1	A	49	LYS
1	A	65	ILE
1	A	91	ILE
1	A	96	ARG
1	A	100	GLU
1	A	144	LEU
1	A	212	MET
1	A	213	VAL
1	A	258	ASN
1	A	259	VAL
1	B	42	GLN
1	B	45	ASP
1	B	49	LYS
1	B	65	ILE
1	B	91	ILE
1	B	96	ARG
1	B	100	GLU
1	B	137	ARG
1	B	144	LEU
1	B	213	VAL
1	C	42	GLN
1	C	45	ASP
1	C	49	LYS
1	C	65	ILE
1	C	91	ILE
1	C	96	ARG
1	C	100	GLU
1	C	137	ARG
1	C	144	LEU
1	C	213	VAL
1	C	260	LEU
1	D	42	GLN
1	D	45	ASP
1	D	49	LYS
1	D	65	ILE
1	D	91	ILE
1	D	96	ARG
1	D	100	GLU
1	D	140	SER
1	D	144	LEU

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Mol	Chain	Res	Type
1	D	213	VAL
1	E	42	GLN
1	E	45	ASP
1	E	49	LYS
1	E	65	ILE
1	E	91	ILE
1	E	96	ARG
1	E	100	GLU
1	E	137	ARG
1	E	144	LEU
1	E	213	VAL
1	E	259	VAL
1	F	42	GLN
1	F	45	ASP
1	F	49	LYS
1	F	65	ILE
1	F	91	ILE
1	F	96	ARG
1	F	100	GLU
1	F	137	ARG
1	F	144	LEU
1	F	213	VAL
1	F	260	LEU
1	G	42	GLN
1	G	45	ASP
1	G	49	LYS
1	G	65	ILE
1	G	91	ILE
1	G	96	ARG
1	G	100	GLU
1	G	137	ARG
1	G	144	LEU
1	G	213	VAL
1	H	42	GLN
1	H	45	ASP
1	H	49	LYS
1	H	65	ILE
1	H	91	ILE
1	H	96	ARG
1	H	100	GLU
1	H	137	ARG
1	H	144	LEU

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Mol	Chain	Res	Type
1	H	212	MET
1	H	213	VAL
1	H	259	VAL
1	H	260	LEU
1	I	42	GLN
1	I	45	ASP
1	I	49	LYS
1	I	65	ILE
1	I	91	ILE
1	I	96	ARG
1	I	100	GLU
1	I	137	ARG
1	I	144	LEU
1	I	213	VAL
1	I	258	ASN
1	I	259	VAL
1	J	42	GLN
1	J	45	ASP
1	J	49	LYS
1	J	65	ILE
1	J	91	ILE
1	J	96	ARG
1	J	100	GLU
1	J	144	LEU
1	J	213	VAL
1	K	42	GLN
1	K	45	ASP
1	K	49	LYS
1	K	65	ILE
1	K	91	ILE
1	K	96	ARG
1	K	100	GLU
1	K	144	LEU
1	K	212	MET
1	K	213	VAL
1	K	258	ASN
1	L	42	GLN
1	L	45	ASP
1	L	49	LYS
1	L	65	ILE
1	L	91	ILE
1	L	96	ARG

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Mol	Chain	Res	Type
1	L	100	GLU
1	L	137	ARG
1	L	144	LEU
1	L	213	VAL
1	M	42	GLN
1	M	45	ASP
1	M	49	LYS
1	M	65	ILE
1	M	91	ILE
1	M	96	ARG
1	M	100	GLU
1	M	137	ARG
1	M	144	LEU
1	M	213	VAL
1	M	258	ASN
1	N	42	GLN
1	N	45	ASP
1	N	49	LYS
1	N	65	ILE
1	N	91	ILE
1	N	96	ARG
1	N	100	GLU
1	N	137	ARG
1	N	144	LEU
1	N	212	MET
1	N	213	VAL
1	N	260	LEU
1	O	42	GLN
1	O	45	ASP
1	O	49	LYS
1	O	65	ILE
1	O	91	ILE
1	O	96	ARG
1	O	100	GLU
1	O	137	ARG
1	O	144	LEU
1	O	213	VAL
1	O	254	VAL
1	P	42	GLN
1	P	45	ASP
1	P	49	LYS
1	P	65	ILE

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Mol	Chain	Res	Type
1	P	91	ILE
1	P	96	ARG
1	P	99	LEU
1	P	100	GLU
1	P	137	ARG
1	P	144	LEU
1	P	213	VAL
1	P	259	VAL
1	P	260	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	138	ASN
1	A	258	ASN
1	D	29	HIS
1	D	138	ASN
1	E	258	ASN
1	F	210	ASN
1	F	258	ASN
1	H	258	ASN
1	I	29	HIS
1	I	258	ASN
1	J	29	HIS
1	J	138	ASN
1	L	258	ASN
1	P	258	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

32 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	261	-	38,48,48	1.59	8 (21%)	47,73,73	3.28	20 (42%)
3	09T	A	262	-	21,22,22	1.32	3 (14%)	27,32,32	1.39	3 (11%)
2	NAD	B	261	-	38,48,48	1.70	10 (26%)	47,73,73	2.00	12 (25%)
3	09T	B	262	-	21,22,22	1.36	2 (9%)	27,32,32	0.90	1 (3%)
2	NAD	C	261	-	38,48,48	1.51	8 (21%)	47,73,73	2.99	18 (38%)
3	09T	C	262	-	21,22,22	2.27	4 (19%)	27,32,32	2.32	8 (29%)
2	NAD	D	261	-	38,48,48	1.75	6 (15%)	47,73,73	3.20	15 (31%)
3	09T	D	262	-	21,22,22	1.81	5 (23%)	27,32,32	1.75	5 (18%)
2	NAD	E	261	-	38,48,48	1.77	7 (18%)	47,73,73	2.86	17 (36%)
3	09T	E	262	-	21,22,22	1.70	4 (19%)	27,32,32	1.26	2 (7%)
2	NAD	F	261	-	38,48,48	1.46	8 (21%)	47,73,73	2.73	11 (23%)
3	09T	F	262	-	21,22,22	1.65	3 (14%)	27,32,32	1.98	7 (25%)
2	NAD	G	261	-	38,48,48	1.96	7 (18%)	47,73,73	3.01	15 (31%)
3	09T	G	262	-	21,22,22	1.64	3 (14%)	27,32,32	1.13	1 (3%)
2	NAD	H	261	-	38,48,48	1.89	9 (23%)	47,73,73	2.51	12 (25%)
3	09T	H	262	-	21,22,22	1.62	3 (14%)	27,32,32	0.83	0
2	NAD	I	261	-	38,48,48	1.41	6 (15%)	47,73,73	2.85	12 (25%)
3	09T	I	262	-	21,22,22	1.96	3 (14%)	27,32,32	1.92	7 (25%)
2	NAD	J	261	-	38,48,48	1.75	4 (10%)	47,73,73	3.24	13 (27%)
3	09T	J	262	-	21,22,22	1.65	4 (19%)	27,32,32	1.75	7 (25%)
2	NAD	K	261	-	38,48,48	1.70	8 (21%)	47,73,73	3.16	17 (36%)
3	09T	K	262	-	21,22,22	1.19	2 (9%)	27,32,32	2.02	3 (11%)
2	NAD	L	261	-	38,48,48	1.67	8 (21%)	47,73,73	2.24	14 (29%)
3	09T	L	262	-	21,22,22	1.22	2 (9%)	27,32,32	1.10	1 (3%)
2	NAD	M	261	-	38,48,48	1.89	7 (18%)	47,73,73	2.95	15 (31%)
3	09T	M	262	-	21,22,22	1.42	3 (14%)	27,32,32	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	N	261	-	38,48,48	1.83	9 (23%)	47,73,73	2.87	13 (27%)
3	09T	N	262	-	21,22,22	1.67	4 (19%)	27,32,32	0.88	0
2	NAD	O	261	-	38,48,48	1.94	10 (26%)	47,73,73	3.14	13 (27%)
3	09T	O	262	-	21,22,22	1.83	4 (19%)	27,32,32	1.19	3 (11%)
2	NAD	P	261	-	38,48,48	1.47	8 (21%)	47,73,73	3.00	19 (40%)
3	09T	P	262	-	21,22,22	1.60	3 (14%)	27,32,32	2.03	7 (25%)

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	261	-	-	0/22/62/62	0/5/5/5
3	09T	A	262	-	-	0/4/4/4	0/3/3/3
2	NAD	B	261	-	-	0/22/62/62	0/5/5/5
3	09T	B	262	-	-	0/4/4/4	0/3/3/3
2	NAD	C	261	-	-	0/22/62/62	0/5/5/5
3	09T	C	262	-	-	0/4/4/4	0/3/3/3
2	NAD	D	261	-	-	0/22/62/62	0/5/5/5
3	09T	D	262	-	-	0/4/4/4	0/3/3/3
2	NAD	E	261	-	-	0/22/62/62	0/5/5/5
3	09T	E	262	-	-	0/4/4/4	0/3/3/3
2	NAD	F	261	-	-	0/22/62/62	0/5/5/5
3	09T	F	262	-	-	0/4/4/4	0/3/3/3
2	NAD	G	261	-	-	0/22/62/62	0/5/5/5
3	09T	G	262	-	-	0/4/4/4	0/3/3/3
2	NAD	H	261	-	-	0/22/62/62	0/5/5/5
3	09T	H	262	-	-	0/4/4/4	0/3/3/3
2	NAD	I	261	-	-	0/22/62/62	0/5/5/5
3	09T	I	262	-	-	0/4/4/4	0/3/3/3
2	NAD	J	261	-	-	0/22/62/62	0/5/5/5
3	09T	J	262	-	-	0/4/4/4	0/3/3/3
2	NAD	K	261	-	-	0/22/62/62	0/5/5/5
3	09T	K	262	-	-	0/4/4/4	0/3/3/3
2	NAD	L	261	-	-	0/22/62/62	0/5/5/5
3	09T	L	262	-	-	0/4/4/4	0/3/3/3
2	NAD	M	261	-	-	0/22/62/62	0/5/5/5
3	09T	M	262	-	-	0/4/4/4	0/3/3/3
2	NAD	N	261	-	-	0/22/62/62	0/5/5/5
3	09T	N	262	-	-	0/4/4/4	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	O	261	-	-	0/22/62/62	0/5/5/5
3	09T	O	262	-	-	0/4/4/4	0/3/3/3
2	NAD	P	261	-	-	0/22/62/62	0/5/5/5
3	09T	P	262	-	-	0/4/4/4	0/3/3/3

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	262	09T	C20-N10	-7.26	1.31	1.39
3	I	262	09T	C20-N10	-6.50	1.31	1.39
3	F	262	09T	C20-N10	-5.34	1.33	1.39
3	D	262	09T	C20-N10	-5.05	1.33	1.39
3	P	262	09T	C20-N10	-4.91	1.33	1.39
3	J	262	09T	C20-N10	-4.83	1.33	1.39
3	O	262	09T	C20-N10	-4.53	1.34	1.39
3	C	262	09T	C9-N10	-3.98	1.42	1.49
3	H	262	09T	C20-N10	-3.90	1.34	1.39
3	E	262	09T	C20-N10	-3.70	1.35	1.39
3	B	262	09T	C20-N10	-3.52	1.35	1.39
3	N	262	09T	C20-N10	-3.23	1.35	1.39
3	G	262	09T	C20-N10	-2.93	1.36	1.39
3	I	262	09T	C9-N10	-2.81	1.44	1.49
3	M	262	09T	C20-N10	-2.50	1.36	1.39
2	C	261	NAD	PN-O1N	-2.47	1.42	1.51
3	L	262	09T	C20-N10	-2.42	1.36	1.39
2	P	261	NAD	PA-O2A	-2.39	1.44	1.54
2	L	261	NAD	PN-O1N	-2.39	1.42	1.51
2	F	261	NAD	PA-O2A	-2.36	1.44	1.54
3	K	262	09T	C20-N10	-2.35	1.36	1.39
2	B	261	NAD	PN-O1N	-2.33	1.42	1.51
2	O	261	NAD	PN-O1N	-2.31	1.42	1.51
3	C	262	09T	C9-C5	-2.30	1.45	1.51
2	K	261	NAD	C6A-N6A	-2.29	1.27	1.34
2	H	261	NAD	PA-O2A	-2.29	1.45	1.54
2	A	261	NAD	C2D-C3D	-2.23	1.47	1.53
3	J	262	09T	C9-N10	-2.14	1.45	1.49
3	D	262	09T	C9-N10	-2.12	1.45	1.49
2	I	261	NAD	PN-O1N	-2.12	1.43	1.51
3	A	262	09T	C14-C13	-2.06	1.38	1.41
2	A	261	NAD	C6A-N6A	-2.04	1.28	1.34
2	F	261	NAD	PN-O1N	-2.03	1.43	1.51
2	C	261	NAD	PA-O2A	-2.00	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	261	NAD	C3N-C7N	2.01	1.53	1.50
2	J	261	NAD	C2A-N3A	2.02	1.35	1.32
3	D	262	09T	C3-C2	2.05	1.43	1.39
2	O	261	NAD	C5N-C4N	2.05	1.43	1.38
2	F	261	NAD	C6N-N1N	2.07	1.41	1.35
2	P	261	NAD	C2A-N1A	2.13	1.37	1.33
2	C	261	NAD	C6N-N1N	2.14	1.41	1.35
2	B	261	NAD	O4B-C4B	2.15	1.50	1.45
2	B	261	NAD	C4N-C3N	2.15	1.43	1.39
2	D	261	NAD	C6N-N1N	2.16	1.41	1.35
2	C	261	NAD	O4B-C4B	2.17	1.50	1.45
2	P	261	NAD	O3D-C3D	2.17	1.48	1.43
3	E	262	09T	C3-C2	2.20	1.43	1.39
2	L	261	NAD	C4A-N3A	2.20	1.38	1.35
2	B	261	NAD	C4A-N3A	2.21	1.38	1.35
2	E	261	NAD	C4N-C3N	2.22	1.43	1.39
2	N	261	NAD	C4N-C3N	2.22	1.43	1.39
3	N	262	09T	C6-C7	2.22	1.42	1.38
2	O	261	NAD	C4N-C3N	2.23	1.43	1.39
2	H	261	NAD	C2A-N1A	2.23	1.38	1.33
2	K	261	NAD	O3B-C3B	2.24	1.48	1.43
2	F	261	NAD	O2D-C2D	2.26	1.48	1.43
2	D	261	NAD	C3N-C7N	2.27	1.54	1.50
2	N	261	NAD	O3D-C3D	2.27	1.48	1.43
2	F	261	NAD	C5N-C4N	2.29	1.43	1.38
2	K	261	NAD	C2N-C3N	2.30	1.42	1.39
2	P	261	NAD	C5N-C4N	2.30	1.43	1.38
2	B	261	NAD	C2A-N1A	2.30	1.38	1.33
2	D	261	NAD	O3D-C3D	2.34	1.48	1.43
2	I	261	NAD	C6N-N1N	2.34	1.41	1.35
3	O	262	09T	C3-C2	2.34	1.44	1.39
2	L	261	NAD	C2N-C3N	2.43	1.42	1.39
2	N	261	NAD	C7N-N7N	2.43	1.37	1.33
2	P	261	NAD	C2N-C3N	2.45	1.42	1.39
2	I	261	NAD	C2N-C3N	2.50	1.42	1.39
2	A	261	NAD	C2A-N1A	2.50	1.38	1.33
2	C	261	NAD	C2A-N1A	2.51	1.38	1.33
2	H	261	NAD	C7N-N7N	2.51	1.38	1.33
2	L	261	NAD	C2A-N1A	2.54	1.38	1.33
2	O	261	NAD	C2A-N3A	2.56	1.36	1.32
2	A	261	NAD	C4N-C3N	2.57	1.43	1.39
2	H	261	NAD	C4N-C3N	2.60	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	261	NAD	C3N-C7N	2.62	1.54	1.50
2	L	261	NAD	C3N-C7N	2.63	1.54	1.50
3	J	262	09T	C7-CL8	2.65	1.80	1.73
2	N	261	NAD	C2A-N1A	2.66	1.39	1.33
2	K	261	NAD	C2A-N3A	2.66	1.36	1.32
2	I	261	NAD	O4B-C4B	2.68	1.51	1.45
2	M	261	NAD	C2A-N1A	2.70	1.39	1.33
3	D	262	09T	C7-CL8	2.70	1.80	1.73
2	I	261	NAD	O2D-C2D	2.71	1.49	1.43
2	A	261	NAD	C2A-N3A	2.75	1.37	1.32
2	F	261	NAD	C2N-C3N	2.76	1.43	1.39
2	N	261	NAD	C6N-N1N	2.76	1.42	1.35
2	I	261	NAD	O4D-C1D	2.77	1.44	1.41
3	A	262	09T	C7-CL8	2.79	1.80	1.73
2	E	261	NAD	C6N-N1N	2.81	1.43	1.35
3	F	262	09T	C7-CL8	2.84	1.80	1.73
2	C	261	NAD	C2N-C3N	2.85	1.43	1.39
2	M	261	NAD	C6N-N1N	2.85	1.43	1.35
2	P	261	NAD	O4D-C1D	2.87	1.44	1.41
3	F	262	09T	C2-CL1	2.88	1.80	1.73
2	G	261	NAD	C2A-N1A	2.89	1.39	1.33
3	J	262	09T	C2-CL1	2.90	1.80	1.73
2	P	261	NAD	C6N-N1N	2.90	1.43	1.35
2	E	261	NAD	C2A-N1A	2.92	1.39	1.33
2	E	261	NAD	C2N-C3N	2.92	1.43	1.39
3	P	262	09T	C2-CL1	2.92	1.80	1.73
2	O	261	NAD	C6N-N1N	2.93	1.43	1.35
2	M	261	NAD	C4N-C3N	2.95	1.44	1.39
2	H	261	NAD	C4A-N3A	3.00	1.40	1.35
2	K	261	NAD	C6N-N1N	3.00	1.43	1.35
2	H	261	NAD	C6N-N1N	3.02	1.43	1.35
3	H	262	09T	C7-CL8	3.04	1.81	1.73
2	P	261	NAD	C4A-N3A	3.06	1.40	1.35
3	P	262	09T	C7-CL8	3.06	1.81	1.73
3	E	262	09T	C7-CL8	3.07	1.81	1.73
3	M	262	09T	C7-CL8	3.08	1.81	1.73
2	F	261	NAD	C4A-N3A	3.10	1.40	1.35
2	G	261	NAD	C6N-N1N	3.11	1.43	1.35
3	O	262	09T	C7-CL8	3.13	1.81	1.73
2	B	261	NAD	C2N-C3N	3.13	1.43	1.39
2	B	261	NAD	C2A-N3A	3.15	1.37	1.32
2	F	261	NAD	O3D-C3D	3.15	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	261	NAD	O4D-C1D	3.17	1.45	1.41
2	J	261	NAD	C2N-C3N	3.17	1.43	1.39
2	L	261	NAD	C6N-N1N	3.19	1.44	1.35
2	K	261	NAD	C4A-N3A	3.29	1.40	1.35
3	K	262	09T	C2-CL1	3.33	1.81	1.73
2	G	261	NAD	C4N-C3N	3.34	1.45	1.39
2	A	261	NAD	C6N-N1N	3.38	1.44	1.35
2	N	261	NAD	C2N-C3N	3.43	1.44	1.39
3	G	262	09T	C7-CL8	3.43	1.82	1.73
2	B	261	NAD	C6N-N1N	3.44	1.44	1.35
2	N	261	NAD	C4A-N3A	3.51	1.40	1.35
2	H	261	NAD	C2N-C3N	3.51	1.44	1.39
2	A	261	NAD	C4A-N3A	3.53	1.40	1.35
2	L	261	NAD	C2A-N3A	3.56	1.38	1.32
3	D	262	09T	C2-CL1	3.59	1.82	1.73
3	N	262	09T	C7-CL8	3.63	1.82	1.73
3	H	262	09T	C2-CL1	3.63	1.82	1.73
2	O	261	NAD	C2A-N1A	3.64	1.40	1.33
2	C	261	NAD	O2D-C2D	3.75	1.51	1.43
3	M	262	09T	C2-CL1	3.76	1.82	1.73
2	G	261	NAD	C2N-C3N	3.77	1.44	1.39
3	N	262	09T	C2-CL1	3.80	1.82	1.73
2	D	261	NAD	C2N-C3N	3.80	1.44	1.39
3	A	262	09T	C2-CL1	3.84	1.83	1.73
2	O	261	NAD	C2N-C3N	3.84	1.44	1.39
2	M	261	NAD	C2N-C3N	3.89	1.44	1.39
3	B	262	09T	C2-CL1	3.96	1.83	1.73
3	E	262	09T	C2-CL1	4.03	1.83	1.73
3	L	262	09T	C2-CL1	4.06	1.83	1.73
3	I	262	09T	C2-CL1	4.17	1.83	1.73
2	N	261	NAD	O4D-C1D	4.26	1.46	1.41
3	C	262	09T	C2-CL1	4.28	1.84	1.73
2	H	261	NAD	C3N-C7N	4.29	1.57	1.50
2	G	261	NAD	C3N-C7N	4.34	1.57	1.50
3	O	262	09T	C2-CL1	4.40	1.84	1.73
2	N	261	NAD	C3N-C7N	4.42	1.57	1.50
2	E	261	NAD	O4D-C1D	4.55	1.47	1.41
3	G	262	09T	C2-CL1	4.64	1.85	1.73
2	M	261	NAD	C4A-N3A	4.72	1.42	1.35
2	E	261	NAD	C3N-C7N	4.73	1.58	1.50
2	O	261	NAD	C3N-C7N	4.80	1.58	1.50
2	L	261	NAD	O4D-C1D	4.92	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	261	NAD	O4D-C1D	4.94	1.47	1.41
2	O	261	NAD	C4A-N3A	4.98	1.43	1.35
2	O	261	NAD	O4D-C1D	5.00	1.47	1.41
2	M	261	NAD	O4D-C1D	5.14	1.47	1.41
2	M	261	NAD	C3N-C7N	5.15	1.58	1.50
2	H	261	NAD	O4D-C1D	5.23	1.47	1.41
2	B	261	NAD	O4D-C1D	5.26	1.47	1.41
2	E	261	NAD	C4A-N3A	5.26	1.43	1.35
2	D	261	NAD	O4D-C1D	5.31	1.47	1.41
2	J	261	NAD	C4A-N3A	5.37	1.43	1.35
2	G	261	NAD	C4A-N3A	5.49	1.43	1.35
2	G	261	NAD	O4D-C1D	5.52	1.48	1.41
2	D	261	NAD	C4A-N3A	5.56	1.43	1.35
2	J	261	NAD	O4D-C1D	5.75	1.48	1.41
2	K	261	NAD	O4D-C1D	6.27	1.49	1.41

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	261	NAD	N3A-C2A-N1A	-15.24	117.22	128.89
2	J	261	NAD	N3A-C2A-N1A	-15.11	117.32	128.89
2	G	261	NAD	N3A-C2A-N1A	-12.39	119.41	128.89
2	A	261	NAD	N3A-C2A-N1A	-12.21	119.55	128.89
2	M	261	NAD	N3A-C2A-N1A	-11.43	120.14	128.89
2	F	261	NAD	N3A-C2A-N1A	-11.37	120.19	128.89
2	K	261	NAD	N3A-C2A-N1A	-11.31	120.24	128.89
2	P	261	NAD	N3A-C2A-N1A	-10.84	120.59	128.89
2	E	261	NAD	N3A-C2A-N1A	-10.46	120.89	128.89
2	I	261	NAD	C4B-O4B-C1B	-10.35	98.35	109.72
2	O	261	NAD	C4B-O4B-C1B	-10.14	98.57	109.72
2	M	261	NAD	C1B-N9A-C4A	-9.79	112.18	126.94
2	G	261	NAD	C1B-N9A-C4A	-9.72	112.28	126.94
2	C	261	NAD	C4B-O4B-C1B	-9.56	99.21	109.72
2	J	261	NAD	C1B-N9A-C4A	-9.49	112.62	126.94
2	N	261	NAD	N3A-C2A-N1A	-9.36	121.72	128.89
2	H	261	NAD	N3A-C2A-N1A	-9.00	122.00	128.89
2	O	261	NAD	C1B-N9A-C4A	-8.88	113.55	126.94
2	O	261	NAD	N3A-C2A-N1A	-8.80	122.16	128.89
2	D	261	NAD	C1B-N9A-C4A	-8.60	113.97	126.94
2	E	261	NAD	C1B-N9A-C4A	-8.56	114.03	126.94
3	K	262	09T	C7-C6-C5	-8.32	114.98	120.36
2	I	261	NAD	N3A-C2A-N1A	-8.13	122.67	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	261	NAD	N3A-C2A-N1A	-7.52	123.14	128.89
2	L	261	NAD	C1B-N9A-C4A	-7.19	116.10	126.94
2	G	261	NAD	C4B-O4B-C1B	-7.07	101.95	109.72
2	I	261	NAD	C2B-C1B-N9A	-6.91	103.74	114.29
3	C	262	09T	C7-C6-C5	-6.90	115.91	120.36
2	C	261	NAD	C2B-C1B-N9A	-6.80	103.90	114.29
2	F	261	NAD	C1B-N9A-C4A	-6.79	116.70	126.94
2	N	261	NAD	C4B-O4B-C1B	-6.61	102.45	109.72
2	M	261	NAD	C4B-O4B-C1B	-6.58	102.49	109.72
2	K	261	NAD	O7N-C7N-C3N	-6.55	112.44	119.59
2	A	261	NAD	C1B-N9A-C4A	-6.53	117.08	126.94
2	I	261	NAD	C1B-N9A-C4A	-6.30	117.44	126.94
2	P	261	NAD	C1B-N9A-C4A	-6.28	117.47	126.94
2	N	261	NAD	C1B-N9A-C4A	-6.27	117.49	126.94
2	N	261	NAD	C2B-C1B-N9A	-6.19	104.84	114.29
2	H	261	NAD	C1B-N9A-C4A	-6.16	117.64	126.94
2	F	261	NAD	C4B-O4B-C1B	-6.13	102.99	109.72
2	E	261	NAD	C4B-O4B-C1B	-6.10	103.02	109.72
2	P	261	NAD	C4B-O4B-C1B	-6.08	103.04	109.72
2	A	261	NAD	O7N-C7N-C3N	-6.02	113.01	119.59
2	H	261	NAD	C4B-O4B-C1B	-5.80	103.34	109.72
3	I	262	09T	C7-C6-C5	-5.73	116.66	120.36
2	B	261	NAD	N3A-C2A-N1A	-5.69	124.53	128.89
2	B	261	NAD	C1B-N9A-C4A	-5.64	118.43	126.94
3	A	262	09T	C7-C6-C5	-5.31	116.93	120.36
2	J	261	NAD	C4B-O4B-C1B	-5.29	103.90	109.72
2	K	261	NAD	C4B-O4B-C1B	-5.26	103.94	109.72
2	L	261	NAD	N3A-C2A-N1A	-5.23	124.89	128.89
2	D	261	NAD	C4B-O4B-C1B	-5.21	103.99	109.72
2	K	261	NAD	C1B-N9A-C4A	-5.10	119.24	126.94
3	C	262	09T	C9-C5-C6	-5.06	112.05	120.30
2	P	261	NAD	O7N-C7N-C3N	-4.86	114.28	119.59
3	D	262	09T	C3-C4-C5	-4.85	114.40	121.04
3	P	262	09T	C5-C9-N10	-4.82	104.25	112.72
2	C	261	NAD	C3N-C7N-N7N	-4.79	112.58	117.82
2	B	261	NAD	C4B-O4B-C1B	-4.79	104.46	109.72
2	C	261	NAD	C1B-N9A-C4A	-4.77	119.75	126.94
2	A	261	NAD	C4B-O4B-C1B	-4.75	104.50	109.72
2	L	261	NAD	C4B-O4B-C1B	-4.72	104.53	109.72
3	F	262	09T	C5-C9-N10	-4.60	104.63	112.72
2	J	261	NAD	C2B-C1B-N9A	-4.57	107.31	114.29
3	F	262	09T	C14-C13-C20	-4.55	116.44	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	262	09T	C14-C13-C20	-4.37	116.62	121.10
2	D	261	NAD	C2B-C1B-N9A	-4.22	107.85	114.29
2	E	261	NAD	O7N-C7N-N7N	-3.99	116.97	122.59
3	I	262	09T	C9-C5-C6	-3.94	113.88	120.30
3	J	262	09T	C3-C4-C5	-3.90	115.69	121.04
2	H	261	NAD	O7N-C7N-C3N	-3.89	115.34	119.59
3	D	262	09T	C9-C5-C6	-3.86	114.00	120.30
2	O	261	NAD	O7N-C7N-N7N	-3.85	117.18	122.59
2	N	261	NAD	O7N-C7N-C3N	-3.81	115.42	119.59
2	P	261	NAD	C2B-C1B-N9A	-3.78	108.51	114.29
2	P	261	NAD	O5D-PN-O1N	-3.76	95.03	109.62
2	K	261	NAD	O3D-C3D-C4D	-3.73	99.85	111.05
2	M	261	NAD	O3-PN-O5D	-3.69	93.14	102.94
2	G	261	NAD	O3-PN-O5D	-3.66	93.24	102.94
3	J	262	09T	C9-C5-C6	-3.53	114.55	120.30
3	P	262	09T	C7-C6-C5	-3.52	118.09	120.36
2	C	261	NAD	C3N-C2N-N1N	-3.43	116.41	120.36
3	C	262	09T	C3-C4-C5	-3.41	116.38	121.04
2	I	261	NAD	C3N-C2N-N1N	-3.34	116.51	120.36
2	J	261	NAD	O2B-C2B-C3B	-3.31	101.07	111.83
3	F	262	09T	C7-C6-C5	-3.26	118.26	120.36
2	E	261	NAD	O5D-PN-O1N	-3.23	97.06	109.62
2	E	261	NAD	C2N-C3N-C4N	-3.22	114.70	118.29
2	I	261	NAD	O5D-PN-O1N	-3.22	97.14	109.62
2	A	261	NAD	O3D-C3D-C2D	-3.18	101.47	111.83
2	K	261	NAD	O5D-C5D-C4D	-3.14	97.53	109.12
2	M	261	NAD	C2N-C3N-C4N	-3.14	114.80	118.29
3	J	262	09T	C14-C13-C20	-3.00	118.03	121.10
2	K	261	NAD	O5D-PN-O1N	-2.96	98.13	109.62
2	O	261	NAD	O3-PN-O5D	-2.89	95.27	102.94
3	J	262	09T	C7-C6-C5	-2.89	118.50	120.36
3	O	262	09T	C6-C7-CL8	-2.85	114.11	118.50
2	A	261	NAD	C3N-C2N-N1N	-2.84	117.09	120.36
2	A	261	NAD	O5D-C5D-C4D	-2.80	98.79	109.12
3	C	262	09T	C14-C13-C20	-2.76	118.27	121.10
2	C	261	NAD	O4D-C4D-C3D	-2.72	99.66	105.15
2	A	261	NAD	O5D-PN-O1N	-2.62	99.45	109.62
3	O	262	09T	C9-C5-C6	-2.61	116.04	120.30
2	D	261	NAD	C3N-C7N-N7N	-2.60	114.97	117.82
2	J	261	NAD	O3-PN-O5D	-2.60	96.03	102.94
3	I	262	09T	C6-C7-CL8	-2.55	114.57	118.50
2	K	261	NAD	O3D-C3D-C2D	-2.55	103.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	262	09T	C6-C7-CL8	-2.54	114.59	118.50
2	L	261	NAD	O3-PA-O5B	-2.52	96.25	102.94
2	O	261	NAD	O4D-C4D-C3D	-2.50	100.10	105.15
2	F	261	NAD	O5D-PN-O1N	-2.50	99.90	109.62
3	A	262	09T	C19-C20-C13	-2.47	118.10	120.54
3	D	262	09T	C14-C13-C20	-2.45	118.60	121.10
2	P	261	NAD	O3D-C3D-C4D	-2.44	103.73	111.05
2	B	261	NAD	O3-PA-O5B	-2.34	96.72	102.94
2	L	261	NAD	O5B-C5B-C4B	-2.32	100.57	109.12
2	A	261	NAD	O3-PA-O5B	-2.31	96.80	102.94
2	M	261	NAD	PN-O3-PA	-2.31	126.24	132.73
3	I	262	09T	C3-C4-C5	-2.30	117.89	121.04
2	M	261	NAD	O7N-C7N-N7N	-2.30	119.36	122.59
2	L	261	NAD	C3N-C2N-N1N	-2.29	117.72	120.36
2	B	261	NAD	C3N-C7N-N7N	-2.24	115.37	117.82
2	L	261	NAD	O4D-C4D-C3D	-2.22	100.67	105.15
3	E	262	09T	C9-C5-C6	-2.20	116.71	120.30
2	D	261	NAD	O5B-C5B-C4B	-2.19	101.06	109.12
2	F	261	NAD	O7N-C7N-C3N	-2.17	117.22	119.59
2	G	261	NAD	O7N-C7N-N7N	-2.16	119.55	122.59
3	P	262	09T	C2-C7-CL8	-2.16	115.47	120.87
2	L	261	NAD	O2B-C2B-C3B	-2.16	104.81	111.83
2	P	261	NAD	O4D-C4D-C3D	-2.15	100.81	105.15
2	D	261	NAD	O3-PN-O5D	-2.14	97.26	102.94
2	A	261	NAD	O2B-C2B-C3B	-2.12	104.93	111.83
2	G	261	NAD	O4B-C4B-C5B	-2.11	101.77	109.32
3	K	262	09T	C14-C13-C20	-2.08	118.97	121.10
2	A	261	NAD	O3D-C3D-C4D	-2.08	104.82	111.05
3	C	262	09T	C5-C9-N10	-2.05	109.12	112.72
2	M	261	NAD	O3-PA-O5B	-2.04	97.51	102.94
2	A	261	NAD	PN-O3-PA	-2.03	127.02	132.73
2	D	261	NAD	O2B-C2B-C3B	-2.03	105.21	111.83
2	M	261	NAD	O4B-C4B-C5B	-2.02	102.09	109.32
2	B	261	NAD	O2B-C2B-C3B	-2.01	105.29	111.83
2	O	261	NAD	O2N-PN-O3	2.02	114.24	105.09
2	F	261	NAD	C2B-C3B-C4B	2.04	106.80	102.61
2	G	261	NAD	O2A-PA-O1A	2.04	123.59	112.53
2	G	261	NAD	N6A-C6A-N1A	2.06	123.61	119.20
2	A	261	NAD	C5D-C4D-C3D	2.06	123.40	115.21
2	H	261	NAD	O5B-PA-O1A	2.06	117.63	109.62
3	F	262	09T	C3-C2-CL1	2.07	122.66	118.39
2	J	261	NAD	O2A-PA-O1A	2.08	123.77	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	261	NAD	C2D-C3D-C4D	2.08	106.89	102.61
2	E	261	NAD	O2N-PN-O1N	2.08	123.82	112.53
2	B	261	NAD	O2A-PA-O1A	2.09	123.86	112.53
2	M	261	NAD	O2A-PA-O1A	2.09	123.87	112.53
3	O	262	09T	C2-C7-CL8	2.10	126.11	120.87
2	N	261	NAD	C5D-C4D-C3D	2.10	123.56	115.21
3	A	262	09T	C4-C5-C6	2.10	121.66	118.55
2	G	261	NAD	O2N-PN-O3	2.11	114.67	105.09
2	D	261	NAD	O2A-PA-O1A	2.11	123.97	112.53
2	E	261	NAD	C4D-O4D-C1D	2.11	112.04	109.72
2	O	261	NAD	C5D-C4D-C3D	2.12	123.61	115.21
2	A	261	NAD	O7N-C7N-N7N	2.12	125.58	122.59
2	O	261	NAD	O2A-PA-O1A	2.12	124.03	112.53
2	E	261	NAD	C3N-C2N-N1N	2.14	122.83	120.36
2	C	261	NAD	O2N-PN-O1N	2.14	124.13	112.53
3	J	262	09T	C5-C9-N10	2.14	116.47	112.72
2	K	261	NAD	C5D-C4D-C3D	2.14	123.72	115.21
2	B	261	NAD	C2D-C3D-C4D	2.15	107.04	102.61
2	B	261	NAD	O2A-PA-O3	2.15	114.86	105.09
2	A	261	NAD	O4B-C4B-C3B	2.18	109.55	105.15
3	F	262	09T	C14-C13-N12	2.19	136.84	130.77
2	G	261	NAD	C3N-C7N-N7N	2.20	120.23	117.82
3	J	262	09T	C9-N10-C11	2.22	128.31	125.67
2	E	261	NAD	C3N-C7N-N7N	2.24	120.27	117.82
2	K	261	NAD	O3B-C3B-C4B	2.27	117.85	111.05
2	H	261	NAD	O2A-PA-O3	2.28	115.45	105.09
2	K	261	NAD	O2D-C2D-C3D	2.30	119.29	111.83
2	C	261	NAD	C2D-C3D-C4D	2.33	107.40	102.61
2	C	261	NAD	O2D-C2D-C3D	2.33	119.40	111.83
3	C	262	09T	C9-N10-C11	2.33	128.45	125.67
2	E	261	NAD	C5D-C4D-C3D	2.33	124.47	115.21
2	C	261	NAD	O2A-PA-O3	2.34	115.72	105.09
3	F	262	09T	C4-C5-C6	2.35	122.02	118.55
2	B	261	NAD	O2N-PN-O3	2.37	115.85	105.09
2	P	261	NAD	O5B-PA-O1A	2.38	118.86	109.62
2	I	261	NAD	O2D-C2D-C3D	2.39	119.58	111.83
2	E	261	NAD	C2A-N1A-C6A	2.39	123.03	118.77
3	P	262	09T	C3-C2-CL1	2.40	123.35	118.39
2	I	261	NAD	O2N-PN-O1N	2.40	125.55	112.53
2	J	261	NAD	O7N-C7N-C3N	2.41	122.21	119.59
2	G	261	NAD	C2D-C3D-C4D	2.42	107.59	102.61
3	B	262	09T	C3-C2-CL1	2.43	123.42	118.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	261	NAD	C2N-C3N-C4N	2.44	121.00	118.29
2	L	261	NAD	C2D-C3D-C4D	2.45	107.64	102.61
2	C	261	NAD	O4B-C4B-C5B	2.46	118.11	109.32
3	C	262	09T	C3-C2-CL1	2.46	123.47	118.39
2	G	261	NAD	C5N-C4N-C3N	2.51	123.49	120.33
2	O	261	NAD	N6A-C6A-N1A	2.52	124.61	119.20
2	J	261	NAD	O2N-PN-O3	2.53	116.58	105.09
2	N	261	NAD	O4D-C1D-N1N	2.55	110.94	108.13
2	C	261	NAD	O3-PN-O5D	2.56	109.74	102.94
2	G	261	NAD	C2A-N1A-C6A	2.59	123.40	118.77
2	K	261	NAD	C4D-O4D-C1D	2.60	112.57	109.72
2	P	261	NAD	O2N-PN-O1N	2.60	126.62	112.53
3	D	262	09T	C9-N10-C11	2.62	128.79	125.67
3	I	262	09T	C3-C2-CL1	2.62	123.81	118.39
2	A	261	NAD	C2N-C3N-C4N	2.64	121.23	118.29
2	C	261	NAD	C2N-C3N-C4N	2.65	121.24	118.29
2	P	261	NAD	O2D-C2D-C3D	2.67	120.52	111.83
2	M	261	NAD	C2A-N1A-C6A	2.68	123.56	118.77
2	E	261	NAD	C5N-C4N-C3N	2.70	123.72	120.33
2	N	261	NAD	O2A-PA-O3	2.70	117.35	105.09
3	L	262	09T	C3-C2-CL1	2.71	124.00	118.39
2	J	261	NAD	C6N-C5N-C4N	2.72	123.56	119.44
2	I	261	NAD	O2A-PA-O3	2.74	117.54	105.09
2	K	261	NAD	O4B-C4B-C3B	2.75	110.68	105.15
2	D	261	NAD	C6N-C5N-C4N	2.76	123.61	119.44
2	H	261	NAD	C2B-C3B-C4B	2.79	108.36	102.61
2	L	261	NAD	O4B-C1B-N9A	2.80	113.96	108.10
2	P	261	NAD	O4B-C1B-N9A	2.82	114.00	108.10
2	H	261	NAD	C5N-C4N-C3N	2.82	123.89	120.33
2	L	261	NAD	C4A-C5A-N7A	2.85	112.10	109.48
2	P	261	NAD	C5D-C4D-C3D	2.87	126.59	115.21
2	H	261	NAD	C4A-C5A-N7A	2.88	112.12	109.48
2	L	261	NAD	C5D-C4D-C3D	2.88	126.66	115.21
2	J	261	NAD	C5D-C4D-C3D	2.91	126.75	115.21
2	F	261	NAD	C5D-C4D-C3D	2.91	126.75	115.21
2	E	261	NAD	O7N-C7N-C3N	2.91	122.76	119.59
3	I	262	09T	C6-C7-C2	2.91	124.60	120.25
2	D	261	NAD	O4D-C1D-N1N	2.91	111.33	108.13
2	P	261	NAD	O2A-PA-O3	2.98	118.63	105.09
3	I	262	09T	C4-C5-C6	3.04	123.05	118.55
2	I	261	NAD	C4A-C5A-N7A	3.06	112.29	109.48
2	K	261	NAD	O2A-PA-O3	3.09	119.12	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	261	NAD	O4D-C1D-N1N	3.11	111.55	108.13
2	H	261	NAD	O3-PN-O5D	3.11	111.20	102.94
2	L	261	NAD	O2A-PA-O1A	3.12	129.42	112.53
2	K	261	NAD	C4A-C5A-N7A	3.16	112.39	109.48
2	I	261	NAD	C4D-O4D-C1D	3.22	113.26	109.72
2	D	261	NAD	O2N-PN-O3	3.23	119.77	105.09
2	M	261	NAD	O4B-C1B-N9A	3.24	114.87	108.10
2	A	261	NAD	C3N-C7N-N7N	3.28	121.41	117.82
2	A	261	NAD	O2A-PA-O3	3.33	120.19	105.09
2	I	261	NAD	O4D-C1D-N1N	3.36	111.82	108.13
3	P	262	09T	C6-C7-CL8	3.36	123.68	118.50
3	G	262	09T	C7-C6-C5	3.45	122.59	120.36
2	B	261	NAD	O4D-C1D-N1N	3.66	112.15	108.13
3	D	262	09T	C4-C5-C6	3.70	124.02	118.55
2	P	261	NAD	O3-PN-O5D	3.78	112.97	102.94
2	J	261	NAD	C4A-C5A-N7A	3.79	112.96	109.48
2	D	261	NAD	C2A-N1A-C6A	3.82	125.59	118.77
2	J	261	NAD	C2A-N1A-C6A	3.82	125.60	118.77
2	D	261	NAD	O7N-C7N-C3N	3.88	123.82	119.59
2	P	261	NAD	C4A-C5A-N7A	3.94	113.11	109.48
2	C	261	NAD	C4A-C5A-N7A	3.96	113.12	109.48
2	N	261	NAD	C4A-C5A-N7A	3.97	113.13	109.48
3	F	262	09T	C9-N10-C11	3.99	130.42	125.67
3	K	262	09T	C4-C5-C6	3.99	124.45	118.55
2	F	261	NAD	C4A-C5A-N7A	4.07	113.22	109.48
2	P	261	NAD	C3N-C7N-N7N	4.08	122.28	117.82
2	F	261	NAD	O3-PN-O5D	4.12	113.86	102.94
2	F	261	NAD	C3N-C7N-N7N	4.16	122.37	117.82
2	C	261	NAD	C4D-O4D-C1D	4.17	114.30	109.72
2	C	261	NAD	O7N-C7N-C3N	4.19	124.16	119.59
2	A	261	NAD	C4A-C5A-N7A	4.20	113.35	109.48
2	F	261	NAD	C4D-O4D-C1D	4.29	114.43	109.72
3	P	262	09T	C9-N10-C11	4.36	130.87	125.67
2	G	261	NAD	O4B-C1B-N9A	4.37	117.24	108.10
2	E	261	NAD	O4B-C1B-N9A	4.37	117.25	108.10
2	N	261	NAD	O4B-C1B-N9A	4.39	117.29	108.10
2	M	261	NAD	C5N-C4N-C3N	4.43	125.90	120.33
2	N	261	NAD	O3-PN-O5D	4.43	114.68	102.94
2	O	261	NAD	C4D-O4D-C1D	4.46	114.62	109.72
3	J	262	09T	C4-C5-C6	4.46	125.15	118.55
2	D	261	NAD	C4A-C5A-N7A	4.49	113.61	109.48
2	H	261	NAD	C4D-O4D-C1D	4.73	114.92	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	261	NAD	C4A-C5A-N7A	4.76	113.86	109.48
2	H	261	NAD	C3N-C7N-N7N	4.77	123.04	117.82
3	C	262	09T	C4-C5-C6	4.78	125.62	118.55
2	P	261	NAD	C4D-O4D-C1D	5.03	115.25	109.72
2	E	261	NAD	C4A-C5A-N7A	5.05	114.12	109.48
2	P	261	NAD	O4D-C1D-N1N	5.09	113.72	108.13
2	N	261	NAD	C3N-C7N-N7N	5.10	123.40	117.82
2	N	261	NAD	C4D-O4D-C1D	5.21	115.44	109.72
2	L	261	NAD	O4D-C1D-N1N	5.29	113.94	108.13
2	O	261	NAD	O7N-C7N-C3N	5.65	125.76	119.59
2	C	261	NAD	O4D-C1D-N1N	5.70	114.40	108.13
2	G	261	NAD	C4A-C5A-N7A	5.95	114.95	109.48
2	K	261	NAD	C3N-C7N-N7N	6.21	124.61	117.82
2	O	261	NAD	C4A-C5A-N7A	7.54	116.42	109.48
2	K	261	NAD	O4D-C1D-N1N	9.24	118.28	108.13
2	A	261	NAD	O4D-C1D-N1N	11.07	120.30	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	261	NAD	2	0
3	A	262	09T	1	0
2	B	261	NAD	6	0
3	B	262	09T	7	0
2	C	261	NAD	1	0
3	C	262	09T	1	0
3	D	262	09T	2	0
2	E	261	NAD	6	0
3	E	262	09T	4	0
2	F	261	NAD	2	0
2	G	261	NAD	4	0
3	G	262	09T	3	0
2	H	261	NAD	3	0
2	I	261	NAD	2	0
3	I	262	09T	1	0
2	J	261	NAD	1	0
3	J	262	09T	2	0
2	K	261	NAD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	262	09T	1	0
2	L	261	NAD	3	0
3	L	262	09T	2	0
2	M	261	NAD	10	0
3	M	262	09T	12	0
2	N	261	NAD	3	0
3	N	262	09T	1	0
2	O	261	NAD	3	0
3	O	262	09T	5	0
2	P	261	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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	259/280 (92%)	0.10	8 (3%) 52 57	6, 15, 37, 72	0
1	B	257/280 (91%)	0.18	9 (3%) 48 53	4, 17, 44, 71	0
1	C	259/280 (92%)	0.08	7 (2%) 58 62	6, 15, 37, 96	0
1	D	256/280 (91%)	0.18	6 (2%) 64 67	6, 17, 45, 70	0
1	E	258/280 (92%)	1.24	59 (22%) 1 1	17, 38, 75, 98	0
1	F	259/280 (92%)	0.91	33 (12%) 5 5	17, 36, 63, 89	0
1	G	257/280 (91%)	1.21	55 (21%) 1 1	15, 40, 78, 97	0
1	H	259/280 (92%)	1.04	44 (16%) 2 2	17, 39, 70, 106	0
1	I	259/280 (92%)	0.07	7 (2%) 58 62	6, 15, 37, 88	0
1	J	257/280 (91%)	0.21	10 (3%) 43 48	5, 17, 45, 76	0
1	K	259/280 (92%)	0.08	6 (2%) 64 67	6, 15, 41, 60	0
1	L	257/280 (91%)	0.18	9 (3%) 48 53	5, 18, 47, 71	0
1	M	257/280 (91%)	1.22	56 (21%) 1 1	16, 39, 77, 110	0
1	N	259/280 (92%)	1.05	40 (15%) 3 3	17, 39, 70, 98	0
1	O	256/280 (91%)	1.25	58 (22%) 1 1	17, 39, 76, 99	0
1	P	259/280 (92%)	0.97	38 (14%) 3 3	14, 37, 66, 84	0
All	All	4127/4480 (92%)	0.62	445 (10%) 8 8	4, 27, 65, 110	0

All (445) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	217	LYS	6.7
1	N	42	GLN	6.1
1	O	106	CYS	5.9
1	E	42	GLN	5.7
1	H	42	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
1	G	100	GLU	5.4
1	O	41	GLY	5.4
1	N	179	GLU	5.2
1	C	42	GLN	5.2
1	O	42	GLN	5.2
1	G	42	GLN	5.2
1	M	198	SER	5.1
1	F	42	GLN	5.0
1	M	42	GLN	4.9
1	M	204	LYS	4.9
1	O	208	ASP	4.8
1	I	42	GLN	4.8
1	M	106	CYS	4.8
1	E	195	LEU	4.7
1	G	201	SER	4.6
1	E	41	GLY	4.6
1	G	200	ILE	4.6
1	G	106	CYS	4.5
1	P	42	GLN	4.4
1	O	195	LEU	4.4
1	E	217	LYS	4.4
1	L	198	SER	4.4
1	M	208	ASP	4.4
1	N	202	ASN	4.3
1	G	208	ASP	4.3
1	H	202	ASN	4.3
1	G	195	LEU	4.3
1	J	202	ASN	4.3
1	E	156	TYR	4.3
1	G	204	LYS	4.3
1	E	204	LYS	4.2
1	J	42	GLN	4.2
1	H	178	GLY	4.2
1	N	65	ILE	4.2
1	N	43	PHE	4.1
1	M	200	ILE	4.1
1	E	208	ASP	4.1
1	N	136	ASN	4.1
1	M	41	GLY	4.1
1	D	42	GLN	4.1
1	M	195	LEU	4.1
1	O	156	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	205	LYS	4.0
1	E	106	CYS	4.0
1	H	181	GLY	3.9
1	E	202	ASN	3.9
1	H	136	ASN	3.9
1	E	158	THR	3.9
1	O	100	GLU	3.8
1	H	43	PHE	3.8
1	E	209	TYR	3.7
1	G	198	SER	3.7
1	O	105	ASP	3.7
1	I	201	SER	3.7
1	E	196	ALA	3.6
1	O	202	ASN	3.6
1	G	156	TYR	3.6
1	A	201	SER	3.6
1	M	100	GLU	3.6
1	M	201	SER	3.6
1	E	203	PHE	3.6
1	E	161	VAL	3.6
1	F	6	GLY	3.6
1	P	6	GLY	3.6
1	J	198	SER	3.6
1	O	201	SER	3.5
1	J	257	GLY	3.5
1	O	204	LYS	3.5
1	O	219	ASN	3.5
1	B	42	GLN	3.5
1	L	42	GLN	3.5
1	H	75	VAL	3.4
1	G	101	GLY	3.4
1	P	136	ASN	3.4
1	N	199	GLY	3.4
1	H	82	ASP	3.4
1	E	219	ASN	3.4
1	A	42	GLN	3.4
1	E	220	VAL	3.4
1	E	201	SER	3.4
1	O	223	MET	3.4
1	E	105	ASP	3.3
1	E	159	MET	3.3
1	N	82	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	161	VAL	3.3
1	F	127	ALA	3.3
1	H	179	GLU	3.3
1	E	21	ALA	3.3
1	C	100	GLU	3.3
1	D	202	ASN	3.3
1	H	199	GLY	3.3
1	K	201	SER	3.3
1	D	198	SER	3.3
1	M	45	ASP	3.2
1	O	198	SER	3.2
1	N	38	THR	3.2
1	A	5	ALA	3.2
1	H	55	ASN	3.2
1	O	203	PHE	3.2
1	G	196	ALA	3.2
1	O	256	MET	3.2
1	F	136	ASN	3.2
1	O	196	ALA	3.2
1	O	212	MET	3.2
1	M	161	VAL	3.2
1	M	209	TYR	3.2
1	N	132	SER	3.2
1	K	136	ASN	3.1
1	O	110	GLU	3.1
1	O	190	GLY	3.1
1	O	200	ILE	3.1
1	C	201	SER	3.1
1	N	55	ASN	3.1
1	E	190	GLY	3.1
1	F	65	ILE	3.1
1	M	156	TYR	3.1
1	O	205	LYS	3.1
1	P	71	LYS	3.1
1	H	38	THR	3.1
1	G	27	ALA	3.1
1	F	180	ASP	3.1
1	O	159	MET	3.1
1	O	161	VAL	3.1
1	E	100	GLU	3.1
1	P	179	GLU	3.1
1	E	22	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	21	ALA	3.1
1	E	216	LEU	3.0
1	G	249	ALA	3.0
1	O	220	VAL	3.0
1	P	100	GLU	3.0
1	B	198	SER	3.0
1	N	178	GLY	3.0
1	G	45	ASP	3.0
1	G	110	GLU	3.0
1	E	96	ARG	3.0
1	N	75	VAL	3.0
1	E	32	GLY	3.0
1	H	182	ILE	3.0
1	P	127	ALA	3.0
1	E	43	PHE	3.0
1	E	200	ILE	3.0
1	M	202	ASN	3.0
1	P	55	ASN	3.0
1	H	132	SER	3.0
1	H	65	ILE	3.0
1	M	193	LYS	3.0
1	F	201	SER	2.9
1	M	205	LYS	2.9
1	P	61	PRO	2.9
1	G	41	GLY	2.9
1	F	58	ALA	2.9
1	G	202	ASN	2.9
1	E	110	GLU	2.9
1	E	198	SER	2.9
1	H	201	SER	2.9
1	J	100	GLU	2.9
1	G	146	TYR	2.9
1	I	100	GLU	2.9
1	E	45	ASP	2.9
1	P	80	VAL	2.9
1	F	177	LEU	2.9
1	D	100	GLU	2.9
1	O	209	TYR	2.9
1	O	32	GLY	2.9
1	M	196	ALA	2.9
1	M	11	ILE	2.9
1	N	201	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	5	ALA	2.9
1	F	100	GLU	2.8
1	O	193	LYS	2.8
1	M	101	GLY	2.8
1	M	212	MET	2.8
1	M	217	LYS	2.8
1	O	102	ASN	2.8
1	N	39	TYR	2.8
1	E	225	VAL	2.8
1	J	258	ASN	2.8
1	P	177	LEU	2.8
1	G	43	PHE	2.8
1	E	99	LEU	2.8
1	K	42	GLN	2.8
1	E	256	MET	2.8
1	M	107	VAL	2.8
1	M	158	THR	2.8
1	N	37	PHE	2.8
1	F	125	ALA	2.8
1	E	193	LYS	2.8
1	J	201	SER	2.8
1	H	68	GLN	2.7
1	P	199	GLY	2.7
1	E	212	MET	2.7
1	N	79	LYS	2.7
1	O	99	LEU	2.7
1	G	105	ASP	2.7
1	K	82	ASP	2.7
1	G	104	ILE	2.7
1	H	79	LYS	2.7
1	H	97	ASP	2.7
1	L	100	GLU	2.7
1	F	43	PHE	2.7
1	H	58	ALA	2.7
1	N	58	ALA	2.7
1	O	152	ALA	2.7
1	F	55	ASN	2.7
1	G	220	VAL	2.7
1	M	213	VAL	2.7
1	M	146	TYR	2.7
1	E	46	ARG	2.7
1	O	46	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	181	GLY	2.7
1	G	102	ASN	2.7
1	H	39	TYR	2.7
1	M	197	ALA	2.7
1	E	258	ASN	2.7
1	H	135	LYS	2.6
1	F	176	ALA	2.6
1	M	136	ASN	2.6
1	P	65	ILE	2.6
1	O	18	LYS	2.6
1	G	209	TYR	2.6
1	H	14	LEU	2.6
1	N	74	PHE	2.6
1	P	5	ALA	2.6
1	I	82	ASP	2.6
1	P	201	SER	2.6
1	G	191	PRO	2.6
1	N	97	ASP	2.6
1	P	180	ASP	2.6
1	C	82	ASP	2.6
1	I	41	GLY	2.6
1	O	97	ASP	2.6
1	P	132	SER	2.6
1	E	97	ASP	2.5
1	O	154	PRO	2.5
1	F	179	GLU	2.5
1	M	104	ILE	2.5
1	G	193	LYS	2.5
1	M	27	ALA	2.5
1	M	203	PHE	2.5
1	H	47	VAL	2.5
1	M	97	ASP	2.5
1	M	192	ILE	2.5
1	M	105	ASP	2.5
1	M	108	THR	2.5
1	E	103	PHE	2.5
1	N	68	GLN	2.5
1	G	223	MET	2.5
1	P	8	LYS	2.5
1	E	94	ALA	2.5
1	F	75	VAL	2.5
1	C	97	ASP	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	38	THR	2.5
1	N	52	ALA	2.5
1	M	110	GLU	2.5
1	M	112	PHE	2.5
1	O	103	PHE	2.5
1	P	43	PHE	2.5
1	E	40	VAL	2.5
1	N	80	VAL	2.5
1	M	223	MET	2.5
1	N	129	GLU	2.5
1	O	40	VAL	2.4
1	G	15	LEU	2.4
1	P	68	GLN	2.4
1	G	190	GLY	2.4
1	M	102	ASN	2.4
1	N	182	ILE	2.4
1	N	135	LYS	2.4
1	F	82	ASP	2.4
1	G	112	PHE	2.4
1	E	44	LYS	2.4
1	F	41	GLY	2.4
1	G	160	GLY	2.4
1	N	78	GLY	2.4
1	O	43	PHE	2.4
1	P	49	LYS	2.4
1	A	136	ASN	2.4
1	G	213	VAL	2.4
1	O	17	ASN	2.4
1	N	51	CYS	2.4
1	N	66	SER	2.4
1	O	45	ASP	2.4
1	E	223	MET	2.4
1	H	124	ALA	2.4
1	H	176	ALA	2.4
1	B	202	ASN	2.4
1	G	136	ASN	2.4
1	O	96	ARG	2.4
1	O	158	THR	2.4
1	P	26	LYS	2.4
1	O	249	ALA	2.4
1	E	49	LYS	2.4
1	N	18	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	20	ILE	2.4
1	O	104	ILE	2.4
1	H	36	ALA	2.4
1	H	143	ALA	2.4
1	E	95	PRO	2.3
1	F	8	LYS	2.3
1	O	93	PHE	2.3
1	A	82	ASP	2.3
1	P	82	ASP	2.3
1	H	80	VAL	2.3
1	O	216	LEU	2.3
1	L	202	ASN	2.3
1	M	96	ARG	2.3
1	B	43	PHE	2.3
1	M	43	PHE	2.3
1	O	22	TYR	2.3
1	P	62	CYS	2.3
1	F	132	SER	2.3
1	G	155	SER	2.3
1	A	202	ASN	2.3
1	M	46	ARG	2.3
1	P	2	GLY	2.3
1	C	99	LEU	2.3
1	E	51	CYS	2.3
1	P	53	GLU	2.3
1	F	68	GLN	2.3
1	N	181	GLY	2.3
1	H	46	ARG	2.3
1	G	216	LEU	2.3
1	D	45	ASP	2.3
1	J	199	GLY	2.3
1	N	41	GLY	2.3
1	N	143	ALA	2.3
1	N	177	LEU	2.3
1	N	258	ASN	2.3
1	B	40	VAL	2.3
1	E	65	ILE	2.2
1	B	82	ASP	2.2
1	L	82	ASP	2.2
1	M	190	GLY	2.2
1	P	50	LEU	2.2
1	P	75	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	105	ASP	2.2
1	G	203	PHE	2.2
1	L	195	LEU	2.2
1	O	225	VAL	2.2
1	H	127	ALA	2.2
1	I	136	ASN	2.2
1	G	96	ARG	2.2
1	F	71	LYS	2.2
1	G	217	LYS	2.2
1	H	184	VAL	2.2
1	F	181	GLY	2.2
1	P	77	LEU	2.2
1	E	162	ALA	2.2
1	G	51	CYS	2.2
1	K	202	ASN	2.2
1	O	116	HIS	2.2
1	G	11	ILE	2.2
1	M	257	GLY	2.2
1	O	20	ILE	2.2
1	O	65	ILE	2.2
1	K	258	ASN	2.2
1	H	57	ALA	2.2
1	H	140	SER	2.2
1	M	159	MET	2.2
1	H	74	PHE	2.2
1	E	102	ASN	2.2
1	L	105	ASP	2.2
1	F	198	SER	2.1
1	M	6	GLY	2.1
1	M	249	ALA	2.1
1	P	41	GLY	2.1
1	F	79	LYS	2.1
1	E	93	PHE	2.1
1	E	82	ASP	2.1
1	E	154	PRO	2.1
1	O	95	PRO	2.1
1	E	247	VAL	2.1
1	G	16	SER	2.1
1	M	160	GLY	2.1
1	G	197	ALA	2.1
1	J	65	ILE	2.1
1	M	93	PHE	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	183	LYS	2.1
1	O	44	LYS	2.1
1	P	198	SER	2.1
1	E	52	ALA	2.1
1	C	136	ASN	2.1
1	G	207	LEU	2.1
1	M	15	LEU	2.1
1	N	73	LEU	2.1
1	P	73	LEU	2.1
1	P	99	LEU	2.1
1	G	6	GLY	2.1
1	M	16	SER	2.1
1	E	152	ALA	2.1
1	H	100	GLU	2.1
1	F	128	LYS	2.1
1	G	219	ASN	2.1
1	F	61	PRO	2.1
1	A	100	GLU	2.1
1	B	100	GLU	2.1
1	H	61	PRO	2.1
1	N	32	GLY	2.1
1	O	191	PRO	2.1
1	D	201	SER	2.1
1	O	151	LYS	2.1
1	M	220	VAL	2.1
1	M	51	CYS	2.1
1	N	46	ARG	2.1
1	F	240	ILE	2.1
1	F	178	GLY	2.1
1	G	116	HIS	2.1
1	M	49	LYS	2.1
1	G	82	ASP	2.1
1	N	180	ASP	2.1
1	B	96	ARG	2.0
1	L	96	ARG	2.0
1	M	21	ALA	2.0
1	O	162	ALA	2.0
1	P	202	ASN	2.0
1	L	40	VAL	2.0
1	G	257	GLY	2.0
1	H	49	LYS	2.0
1	H	105	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	157	ASN	2.0
1	G	205	LYS	2.0
1	E	88	VAL	2.0
1	H	41	GLY	2.0
1	G	97	ASP	2.0
1	G	251	TYR	2.0
1	F	74	PHE	2.0
1	H	66	SER	2.0
1	P	197	ALA	2.0
1	F	2	GLY	2.0
1	G	2	GLY	2.0
1	I	6	GLY	2.0
1	G	114	ILE	2.0
1	H	129	GLU	2.0
1	J	200	ILE	2.0
1	N	105	ASP	2.0
1	H	73	LEU	2.0
1	P	84	LEU	2.0
1	A	204	LYS	2.0
1	F	39	TYR	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	09T	B	262	20/20	0.86	0.23	2.16	39,44,61,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	09T	L	262	20/20	0.85	0.23	1.81	35,39,58,79	0
3	09T	A	262	20/20	0.86	0.21	1.73	20,23,35,54	0
3	09T	K	262	20/20	0.89	0.19	1.33	17,21,38,61	0
3	09T	H	262	20/20	0.86	0.23	0.85	39,54,68,87	0
3	09T	N	262	20/20	0.87	0.23	0.78	36,47,72,94	0
3	09T	D	262	20/20	0.90	0.20	0.68	25,30,48,91	0
3	09T	J	262	20/20	0.89	0.20	0.58	22,28,52,94	0
3	09T	G	262	20/20	0.80	0.30	0.38	42,48,94,98	0
3	09T	M	262	20/20	0.81	0.29	0.21	43,51,103,139	0
3	09T	F	262	20/20	0.89	0.19	0.13	18,20,47,66	0
3	09T	C	262	20/20	0.93	0.16	0.06	10,12,26,49	0
3	09T	I	262	20/20	0.94	0.15	0.02	11,12,27,53	0
3	09T	P	262	20/20	0.89	0.19	0.02	21,26,42,54	0
2	NAD	F	261	44/44	0.91	0.18	-0.34	14,23,68,73	3
2	NAD	N	261	44/44	0.92	0.17	-0.36	22,34,75,77	0
2	NAD	H	261	44/44	0.92	0.17	-0.45	24,37,81,84	0
2	NAD	P	261	44/44	0.92	0.17	-0.46	19,29,70,76	0
2	NAD	B	261	44/44	0.93	0.14	-0.70	15,18,24,25	0
3	09T	O	262	20/20	0.79	0.24	-0.74	37,41,58,74	0
2	NAD	L	261	44/44	0.94	0.13	-0.75	14,18,20,21	0
2	NAD	A	261	44/44	0.96	0.12	-0.84	4,7,15,15	0
2	NAD	E	261	44/44	0.87	0.20	-0.88	30,40,52,55	0
2	NAD	G	261	44/44	0.86	0.20	-0.88	23,42,66,75	0
2	NAD	J	261	44/44	0.95	0.12	-0.90	10,13,16,20	0
2	NAD	K	261	44/44	0.95	0.12	-0.94	5,7,17,17	0
2	NAD	D	261	44/44	0.95	0.12	-1.07	12,14,18,22	0
3	09T	E	262	20/20	0.84	0.21	-1.24	33,37,58,71	0
2	NAD	C	261	44/44	0.96	0.11	-1.32	5,8,23,24	0
2	NAD	O	261	44/44	0.90	0.18	-1.36	25,34,51,57	0
2	NAD	I	261	44/44	0.97	0.11	-1.39	5,8,22,23	0
2	NAD	M	261	44/44	0.89	0.17	-1.50	24,40,52,58	0

## 6.5 Other polymers

There are no such residues in this entry.