



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2017 – 07:26 PM EDT

PDB ID : 5IFL
Title : Crystal structure of B. pseudomallei FabI in complex with NAD and triclosan
Authors : Hirschbeck, M.W.; Eltschkner, S.; Tonge, P.J.; Kisker, C.
Deposited on : unknown
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

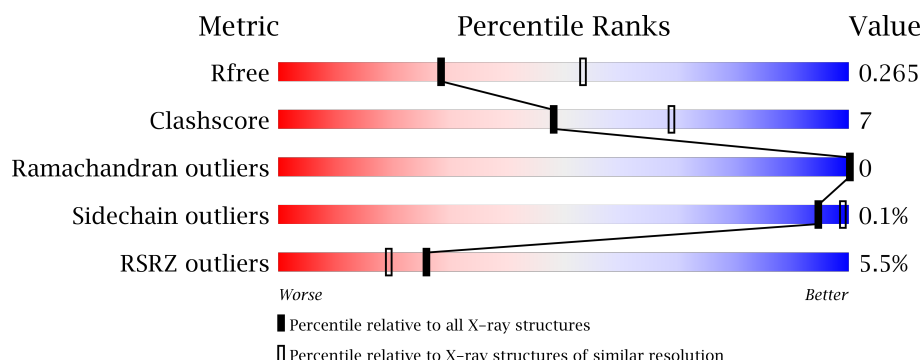
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	276	
1	B	276	
1	C	276	
1	D	276	
1	E	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	276	
1	G	276	
1	H	276	
1	I	276	
1	J	276	
1	K	276	
1	L	276	
1	M	276	
1	N	276	
1	O	276	
1	P	276	

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
2	TCL	K	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32377 atoms, of which 432 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	B	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	A	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	C	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	D	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	E	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	F	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	G	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	H	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	I	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	J	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	K	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	L	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	M	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	N	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	O	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0
1	P	255	Total 1900	C 1211	N 323	O 361	S 5	0	0	0

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	LYS	-	expression tag	UNP A0A069B9A4
B	265	LEU	-	expression tag	UNP A0A069B9A4
B	266	ALA	-	expression tag	UNP A0A069B9A4
B	267	ALA	-	expression tag	UNP A0A069B9A4
B	268	ALA	-	expression tag	UNP A0A069B9A4
B	269	LEU	-	expression tag	UNP A0A069B9A4
B	270	GLU	-	expression tag	UNP A0A069B9A4
B	271	HIS	-	expression tag	UNP A0A069B9A4
B	272	HIS	-	expression tag	UNP A0A069B9A4
B	273	HIS	-	expression tag	UNP A0A069B9A4
B	274	HIS	-	expression tag	UNP A0A069B9A4
B	275	HIS	-	expression tag	UNP A0A069B9A4
B	276	HIS	-	expression tag	UNP A0A069B9A4
A	264	LYS	-	expression tag	UNP A0A069B9A4
A	265	LEU	-	expression tag	UNP A0A069B9A4
A	266	ALA	-	expression tag	UNP A0A069B9A4
A	267	ALA	-	expression tag	UNP A0A069B9A4
A	268	ALA	-	expression tag	UNP A0A069B9A4
A	269	LEU	-	expression tag	UNP A0A069B9A4
A	270	GLU	-	expression tag	UNP A0A069B9A4
A	271	HIS	-	expression tag	UNP A0A069B9A4
A	272	HIS	-	expression tag	UNP A0A069B9A4
A	273	HIS	-	expression tag	UNP A0A069B9A4
A	274	HIS	-	expression tag	UNP A0A069B9A4
A	275	HIS	-	expression tag	UNP A0A069B9A4
A	276	HIS	-	expression tag	UNP A0A069B9A4
C	264	LYS	-	expression tag	UNP A0A069B9A4
C	265	LEU	-	expression tag	UNP A0A069B9A4
C	266	ALA	-	expression tag	UNP A0A069B9A4
C	267	ALA	-	expression tag	UNP A0A069B9A4
C	268	ALA	-	expression tag	UNP A0A069B9A4
C	269	LEU	-	expression tag	UNP A0A069B9A4
C	270	GLU	-	expression tag	UNP A0A069B9A4
C	271	HIS	-	expression tag	UNP A0A069B9A4
C	272	HIS	-	expression tag	UNP A0A069B9A4
C	273	HIS	-	expression tag	UNP A0A069B9A4
C	274	HIS	-	expression tag	UNP A0A069B9A4
C	275	HIS	-	expression tag	UNP A0A069B9A4
C	276	HIS	-	expression tag	UNP A0A069B9A4
D	264	LYS	-	expression tag	UNP A0A069B9A4
D	265	LEU	-	expression tag	UNP A0A069B9A4
D	266	ALA	-	expression tag	UNP A0A069B9A4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	267	ALA	-	expression tag	UNP A0A069B9A4
D	268	ALA	-	expression tag	UNP A0A069B9A4
D	269	LEU	-	expression tag	UNP A0A069B9A4
D	270	GLU	-	expression tag	UNP A0A069B9A4
D	271	HIS	-	expression tag	UNP A0A069B9A4
D	272	HIS	-	expression tag	UNP A0A069B9A4
D	273	HIS	-	expression tag	UNP A0A069B9A4
D	274	HIS	-	expression tag	UNP A0A069B9A4
D	275	HIS	-	expression tag	UNP A0A069B9A4
D	276	HIS	-	expression tag	UNP A0A069B9A4
E	264	LYS	-	expression tag	UNP A0A069B9A4
E	265	LEU	-	expression tag	UNP A0A069B9A4
E	266	ALA	-	expression tag	UNP A0A069B9A4
E	267	ALA	-	expression tag	UNP A0A069B9A4
E	268	ALA	-	expression tag	UNP A0A069B9A4
E	269	LEU	-	expression tag	UNP A0A069B9A4
E	270	GLU	-	expression tag	UNP A0A069B9A4
E	271	HIS	-	expression tag	UNP A0A069B9A4
E	272	HIS	-	expression tag	UNP A0A069B9A4
E	273	HIS	-	expression tag	UNP A0A069B9A4
E	274	HIS	-	expression tag	UNP A0A069B9A4
E	275	HIS	-	expression tag	UNP A0A069B9A4
E	276	HIS	-	expression tag	UNP A0A069B9A4
F	264	LYS	-	expression tag	UNP A0A069B9A4
F	265	LEU	-	expression tag	UNP A0A069B9A4
F	266	ALA	-	expression tag	UNP A0A069B9A4
F	267	ALA	-	expression tag	UNP A0A069B9A4
F	268	ALA	-	expression tag	UNP A0A069B9A4
F	269	LEU	-	expression tag	UNP A0A069B9A4
F	270	GLU	-	expression tag	UNP A0A069B9A4
F	271	HIS	-	expression tag	UNP A0A069B9A4
F	272	HIS	-	expression tag	UNP A0A069B9A4
F	273	HIS	-	expression tag	UNP A0A069B9A4
F	274	HIS	-	expression tag	UNP A0A069B9A4
F	275	HIS	-	expression tag	UNP A0A069B9A4
F	276	HIS	-	expression tag	UNP A0A069B9A4
G	264	LYS	-	expression tag	UNP A0A069B9A4
G	265	LEU	-	expression tag	UNP A0A069B9A4
G	266	ALA	-	expression tag	UNP A0A069B9A4
G	267	ALA	-	expression tag	UNP A0A069B9A4
G	268	ALA	-	expression tag	UNP A0A069B9A4
G	269	LEU	-	expression tag	UNP A0A069B9A4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	270	GLU	-	expression tag	UNP A0A069B9A4
G	271	HIS	-	expression tag	UNP A0A069B9A4
G	272	HIS	-	expression tag	UNP A0A069B9A4
G	273	HIS	-	expression tag	UNP A0A069B9A4
G	274	HIS	-	expression tag	UNP A0A069B9A4
G	275	HIS	-	expression tag	UNP A0A069B9A4
G	276	HIS	-	expression tag	UNP A0A069B9A4
H	264	LYS	-	expression tag	UNP A0A069B9A4
H	265	LEU	-	expression tag	UNP A0A069B9A4
H	266	ALA	-	expression tag	UNP A0A069B9A4
H	267	ALA	-	expression tag	UNP A0A069B9A4
H	268	ALA	-	expression tag	UNP A0A069B9A4
H	269	LEU	-	expression tag	UNP A0A069B9A4
H	270	GLU	-	expression tag	UNP A0A069B9A4
H	271	HIS	-	expression tag	UNP A0A069B9A4
H	272	HIS	-	expression tag	UNP A0A069B9A4
H	273	HIS	-	expression tag	UNP A0A069B9A4
H	274	HIS	-	expression tag	UNP A0A069B9A4
H	275	HIS	-	expression tag	UNP A0A069B9A4
H	276	HIS	-	expression tag	UNP A0A069B9A4
I	264	LYS	-	expression tag	UNP A0A069B9A4
I	265	LEU	-	expression tag	UNP A0A069B9A4
I	266	ALA	-	expression tag	UNP A0A069B9A4
I	267	ALA	-	expression tag	UNP A0A069B9A4
I	268	ALA	-	expression tag	UNP A0A069B9A4
I	269	LEU	-	expression tag	UNP A0A069B9A4
I	270	GLU	-	expression tag	UNP A0A069B9A4
I	271	HIS	-	expression tag	UNP A0A069B9A4
I	272	HIS	-	expression tag	UNP A0A069B9A4
I	273	HIS	-	expression tag	UNP A0A069B9A4
I	274	HIS	-	expression tag	UNP A0A069B9A4
I	275	HIS	-	expression tag	UNP A0A069B9A4
I	276	HIS	-	expression tag	UNP A0A069B9A4
J	264	LYS	-	expression tag	UNP A0A069B9A4
J	265	LEU	-	expression tag	UNP A0A069B9A4
J	266	ALA	-	expression tag	UNP A0A069B9A4
J	267	ALA	-	expression tag	UNP A0A069B9A4
J	268	ALA	-	expression tag	UNP A0A069B9A4
J	269	LEU	-	expression tag	UNP A0A069B9A4
J	270	GLU	-	expression tag	UNP A0A069B9A4
J	271	HIS	-	expression tag	UNP A0A069B9A4
J	272	HIS	-	expression tag	UNP A0A069B9A4

Continued on next page...

Continued from previous page...

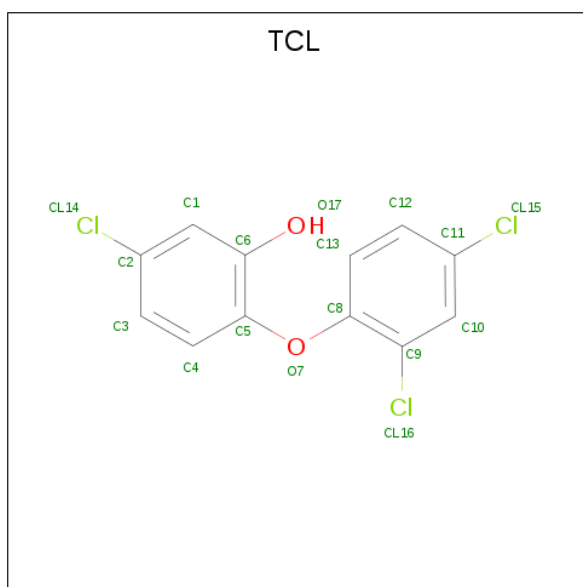
Chain	Residue	Modelled	Actual	Comment	Reference
J	273	HIS	-	expression tag	UNP A0A069B9A4
J	274	HIS	-	expression tag	UNP A0A069B9A4
J	275	HIS	-	expression tag	UNP A0A069B9A4
J	276	HIS	-	expression tag	UNP A0A069B9A4
K	264	LYS	-	expression tag	UNP A0A069B9A4
K	265	LEU	-	expression tag	UNP A0A069B9A4
K	266	ALA	-	expression tag	UNP A0A069B9A4
K	267	ALA	-	expression tag	UNP A0A069B9A4
K	268	ALA	-	expression tag	UNP A0A069B9A4
K	269	LEU	-	expression tag	UNP A0A069B9A4
K	270	GLU	-	expression tag	UNP A0A069B9A4
K	271	HIS	-	expression tag	UNP A0A069B9A4
K	272	HIS	-	expression tag	UNP A0A069B9A4
K	273	HIS	-	expression tag	UNP A0A069B9A4
K	274	HIS	-	expression tag	UNP A0A069B9A4
K	275	HIS	-	expression tag	UNP A0A069B9A4
K	276	HIS	-	expression tag	UNP A0A069B9A4
L	264	LYS	-	expression tag	UNP A0A069B9A4
L	265	LEU	-	expression tag	UNP A0A069B9A4
L	266	ALA	-	expression tag	UNP A0A069B9A4
L	267	ALA	-	expression tag	UNP A0A069B9A4
L	268	ALA	-	expression tag	UNP A0A069B9A4
L	269	LEU	-	expression tag	UNP A0A069B9A4
L	270	GLU	-	expression tag	UNP A0A069B9A4
L	271	HIS	-	expression tag	UNP A0A069B9A4
L	272	HIS	-	expression tag	UNP A0A069B9A4
L	273	HIS	-	expression tag	UNP A0A069B9A4
L	274	HIS	-	expression tag	UNP A0A069B9A4
L	275	HIS	-	expression tag	UNP A0A069B9A4
L	276	HIS	-	expression tag	UNP A0A069B9A4
M	264	LYS	-	expression tag	UNP A0A069B9A4
M	265	LEU	-	expression tag	UNP A0A069B9A4
M	266	ALA	-	expression tag	UNP A0A069B9A4
M	267	ALA	-	expression tag	UNP A0A069B9A4
M	268	ALA	-	expression tag	UNP A0A069B9A4
M	269	LEU	-	expression tag	UNP A0A069B9A4
M	270	GLU	-	expression tag	UNP A0A069B9A4
M	271	HIS	-	expression tag	UNP A0A069B9A4
M	272	HIS	-	expression tag	UNP A0A069B9A4
M	273	HIS	-	expression tag	UNP A0A069B9A4
M	274	HIS	-	expression tag	UNP A0A069B9A4
M	275	HIS	-	expression tag	UNP A0A069B9A4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	276	HIS	-	expression tag	UNP A0A069B9A4
N	264	LYS	-	expression tag	UNP A0A069B9A4
N	265	LEU	-	expression tag	UNP A0A069B9A4
N	266	ALA	-	expression tag	UNP A0A069B9A4
N	267	ALA	-	expression tag	UNP A0A069B9A4
N	268	ALA	-	expression tag	UNP A0A069B9A4
N	269	LEU	-	expression tag	UNP A0A069B9A4
N	270	GLU	-	expression tag	UNP A0A069B9A4
N	271	HIS	-	expression tag	UNP A0A069B9A4
N	272	HIS	-	expression tag	UNP A0A069B9A4
N	273	HIS	-	expression tag	UNP A0A069B9A4
N	274	HIS	-	expression tag	UNP A0A069B9A4
N	275	HIS	-	expression tag	UNP A0A069B9A4
N	276	HIS	-	expression tag	UNP A0A069B9A4
O	264	LYS	-	expression tag	UNP A0A069B9A4
O	265	LEU	-	expression tag	UNP A0A069B9A4
O	266	ALA	-	expression tag	UNP A0A069B9A4
O	267	ALA	-	expression tag	UNP A0A069B9A4
O	268	ALA	-	expression tag	UNP A0A069B9A4
O	269	LEU	-	expression tag	UNP A0A069B9A4
O	270	GLU	-	expression tag	UNP A0A069B9A4
O	271	HIS	-	expression tag	UNP A0A069B9A4
O	272	HIS	-	expression tag	UNP A0A069B9A4
O	273	HIS	-	expression tag	UNP A0A069B9A4
O	274	HIS	-	expression tag	UNP A0A069B9A4
O	275	HIS	-	expression tag	UNP A0A069B9A4
O	276	HIS	-	expression tag	UNP A0A069B9A4
P	264	LYS	-	expression tag	UNP A0A069B9A4
P	265	LEU	-	expression tag	UNP A0A069B9A4
P	266	ALA	-	expression tag	UNP A0A069B9A4
P	267	ALA	-	expression tag	UNP A0A069B9A4
P	268	ALA	-	expression tag	UNP A0A069B9A4
P	269	LEU	-	expression tag	UNP A0A069B9A4
P	270	GLU	-	expression tag	UNP A0A069B9A4
P	271	HIS	-	expression tag	UNP A0A069B9A4
P	272	HIS	-	expression tag	UNP A0A069B9A4
P	273	HIS	-	expression tag	UNP A0A069B9A4
P	274	HIS	-	expression tag	UNP A0A069B9A4
P	275	HIS	-	expression tag	UNP A0A069B9A4
P	276	HIS	-	expression tag	UNP A0A069B9A4

- Molecule 2 is TRICLOSAN (three-letter code: TCL) (formula: C₁₂H₇Cl₃O₂).



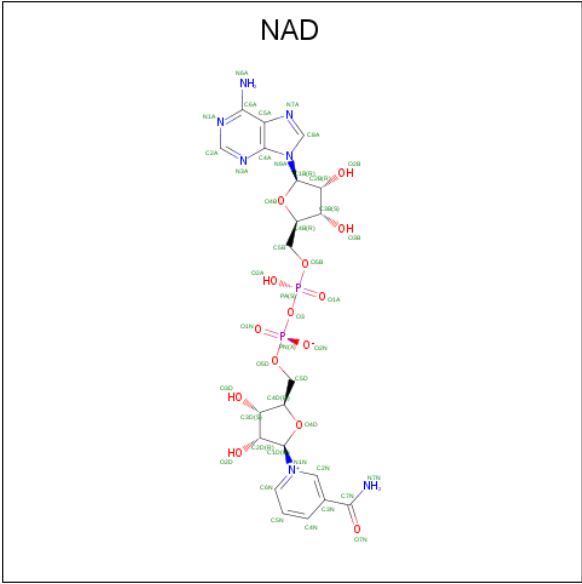
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	D	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	E	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	F	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	G	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	H	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	I	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	J	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	K	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	L	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	M	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	N	1	Total	C	Cl	O	0	0
			17	12	3	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	A	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	C	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	D	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	E	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	F	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	G	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	H	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	I	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	J	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	K	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	L	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	M	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	N	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	O	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
3	P	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	60	Total	O	0	0
			60	60		
4	A	44	Total	O	0	0
			44	44		
4	C	35	Total	O	0	0
			35	35		
4	D	45	Total	O	0	0
			45	45		
4	E	47	Total	O	0	0
			47	47		
4	F	28	Total	O	0	0
			28	28		
4	G	36	Total	O	0	0
			36	36		
4	H	23	Total	O	0	0
			23	23		
4	I	36	Total	O	0	0
			36	36		
4	J	29	Total	O	0	0
			29	29		
4	K	46	Total	O	0	0
			46	46		
4	L	29	Total	O	0	0
			29	29		

Continued on next page...

Continued from previous page...


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	21	Total 21	O 21	0	0
4	N	26	Total 26	O 26	0	0
4	O	39	Total 39	O 39	0	0
4	P	25	Total 25	O 25	0	0

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



MET
ALA
GLY
LEU
GLU
GLU
LYS
LEU
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS


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

Chain E:  82% 10% 8%

MET G2 R18 T38 R43 F51 E54 F61 F75 K79 W82 L88 F124 P125 A131 L132 P133 L141 P154 N155 L177 V182 L195 P215 N219 F231 V240 M245 S249 G256 GLY MET ALA GLY LEU GLU

GLU
LYS
LEU
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS


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

Chain F:  2% 80% 12% 8%

MET G2 R8 L15 R18 E34 T38 D42 K45 D46 E50 F61 F75 K79 W82 D83 L88 R97 G102 D103 F104 L105 L108 F124 P125 A131 L132 P133 L141 P154 N155 I192 K193 T194 L195 I200 I206

P215 R218 V240 M245 S249 G256 GLY MET ALA GLY LEU GLU GLU LYS ALA LEU ALA ALA LEU GLU HIS HIS HIS HIS HIS


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

Chain G:  0% 81% 12% 8%

MET G2 F3 S16 N17 R18 R30 R43 F51 E54 V65 F75 K79 W82 L88 R114 P124 P125 A131 L132 P133 D137 L141 P154 N155 L177 V182 K193 T194 L195 I200 P215 L216 V240 M245 S249

G256 GLY MET ALA GLY LEU GLU GLU LYS LEU ALA ALA ALA GLU HIS HIS HIS HIS HIS


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

Chain H:  2% 80% 12% 8%

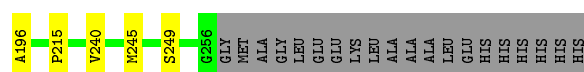
MET G2 L15 R18 V40 F51 E54 V65 F75 K79 W82 L88 R114 F124 P125 A131 L132 P133 H138 L139 L141 Y146 A149 P154 N155 K163 L177 V182 I187 K193 T194 L195 G199 I200 I201 P215

V240 M245 V247 P248 S249 G256 GLY MET ALA GLY LEU GLU GLU LYS LEU ALA ALA ALA GLU HIS HIS HIS HIS HIS

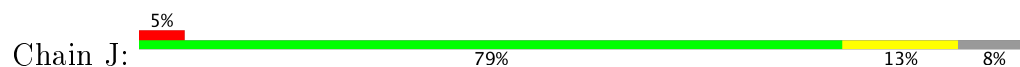
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain I:  3% 81% 12% 8%

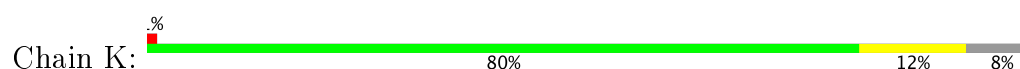
MET G2 L15 R18 S19 I20 V39 Y40 G41 D42 R43 F44 I48 T49 E50 F51 E54 L59 W60 V65 F75 K79 W82 L88 P86 R87 I115 F124 P125 A131 L132 P133 L141 P154 N155 L177 V182 I192 L195



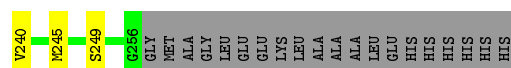
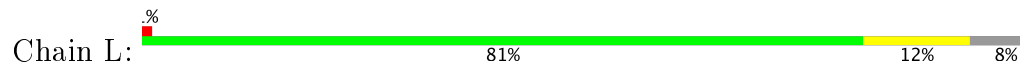
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



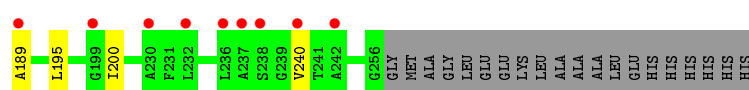
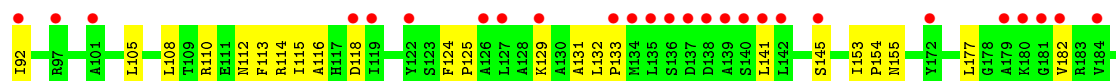
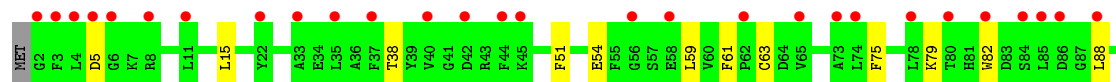
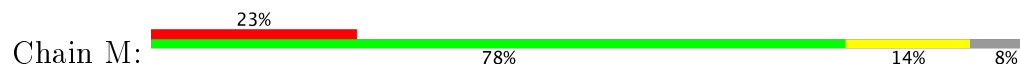
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- 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	Depositor
Cell constants a, b, c, α , β , γ	70.36 Å 99.92 Å 139.86 Å 82.87° 89.20° 78.13°	Depositor
Resolution (Å)	48.58 – 2.60 68.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.58-2.60) 94.5 (68.85-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.62 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.262 0.229 , 0.265	Depositor DCC
R_{free} test set	5630 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TCL, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/1933	0.40	0/2616
1	B	0.22	0/1933	0.40	0/2616
1	C	0.22	0/1933	0.40	0/2616
1	D	0.22	0/1933	0.40	0/2616
1	E	0.22	0/1933	0.40	0/2616
1	F	0.22	0/1933	0.40	0/2616
1	G	0.22	0/1933	0.41	0/2616
1	H	0.22	0/1933	0.42	0/2616
1	I	0.22	0/1933	0.40	0/2616
1	J	0.24	0/1933	0.43	1/2616 (0.0%)
1	K	0.22	0/1933	0.40	0/2616
1	L	0.22	0/1933	0.40	0/2616
1	M	0.22	0/1933	0.41	0/2616
1	N	0.23	0/1933	0.41	0/2616
1	O	0.22	0/1933	0.40	0/2616
1	P	0.22	0/1933	0.41	0/2616
All	All	0.22	0/30928	0.41	1/41856 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	18	ARG	NE-CZ-NH2	5.91	123.26	120.30

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	1900	0	1907	29	1
1	B	1900	0	1907	29	0
1	C	1900	0	1907	23	2
1	D	1900	0	1907	24	0
1	E	1900	0	1907	22	0
1	F	1900	0	1907	34	0
1	G	1900	0	1907	29	0
1	H	1900	0	1907	32	0
1	I	1900	0	1907	35	0
1	J	1900	0	1907	28	2
1	K	1900	0	1907	28	0
1	L	1900	0	1907	27	1
1	M	1900	0	1907	40	0
1	N	1900	0	1907	40	0
1	O	1900	0	1907	36	0
1	P	1900	0	1907	37	0
2	A	17	0	7	2	0
2	B	17	0	7	3	0
2	C	17	0	7	0	0
2	D	17	0	7	2	0
2	E	17	0	7	0	0
2	F	17	0	7	1	0
2	G	17	0	7	1	0
2	H	17	0	7	0	0
2	I	17	0	7	0	0
2	J	17	0	7	2	0
2	K	17	0	7	1	0
2	L	17	0	7	1	0
2	M	17	0	7	3	0
2	N	17	0	7	2	0
2	O	17	0	7	2	0
2	P	17	0	7	4	0
3	A	44	27	26	2	0
3	B	44	27	26	1	0
3	C	44	27	26	1	0
3	D	44	27	26	3	0
3	E	44	27	26	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	44	27	26	1	0
3	G	44	27	26	1	0
3	H	44	27	26	4	0
3	I	44	27	26	4	0
3	J	44	27	26	4	0
3	K	44	27	26	2	0
3	L	44	27	26	3	0
3	M	44	27	26	8	0
3	N	44	27	26	4	0
3	O	44	27	26	3	0
3	P	44	27	26	6	0
4	A	44	0	0	1	0
4	B	60	0	0	1	0
4	C	35	0	0	1	0
4	D	45	0	0	2	0
4	E	47	0	0	5	0
4	F	28	0	0	3	0
4	G	36	0	0	3	0
4	H	23	0	0	1	0
4	I	36	0	0	3	0
4	J	29	0	0	2	0
4	K	46	0	0	2	0
4	L	29	0	0	2	0
4	M	21	0	0	6	0
4	N	26	0	0	3	0
4	O	39	0	0	3	0
4	P	25	0	0	5	0
All	All	31945	432	31040	428	3

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 7.

All (428) 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:F:50:GLU:OE2	1:I:97:ARG:NH1	2.14	0.81
1:P:191:PRO:HA	3:P:302:NAD:O7N	1.80	0.80
1:M:15:LEU:HD23	1:M:195:LEU:HD22	1.63	0.80
1:P:18:ARG:NH1	1:P:193:LYS:O	2.15	0.79
1:B:200:ILE:HD11	2:B:301:TCL:H131	1.64	0.79
1:M:114:ARG:HG3	1:N:114:ARG:HG3	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:116:ALA:N	4:M:401:HOH:O	2.15	0.78
1:H:193:LYS:HZ1	1:P:69:ALA:HA	1.50	0.76
1:M:112:ASN:O	4:M:401:HOH:O	2.04	0.74
1:F:15:LEU:HD23	1:F:195:LEU:HD22	1.70	0.73
1:H:65:VAL:HG22	3:H:302:NAD:N1A	2.03	0.72
1:N:252:ASN:OD1	1:N:253:ALA:N	2.22	0.71
1:N:252:ASN:HA	4:N:415:HOH:O	1.91	0.71
1:P:95:ALA:N	2:P:301:TCL:CL15	2.61	0.70
1:L:205:LYS:NZ	4:L:401:HOH:O	2.19	0.70
1:F:103:ASP:OD2	4:F:401:HOH:O	2.10	0.70
1:E:240:VAL:HG21	1:H:245:MET:HE2	1.74	0.69
1:O:43:ARG:NH2	4:O:401:HOH:O	2.26	0.69
1:K:18:ARG:NH1	4:K:402:HOH:O	2.25	0.69
1:N:200:ILE:HD11	2:N:301:TCL:H131	1.75	0.68
1:L:88:LEU:HB3	1:L:141:LEU:HD22	1.75	0.68
1:P:189:ALA:HB3	3:P:302:NAD:C5N	2.24	0.68
1:F:88:LEU:HB3	1:F:141:LEU:HD22	1.77	0.67
1:B:97:ARG:NH1	1:F:218:ARG:HD2	2.09	0.67
1:B:88:LEU:HB3	1:B:141:LEU:HD22	1.77	0.67
1:G:18:ARG:NH1	1:G:194:THR:HA	2.08	0.67
1:D:88:LEU:HB3	1:D:141:LEU:HD22	1.77	0.66
1:P:251:PHE:O	1:P:254:VAL:HG22	1.96	0.66
1:J:88:LEU:HB3	1:J:141:LEU:HD22	1.77	0.65
1:P:65:VAL:N	4:P:401:HOH:O	2.29	0.65
1:H:75:PHE:CE1	1:H:131:ALA:HB2	2.32	0.65
1:I:75:PHE:CE1	1:I:131:ALA:HB2	2.32	0.65
1:K:88:LEU:HB3	1:K:141:LEU:HD22	1.79	0.64
1:K:200:ILE:HD11	2:K:301:TCL:H131	1.78	0.64
1:O:18:ARG:NH2	1:O:195:LEU:HD22	2.11	0.64
1:K:75:PHE:CE1	1:K:131:ALA:HB2	2.32	0.64
1:C:75:PHE:CE1	1:C:131:ALA:HB2	2.33	0.63
1:F:45:LYS:HZ3	1:I:115:ILE:HD12	1.61	0.63
1:I:132:LEU:HB3	1:I:133:PRO:HD3	1.80	0.63
1:B:97:ARG:HH11	1:F:218:ARG:HD2	1.63	0.63
1:J:75:PHE:CE1	1:J:131:ALA:HB2	2.34	0.63
1:D:18:ARG:HH22	1:D:195:LEU:HD13	1.63	0.63
1:K:132:LEU:HB3	1:K:133:PRO:HD3	1.81	0.63
1:P:194:THR:OG1	3:P:302:NAD:O1N	2.16	0.63
1:G:18:ARG:HH12	1:G:194:THR:HA	1.63	0.63
1:B:75:PHE:CE1	1:B:131:ALA:HB2	2.34	0.63
1:N:132:LEU:HB3	1:N:133:PRO:HD3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:75:PHE:CE1	1:N:131:ALA:HB2	2.34	0.63
3:D:302:NAD:O1N	3:D:302:NAD:N7N	2.28	0.62
1:M:75:PHE:CE1	1:M:131:ALA:HB2	2.34	0.62
1:D:132:LEU:HB3	1:D:133:PRO:HD3	1.82	0.62
1:I:88:LEU:HB3	1:I:141:LEU:HD22	1.80	0.62
1:A:79:LYS:HA	1:A:82:TRP:O	2.00	0.61
1:G:75:PHE:CE1	1:G:131:ALA:HB2	2.34	0.61
1:J:132:LEU:HB3	1:J:133:PRO:HD3	1.82	0.61
1:E:132:LEU:HB3	1:E:133:PRO:HD3	1.81	0.61
1:F:8:ARG:NE	1:F:34:GLU:OE1	2.28	0.61
1:G:65:VAL:HG22	3:G:302:NAD:N1A	2.16	0.61
1:D:75:PHE:CE1	1:D:131:ALA:HB2	2.35	0.61
1:F:192:ILE:N	3:F:302:NAD:O7N	2.34	0.61
1:M:15:LEU:CD2	1:M:195:LEU:HD22	2.31	0.61
1:O:15:LEU:HB2	3:O:302:NAD:O3B	2.01	0.61
1:F:15:LEU:CD2	1:F:195:LEU:HD22	2.30	0.60
1:K:65:VAL:HG22	3:K:302:NAD:N1A	2.17	0.60
1:M:132:LEU:HB3	1:M:133:PRO:HD3	1.83	0.60
1:A:75:PHE:CE1	1:A:131:ALA:HB2	2.35	0.60
1:E:75:PHE:CE1	1:E:131:ALA:HB2	2.37	0.60
1:H:132:LEU:HB3	1:H:133:PRO:HD3	1.83	0.60
1:C:132:LEU:HB3	1:C:133:PRO:HD3	1.83	0.60
1:A:245:MET:HE2	1:D:240:VAL:HG21	1.83	0.60
1:L:132:LEU:HB3	1:L:133:PRO:HD3	1.83	0.60
1:G:30:ARG:NH1	4:G:403:HOH:O	2.23	0.60
1:N:246:HIS:CG	1:N:252:ASN:ND2	2.70	0.60
1:A:245:MET:CE	1:D:240:VAL:HG21	2.32	0.59
1:G:88:LEU:HB3	1:G:141:LEU:HD22	1.83	0.59
1:P:132:LEU:HB3	1:P:133:PRO:HD3	1.83	0.59
1:B:195:LEU:HD12	1:G:137:ASP:OD2	2.02	0.59
1:D:15:LEU:HB2	3:D:302:NAD:O3B	2.02	0.59
3:E:302:NAD:O1A	4:E:401:HOH:O	2.16	0.59
1:M:115:ILE:O	1:M:118:ASP:HB3	2.02	0.59
1:M:59:LEU:HG	4:M:411:HOH:O	2.02	0.59
1:P:88:LEU:HB3	1:P:141:LEU:HD22	1.84	0.59
1:O:75:PHE:CE1	1:O:131:ALA:HB2	2.37	0.59
1:P:94:PHE:HA	2:P:301:TCL:H101	1.83	0.59
1:L:75:PHE:CE1	1:L:131:ALA:HB2	2.37	0.59
1:M:15:LEU:HD22	3:M:302:NAD:H51A	1.85	0.59
1:F:75:PHE:CE1	1:F:131:ALA:HB2	2.38	0.58
1:M:92:ILE:HG23	3:M:302:NAD:N3A	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:LEU:HB3	1:E:141:LEU:HD22	1.84	0.58
1:M:200:ILE:HD12	2:M:301:TCL:C3	2.34	0.58
1:F:79:LYS:HA	1:F:82:TRP:O	2.03	0.58
1:M:88:LEU:HB3	1:M:141:LEU:HD22	1.85	0.58
1:B:245:MET:CE	1:C:240:VAL:HG21	2.33	0.57
1:E:240:VAL:HG21	1:H:245:MET:CE	2.33	0.57
1:O:65:VAL:HG22	3:O:302:NAD:N1A	2.18	0.57
1:P:75:PHE:CE1	1:P:131:ALA:HB2	2.40	0.57
1:I:192:ILE:N	3:I:302:NAD:O7N	2.30	0.57
1:J:196:ALA:HB1	2:J:301:TCL:C9	2.35	0.57
1:A:132:LEU:HB3	1:A:133:PRO:HD3	1.86	0.57
1:A:200:ILE:HD11	2:A:301:TCL:H131	1.87	0.57
1:D:65:VAL:HG22	3:D:302:NAD:N1A	2.20	0.57
1:I:124:PHE:HB3	1:I:125:PRO:CD	2.35	0.56
1:O:18:ARG:NH1	1:O:194:THR:HA	2.20	0.56
1:L:205:LYS:NZ	4:L:402:HOH:O	2.32	0.56
1:O:132:LEU:HB3	1:O:133:PRO:HD3	1.87	0.56
1:G:18:ARG:HH12	1:G:194:THR:CA	2.17	0.56
1:J:124:PHE:HB3	1:J:125:PRO:CD	2.35	0.56
1:F:132:LEU:HB3	1:F:133:PRO:HD3	1.88	0.56
1:K:124:PHE:HB3	1:K:125:PRO:CD	2.35	0.56
1:M:92:ILE:HD13	3:M:302:NAD:H2A	1.86	0.56
1:C:88:LEU:HB3	1:C:141:LEU:HD22	1.86	0.56
1:B:132:LEU:HB3	1:B:133:PRO:HD3	1.87	0.56
1:N:88:LEU:HB3	1:N:141:LEU:HD22	1.86	0.56
1:A:240:VAL:HG21	1:D:245:MET:HE2	1.88	0.56
1:M:108:LEU:HD22	1:N:125:PRO:HB2	1.87	0.56
1:P:64:ASP:OD1	4:P:401:HOH:O	2.18	0.56
1:G:132:LEU:HB3	1:G:133:PRO:HD3	1.87	0.55
1:N:15:LEU:HD23	1:N:195:LEU:HD22	1.87	0.55
1:A:83:ASP:CG	1:I:195:LEU:HD21	2.26	0.55
1:A:124:PHE:HB3	1:A:125:PRO:CD	2.36	0.55
1:L:124:PHE:HB3	1:L:125:PRO:CD	2.36	0.55
1:N:13:GLY:HA2	3:N:302:NAD:O2B	2.06	0.55
1:H:79:LYS:HA	1:H:82:TRP:O	2.06	0.55
1:I:240:VAL:HG21	1:L:245:MET:HE2	1.87	0.55
1:P:124:PHE:HB3	1:P:125:PRO:CD	2.37	0.55
1:E:43:ARG:HG2	4:E:447:HOH:O	2.07	0.55
1:J:79:LYS:HA	1:J:82:TRP:O	2.07	0.54
1:P:246:HIS:CG	1:P:252:ASN:HD21	2.25	0.54
1:C:124:PHE:HB3	1:C:125:PRO:CD	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:OD2	1:I:195:LEU:HD21	2.07	0.54
1:N:124:PHE:HB3	1:N:125:PRO:CD	2.37	0.54
1:O:200:ILE:HD11	2:O:301:TCL:H131	1.88	0.54
1:O:88:LEU:HB3	1:O:141:LEU:HD22	1.88	0.54
1:F:240:VAL:HG21	1:G:245:MET:HE2	1.88	0.54
1:E:124:PHE:HB3	1:E:125:PRO:CD	2.38	0.54
1:O:124:PHE:HB3	1:O:125:PRO:CD	2.37	0.54
1:L:79:LYS:HA	1:L:82:TRP:O	2.06	0.54
1:G:79:LYS:HA	1:G:82:TRP:O	2.07	0.54
1:I:79:LYS:HA	1:I:82:TRP:O	2.08	0.54
1:K:124:PHE:HB3	1:K:125:PRO:HD3	1.90	0.54
1:K:79:LYS:HA	1:K:82:TRP:O	2.08	0.54
1:H:124:PHE:HB3	1:H:125:PRO:CD	2.37	0.54
1:N:79:LYS:HA	1:N:82:TRP:O	2.07	0.54
1:A:124:PHE:HB3	1:A:125:PRO:HD3	1.90	0.53
1:F:8:ARG:HG2	1:F:34:GLU:HB2	1.90	0.53
1:N:178:GLY:HA3	1:O:215:PRO:O	2.08	0.53
1:B:124:PHE:HB3	1:B:125:PRO:CD	2.38	0.53
1:C:124:PHE:HB3	1:C:125:PRO:HD3	1.91	0.53
1:I:124:PHE:HB3	1:I:125:PRO:HD3	1.89	0.53
1:N:75:PHE:CZ	1:N:131:ALA:HB2	2.43	0.53
1:N:218:ARG:NH2	1:O:238:SER:O	2.41	0.53
1:I:75:PHE:CZ	1:I:131:ALA:HB2	2.44	0.53
1:B:240:VAL:HG21	1:C:245:MET:HE2	1.90	0.53
1:G:124:PHE:HB3	1:G:125:PRO:CD	2.38	0.53
1:K:114:ARG:HG3	1:L:114:ARG:HG3	1.90	0.53
1:L:124:PHE:HB3	1:L:125:PRO:HD3	1.91	0.53
1:M:79:LYS:HA	1:M:82:TRP:O	2.08	0.52
1:J:124:PHE:HB3	1:J:125:PRO:HD3	1.92	0.52
1:P:70:GLN:O	4:P:402:HOH:O	2.19	0.52
1:D:124:PHE:HB3	1:D:125:PRO:CD	2.38	0.52
1:O:18:ARG:HH12	1:O:194:THR:HA	1.74	0.52
1:M:195:LEU:HB2	3:M:302:NAD:O1A	2.09	0.52
1:D:79:LYS:HA	1:D:82:TRP:O	2.10	0.52
1:C:79:LYS:HA	1:C:82:TRP:O	2.09	0.52
1:O:124:PHE:HB3	1:O:125:PRO:HD3	1.91	0.52
1:E:195:LEU:HD23	4:E:401:HOH:O	2.09	0.51
1:H:124:PHE:HB3	1:H:125:PRO:HD3	1.92	0.51
1:M:129:LYS:HB2	1:N:105:LEU:HD22	1.92	0.51
1:A:51:PHE:O	1:A:54:GLU:HB3	2.10	0.51
1:B:245:MET:HE2	1:C:240:VAL:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:PHE:O	4:D:401:HOH:O	2.18	0.51
1:E:124:PHE:HB3	1:E:125:PRO:HD3	1.92	0.51
1:N:124:PHE:HB3	1:N:125:PRO:HD3	1.92	0.51
1:N:47:ARG:HG3	4:N:410:HOH:O	2.10	0.51
1:C:75:PHE:CZ	1:C:131:ALA:HB2	2.46	0.51
1:P:124:PHE:HB3	1:P:125:PRO:HD3	1.91	0.51
1:F:124:PHE:HB3	1:F:125:PRO:CD	2.41	0.50
1:H:88:LEU:HB3	1:H:141:LEU:HD22	1.92	0.50
1:P:194:THR:HG21	3:P:302:NAD:O2N	2.11	0.50
1:M:108:LEU:CD2	1:N:125:PRO:HB2	2.42	0.50
1:N:64:ASP:HA	3:N:302:NAD:N1A	2.27	0.50
1:F:45:LYS:NZ	1:I:115:ILE:HD12	2.27	0.50
1:O:79:LYS:HA	1:O:82:TRP:O	2.10	0.50
1:B:124:PHE:HB3	1:B:125:PRO:HD3	1.93	0.50
1:B:79:LYS:HA	1:B:82:TRP:O	2.12	0.50
1:E:79:LYS:HA	1:E:82:TRP:O	2.10	0.50
1:M:124:PHE:HB3	1:M:125:PRO:CD	2.41	0.50
1:L:177:LEU:HB3	1:L:182:VAL:HB	1.94	0.50
1:J:75:PHE:CZ	1:J:131:ALA:HB2	2.47	0.50
1:N:246:HIS:CG	1:N:252:ASN:HD22	2.29	0.50
1:B:75:PHE:CZ	1:B:131:ALA:HB2	2.47	0.50
1:M:75:PHE:CZ	1:M:131:ALA:HB2	2.47	0.50
1:P:79:LYS:HA	1:P:82:TRP:O	2.11	0.50
1:B:65:VAL:HG22	3:B:302:NAD:N1A	2.28	0.49
1:M:92:ILE:HG12	3:M:302:NAD:HO2A	1.77	0.49
1:O:8:ARG:HB3	1:O:82:TRP:CZ3	2.47	0.49
1:H:75:PHE:CZ	1:H:131:ALA:HB2	2.47	0.49
1:K:75:PHE:CZ	1:K:131:ALA:HB2	2.48	0.49
1:L:51:PHE:O	1:L:54:GLU:HB3	2.12	0.49
1:C:65:VAL:HG22	3:C:302:NAD:N1A	2.27	0.49
1:H:177:LEU:HB3	1:H:182:VAL:HB	1.95	0.49
1:I:65:VAL:HG22	3:I:302:NAD:N1A	2.28	0.49
1:A:83:ASP:OD2	1:I:195:LEU:HD11	2.13	0.49
1:F:46:ASP:CG	1:I:97:ARG:H	2.15	0.49
1:N:241:THR:HG21	1:O:216:LEU:HG	1.95	0.49
1:E:75:PHE:CZ	1:E:131:ALA:HB2	2.48	0.49
1:I:240:VAL:HG21	1:L:245:MET:CE	2.42	0.49
1:H:154:PRO:O	1:H:155:ASN:HB2	2.13	0.49
1:G:124:PHE:HB3	1:G:125:PRO:HD3	1.93	0.49
1:D:124:PHE:HB3	1:D:125:PRO:HD3	1.94	0.48
1:I:154:PRO:O	1:I:155:ASN:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:PRO:O	1:M:155:ASN:HB2	2.13	0.48
1:O:154:PRO:O	1:O:155:ASN:HB2	2.13	0.48
1:A:88:LEU:HB3	1:A:141:LEU:HD22	1.95	0.48
1:D:75:PHE:CZ	1:D:131:ALA:HB2	2.48	0.48
1:J:15:LEU:HB2	3:J:302:NAD:H3B	1.95	0.48
1:L:154:PRO:O	1:L:155:ASN:HB2	2.13	0.48
1:L:200:ILE:HD11	2:L:301:TCL:H131	1.96	0.48
1:E:154:PRO:O	1:E:155:ASN:HB2	2.12	0.48
1:J:192:ILE:N	3:J:302:NAD:O7N	2.39	0.48
1:K:154:PRO:O	1:K:155:ASN:HB2	2.14	0.48
1:D:200:ILE:HD11	2:D:301:TCL:H131	1.95	0.48
1:F:124:PHE:HB3	1:F:125:PRO:HD3	1.95	0.48
1:G:154:PRO:O	1:G:155:ASN:HB2	2.13	0.48
1:J:154:PRO:O	1:J:155:ASN:HB2	2.14	0.48
1:P:75:PHE:CZ	1:P:131:ALA:HB2	2.49	0.48
1:L:132:LEU:HA	1:L:135:LEU:HD12	1.96	0.48
1:J:200:ILE:HD11	2:J:301:TCL:H131	1.94	0.48
1:O:215:PRO:HD2	1:O:249:SER:O	2.13	0.48
1:P:154:PRO:O	1:P:155:ASN:HB2	2.13	0.48
1:E:245:MET:CE	1:H:240:VAL:HG21	2.44	0.48
1:O:177:LEU:HB3	1:O:182:VAL:HB	1.96	0.48
1:O:92:ILE:HG23	3:O:302:NAD:C4A	2.43	0.48
1:H:193:LYS:NZ	1:P:69:ALA:CB	2.77	0.48
2:N:301:TCL:CL16	3:N:302:NAD:H3D	2.51	0.48
1:O:163:LYS:NZ	4:O:404:HOH:O	2.27	0.48
1:C:7:LYS:NZ	1:C:138:ASP:OD2	2.47	0.47
1:B:154:PRO:O	1:B:155:ASN:HB2	2.14	0.47
1:D:154:PRO:O	1:D:155:ASN:HB2	2.14	0.47
1:J:245:MET:HE2	1:K:240:VAL:HG21	1.95	0.47
1:A:83:ASP:OD1	1:I:195:LEU:HD11	2.14	0.47
1:M:105:LEU:HD21	1:N:173:LEU:HD21	1.96	0.47
1:O:18:ARG:HH12	1:O:194:THR:CA	2.28	0.47
1:A:240:VAL:HG21	1:D:245:MET:CE	2.44	0.47
1:B:177:LEU:HB3	1:B:182:VAL:HB	1.97	0.47
1:C:154:PRO:O	1:C:155:ASN:HB2	2.15	0.47
1:M:124:PHE:HB3	1:M:125:PRO:HD3	1.95	0.47
1:N:246:HIS:CD2	1:N:252:ASN:HD22	2.32	0.47
1:E:219:ASN:HB3	4:E:425:HOH:O	2.13	0.47
2:M:301:TCL:C4	2:M:301:TCL:H131	2.44	0.47
1:M:189:ALA:HB3	3:M:302:NAD:C5N	2.45	0.47
1:A:75:PHE:CZ	1:A:131:ALA:HB2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:PHE:CE1	2:B:301:TCL:H31	2.49	0.47
1:A:154:PRO:O	1:A:155:ASN:HB2	2.14	0.47
1:O:75:PHE:CZ	1:O:131:ALA:HB2	2.50	0.47
1:O:205:LYS:NZ	4:O:406:HOH:O	2.31	0.47
1:H:132:LEU:HA	1:H:135:LEU:HD12	1.96	0.47
1:A:8:ARG:CZ	1:I:18:ARG:HH11	2.28	0.46
1:C:216:LEU:HB2	1:C:249:SER:HB3	1.97	0.46
1:E:215:PRO:HD2	1:E:249:SER:O	2.15	0.46
1:F:154:PRO:O	1:F:155:ASN:HB2	2.15	0.46
1:G:75:PHE:CZ	1:G:131:ALA:HB2	2.50	0.46
1:I:40:VAL:HG21	3:I:302:NAD:N3A	2.30	0.46
1:M:63:CYS:O	4:M:402:HOH:O	2.21	0.46
1:H:193:LYS:HZ3	1:P:69:ALA:CB	2.29	0.46
1:C:114:ARG:HG3	1:D:114:ARG:HG3	1.97	0.46
1:D:177:LEU:HB3	1:D:182:VAL:HB	1.96	0.46
1:H:15:LEU:HB2	3:H:302:NAD:O3B	2.16	0.46
1:I:43:ARG:O	4:I:401:HOH:O	2.20	0.46
1:M:110:ARG:NH2	1:N:65:VAL:O	2.35	0.46
1:G:200:ILE:HD11	2:G:301:TCL:H131	1.96	0.46
1:P:20:ILE:HG13	3:P:302:NAD:O2N	2.16	0.46
1:H:18:ARG:O	1:H:194:THR:HG22	2.16	0.46
1:M:145:SER:O	3:M:302:NAD:H5N	2.16	0.46
1:N:154:PRO:O	1:N:155:ASN:HB2	2.14	0.46
1:D:196:ALA:HB1	2:D:301:TCL:C9	2.46	0.46
1:F:75:PHE:CZ	1:F:131:ALA:HB2	2.50	0.46
1:H:15:LEU:HD23	1:H:195:LEU:HD22	1.96	0.46
1:I:196:ALA:HB2	3:I:302:NAD:O2A	2.15	0.46
1:N:15:LEU:HB2	3:N:302:NAD:O3B	2.16	0.46
1:F:8:ARG:HB3	1:F:82:TRP:CZ3	2.51	0.45
1:G:18:ARG:NH1	1:G:193:LYS:O	2.50	0.45
1:F:245:MET:HE2	1:G:240:VAL:HG21	1.97	0.45
1:J:240:VAL:HG21	1:K:245:MET:CE	2.46	0.45
1:B:2:GLY:N	4:B:409:HOH:O	2.49	0.45
1:C:185:ASN:HB2	4:C:426:HOH:O	2.16	0.45
1:D:194:THR:HB	4:D:407:HOH:O	2.16	0.45
1:E:245:MET:HE2	1:H:240:VAL:HG21	1.99	0.45
1:K:125:PRO:HB2	1:L:108:LEU:HD22	1.97	0.45
3:P:302:NAD:PA	3:P:302:NAD:HO3A	2.39	0.45
1:K:15:LEU:HB2	3:K:302:NAD:O3B	2.17	0.45
1:K:177:LEU:HB3	1:K:182:VAL:HB	1.98	0.45
1:M:115:ILE:HB	4:M:401:HOH:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:188:SER:HB3	1:N:246:HIS:CD2	2.51	0.45
1:P:7:LYS:NZ	1:P:138:ASP:OD2	2.50	0.45
1:E:38:THR:HA	1:E:61:PHE:O	2.17	0.45
1:M:114:ARG:O	1:M:118:ASP:HB2	2.16	0.45
1:I:245:MET:HE2	1:L:240:VAL:HG21	1.97	0.45
1:P:100:ILE:HD13	2:P:301:TCL:H121	1.98	0.45
1:B:215:PRO:O	1:C:178:GLY:HA3	2.16	0.45
1:I:51:PHE:O	1:I:54:GLU:HB3	2.17	0.45
1:M:240:VAL:HG21	1:P:245:MET:HE2	1.98	0.45
1:M:92:ILE:HG12	3:M:302:NAD:O2B	2.17	0.44
1:N:251:PHE:O	1:N:254:VAL:HG22	2.16	0.44
1:H:146:TYR:HB2	3:H:302:NAD:H5N	1.98	0.44
1:M:5:ASP:HB2	4:M:418:HOH:O	2.17	0.44
1:G:18:ARG:HG3	4:G:401:HOH:O	2.16	0.44
1:K:215:PRO:HD2	1:K:249:SER:O	2.18	0.44
1:K:51:PHE:O	1:K:54:GLU:HB3	2.17	0.44
1:K:38:THR:HA	1:K:61:PHE:O	2.18	0.44
1:B:100:ILE:HD13	2:B:301:TCL:CL15	2.54	0.44
1:A:83:ASP:CG	1:I:195:LEU:HD11	2.38	0.44
1:I:215:PRO:HD2	1:I:249:SER:O	2.18	0.44
1:J:65:VAL:HG22	3:J:302:NAD:N1A	2.33	0.44
1:N:103:ASP:HA	4:N:412:HOH:O	2.17	0.44
1:M:125:PRO:HB2	1:N:108:LEU:HD22	1.98	0.44
1:O:125:PRO:HB2	1:P:108:LEU:CD2	2.48	0.44
1:P:132:LEU:HA	1:P:135:LEU:HD12	1.99	0.44
1:D:215:PRO:HD2	1:D:249:SER:O	2.18	0.44
1:F:102:GLY:HA2	4:F:425:HOH:O	2.18	0.44
1:J:19:SER:HB3	4:J:414:HOH:O	2.18	0.44
1:J:40:VAL:HG21	3:J:302:NAD:N3A	2.33	0.44
1:L:15:LEU:HB2	3:L:302:NAD:O3B	2.17	0.44
1:J:178:GLY:HA3	1:K:215:PRO:O	2.18	0.43
1:L:75:PHE:CZ	1:L:131:ALA:HB2	2.53	0.43
1:H:187:ILE:HG23	1:H:247:VAL:HG23	2.00	0.43
1:I:20:ILE:N	4:I:406:HOH:O	2.50	0.43
1:H:193:LYS:NZ	1:P:69:ALA:HA	2.28	0.43
1:O:216:LEU:HB2	1:O:249:SER:HB3	2.01	0.43
3:E:302:NAD:O1N	3:E:302:NAD:H2N	2.18	0.43
1:K:132:LEU:HA	1:K:135:LEU:HD12	2.00	0.43
1:A:237:ALA:HA	4:A:412:HOH:O	2.18	0.43
1:P:177:LEU:HB3	1:P:182:VAL:HB	2.00	0.43
1:P:246:HIS:CG	1:P:252:ASN:ND2	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:VAL:HG21	1:G:245:MET:CE	2.48	0.43
1:G:177:LEU:HB3	1:G:182:VAL:HB	2.01	0.43
1:M:113:PHE:HE1	1:N:117:HIS:HB3	1.84	0.43
1:E:177:LEU:HB3	1:E:182:VAL:HB	2.01	0.43
1:F:245:MET:CE	1:G:240:VAL:HG21	2.49	0.43
1:G:51:PHE:O	1:G:54:GLU:HB3	2.19	0.43
1:H:215:PRO:HD2	1:H:249:SER:O	2.18	0.43
1:B:7:LYS:NZ	1:B:138:ASP:OD2	2.51	0.43
1:E:231:PHE:HE2	1:H:245:MET:HE3	1.84	0.43
1:C:51:PHE:O	1:C:54:GLU:HB3	2.19	0.43
1:C:215:PRO:HD2	1:C:249:SER:O	2.18	0.42
1:H:163:LYS:NZ	3:H:302:NAD:O2D	2.49	0.42
1:O:196:ALA:HB1	2:O:301:TCL:C9	2.48	0.42
1:P:63:CYS:HA	4:P:402:HOH:O	2.18	0.42
1:I:177:LEU:HB3	1:I:182:VAL:HB	2.00	0.42
1:I:44:PHE:HA	4:I:422:HOH:O	2.19	0.42
1:I:215:PRO:O	1:L:178:GLY:HA3	2.19	0.42
1:G:16:SER:HB3	1:G:195:LEU:HD21	2.00	0.42
1:J:177:LEU:HB3	1:J:182:VAL:HB	1.99	0.42
1:F:45:LYS:NZ	1:I:96:PRO:HG2	2.34	0.42
1:I:245:MET:CE	1:L:240:VAL:HG21	2.48	0.42
1:N:240:VAL:HG21	1:O:245:MET:HE2	2.02	0.42
1:C:177:LEU:HB3	1:C:182:VAL:HB	2.00	0.42
1:J:187:ILE:HG23	1:J:247:VAL:HG23	2.01	0.42
1:J:218:ARG:NH2	1:K:238:SER:O	2.50	0.42
1:M:51:PHE:O	1:M:54:GLU:HB3	2.19	0.42
1:A:65:VAL:HG22	3:A:302:NAD:N1A	2.35	0.42
1:H:51:PHE:O	1:H:54:GLU:HB3	2.20	0.42
1:M:38:THR:HA	1:M:61:PHE:O	2.20	0.42
1:M:177:LEU:HB3	1:M:182:VAL:HB	2.01	0.42
1:O:3:PHE:CZ	1:O:31:GLU:HG3	2.55	0.42
1:A:215:PRO:HD2	1:A:249:SER:O	2.20	0.42
2:M:301:TCL:C4	2:M:301:TCL:C13	2.95	0.42
1:B:114:ARG:HG3	1:A:114:ARG:HG3	2.01	0.42
1:O:8:ARG:HB3	1:O:82:TRP:CH2	2.55	0.42
1:G:216:LEU:HB2	1:G:249:SER:HB3	2.02	0.42
1:B:215:PRO:HD2	1:B:249:SER:O	2.20	0.41
1:G:17:ASN:OD1	4:G:401:HOH:O	2.21	0.41
1:H:54:GLU:HB2	4:H:411:HOH:O	2.18	0.41
1:N:51:PHE:O	1:N:54:GLU:HB3	2.20	0.41
2:A:301:TCL:CL16	3:A:302:NAD:H3D	2.57	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:VAL:HG22	3:L:302:NAD:N1A	2.35	0.41
1:P:156:TYR:CE1	2:P:301:TCL:H11	2.55	0.41
1:B:125:PRO:HB2	1:A:108:LEU:HD22	2.01	0.41
1:B:240:VAL:HG21	1:C:245:MET:CE	2.50	0.41
1:D:3:PHE:CZ	1:D:31:GLU:HG3	2.55	0.41
1:F:105:LEU:N	4:F:401:HOH:O	2.52	0.41
1:G:215:PRO:HD2	1:G:249:SER:O	2.20	0.41
1:N:149:ALA:HB2	1:N:163:LYS:HB3	2.02	0.41
1:A:79:LYS:HD2	1:A:83:ASP:HA	2.01	0.41
1:E:18:ARG:NH2	1:E:195:LEU:HD22	2.35	0.41
1:J:240:VAL:HG21	1:K:245:MET:HE2	2.03	0.41
1:L:196:ALA:HB2	3:L:302:NAD:O2A	2.20	0.41
1:F:200:ILE:HD11	2:F:301:TCL:H131	2.02	0.41
1:J:7:LYS:NZ	1:J:138:ASP:OD2	2.54	0.41
1:J:245:MET:CE	1:K:240:VAL:HG21	2.50	0.41
1:N:215:PRO:HD2	1:N:249:SER:O	2.21	0.41
1:O:39:TYR:CD1	1:O:48:ILE:HG21	2.55	0.41
1:B:108:LEU:CD2	1:A:125:PRO:HB2	2.51	0.41
1:D:51:PHE:O	1:D:54:GLU:HB3	2.21	0.41
1:F:42:ASP:OD1	1:I:115:ILE:HD13	2.20	0.41
1:K:108:LEU:HD22	1:L:125:PRO:HB2	2.03	0.41
1:K:44:PHE:HE1	1:K:47:ARG:NH1	2.17	0.41
1:L:215:PRO:HD2	1:L:249:SER:O	2.21	0.41
1:A:177:LEU:HB3	1:A:182:VAL:HB	2.02	0.41
1:O:173:LEU:CD2	1:P:105:LEU:HD21	2.51	0.41
1:J:121:ALA:O	1:J:125:PRO:HD2	2.21	0.41
1:J:51:PHE:O	1:J:54:GLU:HB3	2.21	0.41
1:N:132:LEU:HA	1:N:135:LEU:HD12	2.03	0.41
1:B:125:PRO:HB2	1:A:108:LEU:CD2	2.51	0.41
1:H:149:ALA:HB2	1:H:163:LYS:HB3	2.02	0.41
1:M:153:ILE:HA	1:M:154:PRO:HD3	1.98	0.41
1:P:57:SER:HA	4:P:409:HOH:O	2.21	0.41
1:B:132:LEU:HA	1:B:135:LEU:HD12	2.03	0.40
1:E:2:GLY:N	4:E:413:HOH:O	2.54	0.40
1:F:79:LYS:HD2	1:F:83:ASP:HA	2.03	0.40
1:G:18:ARG:NH2	1:G:195:LEU:HD22	2.36	0.40
1:H:193:LYS:HZ1	1:P:69:ALA:CA	2.27	0.40
1:K:256:GLY:O	4:K:401:HOH:O	2.22	0.40
1:N:183:ARG:HD2	1:N:240:VAL:O	2.21	0.40
1:C:216:LEU:HD12	1:C:249:SER:HA	2.03	0.40
1:F:38:THR:HA	1:F:61:PHE:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:ASP:HA	4:J:406:HOH:O	2.21	0.40
1:O:170:VAL:HG21	1:O:186:ALA:HB2	2.03	0.40
1:O:246:HIS:CG	1:O:252:ASN:ND2	2.89	0.40
1:O:8:ARG:NH1	1:O:82:TRP:CD1	2.89	0.40
1:E:51:PHE:O	1:E:54:GLU:HB3	2.21	0.40
1:F:215:PRO:HD2	1:F:249:SER:O	2.20	0.40
1:F:8:ARG:NH1	1:F:82:TRP:CD1	2.88	0.40
1:G:114:ARG:HG3	1:H:114:ARG:HG3	2.04	0.40
1:L:18:ARG:O	1:L:194:THR:HG22	2.22	0.40
1:N:216:LEU:HB2	1:N:249:SER:HB3	2.03	0.40
1:C:153:ILE:HA	1:C:154:PRO:HD3	1.98	0.40
1:J:183:ARG:HD2	1:J:240:VAL:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:OH	1:C:137:ASP:OD2[1_655]	1.92	0.28
1:C:106:ASP:O	1:J:97:ARG:NH1[1_545]	2.05	0.15
1:J:137:ASP:OD2	1:L:22:TYR:OH[1_455]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	B	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	C	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	D	253/276 (92%)	242 (96%)	11 (4%)	0	100	100
1	E	253/276 (92%)	242 (96%)	11 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	G	253/276 (92%)	242 (96%)	11 (4%)	0	100	100
1	H	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	I	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	J	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	K	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	L	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	M	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
1	N	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	O	253/276 (92%)	243 (96%)	10 (4%)	0	100	100
1	P	253/276 (92%)	244 (96%)	9 (4%)	0	100	100
All	All	4048/4416 (92%)	3893 (96%)	155 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/209 (93%)	193 (100%)	1 (0%)	91	97
1	B	194/209 (93%)	194 (100%)	0	100	100
1	C	194/209 (93%)	194 (100%)	0	100	100
1	D	194/209 (93%)	194 (100%)	0	100	100
1	E	194/209 (93%)	194 (100%)	0	100	100
1	F	194/209 (93%)	194 (100%)	0	100	100
1	G	194/209 (93%)	194 (100%)	0	100	100
1	H	194/209 (93%)	194 (100%)	0	100	100
1	I	194/209 (93%)	194 (100%)	0	100	100
1	J	194/209 (93%)	194 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	194/209 (93%)	193 (100%)	1 (0%)	91	97
1	L	194/209 (93%)	194 (100%)	0	100	100
1	M	194/209 (93%)	194 (100%)	0	100	100
1	N	194/209 (93%)	194 (100%)	0	100	100
1	O	194/209 (93%)	194 (100%)	0	100	100
1	P	194/209 (93%)	194 (100%)	0	100	100
All	All	3104/3344 (93%)	3102 (100%)	2 (0%)	94	99

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	K	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	246	HIS
1	P	246	HIS
1	P	252	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	TCL	A	301	-	18,18,18	0.43	0	25,25,25	0.81	0
3	NAD	A	302	-	41,48,48	0.65	1 (2%)	43,73,73	0.92	1 (2%)
2	TCL	B	301	-	18,18,18	0.51	0	25,25,25	0.80	0
3	NAD	B	302	-	41,48,48	0.66	1 (2%)	43,73,73	1.00	1 (2%)
2	TCL	C	301	-	18,18,18	0.50	0	25,25,25	0.75	1 (4%)
3	NAD	C	302	-	41,48,48	0.65	1 (2%)	43,73,73	1.02	1 (2%)
2	TCL	D	301	-	18,18,18	0.48	0	25,25,25	0.62	0
3	NAD	D	302	-	41,48,48	0.62	1 (2%)	43,73,73	0.98	1 (2%)
2	TCL	E	301	-	18,18,18	0.47	0	25,25,25	0.84	1 (4%)
3	NAD	E	302	-	41,48,48	0.64	0	43,73,73	0.87	1 (2%)
2	TCL	F	301	-	18,18,18	0.45	0	25,25,25	0.72	0
3	NAD	F	302	-	41,48,48	0.64	1 (2%)	43,73,73	0.81	1 (2%)
2	TCL	G	301	-	18,18,18	0.46	0	25,25,25	0.76	1 (4%)
3	NAD	G	302	-	41,48,48	0.70	1 (2%)	43,73,73	0.98	2 (4%)
2	TCL	H	301	-	18,18,18	0.47	0	25,25,25	0.76	0
3	NAD	H	302	-	41,48,48	0.67	1 (2%)	43,73,73	0.84	1 (2%)
2	TCL	I	301	-	18,18,18	0.49	0	25,25,25	0.71	0
3	NAD	I	302	-	41,48,48	0.68	1 (2%)	43,73,73	0.91	1 (2%)
2	TCL	J	301	-	18,18,18	0.48	0	25,25,25	0.72	0
3	NAD	J	302	-	41,48,48	0.62	1 (2%)	43,73,73	0.63	0
2	TCL	K	301	-	18,18,18	0.50	0	25,25,25	0.82	1 (4%)
3	NAD	K	302	-	41,48,48	0.69	1 (2%)	43,73,73	0.89	1 (2%)
2	TCL	L	301	-	18,18,18	0.45	0	25,25,25	0.76	1 (4%)
3	NAD	L	302	-	41,48,48	0.68	1 (2%)	43,73,73	0.84	1 (2%)
2	TCL	M	301	-	18,18,18	0.39	0	25,25,25	0.74	1 (4%)
3	NAD	M	302	-	41,48,48	0.68	1 (2%)	43,73,73	0.77	2 (4%)
2	TCL	N	301	-	18,18,18	0.49	0	25,25,25	0.85	0
3	NAD	N	302	-	41,48,48	0.81	1 (2%)	43,73,73	0.85	2 (4%)
2	TCL	O	301	-	18,18,18	0.47	0	25,25,25	0.79	1 (4%)
3	NAD	O	302	-	41,48,48	0.67	1 (2%)	43,73,73	1.04	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TCL	P	301	-	18,18,18	0.49	0	25,25,25	0.86	1 (4%)
3	NAD	P	302	-	41,48,48	0.89	1 (2%)	43,73,73	1.01	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TCL	A	301	-	-	0/4/4/4	0/2/2/2
3	NAD	A	302	-	-	0/22/62/62	0/5/5/5
2	TCL	B	301	-	-	0/4/4/4	0/2/2/2
3	NAD	B	302	-	-	0/22/62/62	0/5/5/5
2	TCL	C	301	-	-	0/4/4/4	0/2/2/2
3	NAD	C	302	-	-	0/22/62/62	0/5/5/5
2	TCL	D	301	-	-	0/4/4/4	0/2/2/2
3	NAD	D	302	-	-	0/22/62/62	0/5/5/5
2	TCL	E	301	-	-	0/4/4/4	0/2/2/2
3	NAD	E	302	-	-	0/22/62/62	0/5/5/5
2	TCL	F	301	-	-	0/4/4/4	0/2/2/2
3	NAD	F	302	-	-	0/22/62/62	0/5/5/5
2	TCL	G	301	-	-	0/4/4/4	0/2/2/2
3	NAD	G	302	-	-	0/22/62/62	0/5/5/5
2	TCL	H	301	-	-	0/4/4/4	0/2/2/2
3	NAD	H	302	-	-	0/22/62/62	0/5/5/5
2	TCL	I	301	-	-	0/4/4/4	0/2/2/2
3	NAD	I	302	-	-	0/22/62/62	0/5/5/5
2	TCL	J	301	-	-	0/4/4/4	0/2/2/2
3	NAD	J	302	-	-	0/22/62/62	0/5/5/5
2	TCL	K	301	-	-	0/4/4/4	0/2/2/2
3	NAD	K	302	-	-	0/22/62/62	0/5/5/5
2	TCL	L	301	-	-	0/4/4/4	0/2/2/2
3	NAD	L	302	-	-	0/22/62/62	0/5/5/5
2	TCL	M	301	-	-	0/4/4/4	0/2/2/2
3	NAD	M	302	-	-	0/22/62/62	0/5/5/5
2	TCL	N	301	-	-	0/4/4/4	0/2/2/2
3	NAD	N	302	-	-	0/22/62/62	0/5/5/5
2	TCL	O	301	-	-	0/4/4/4	0/2/2/2
3	NAD	O	302	-	-	0/22/62/62	0/5/5/5
2	TCL	P	301	-	-	0/4/4/4	0/2/2/2
3	NAD	P	302	-	-	0/22/62/62	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	302	NAD	O4D-C1D	-4.50	1.35	1.41
3	N	302	NAD	O4D-C1D	-3.97	1.35	1.41
3	G	302	NAD	O4D-C1D	-3.12	1.36	1.41
3	L	302	NAD	O4D-C1D	-2.87	1.37	1.41
3	K	302	NAD	O4D-C1D	-2.79	1.37	1.41
3	I	302	NAD	O4D-C1D	-2.78	1.37	1.41
3	B	302	NAD	O4D-C1D	-2.77	1.37	1.41
3	O	302	NAD	O4D-C1D	-2.75	1.37	1.41
3	C	302	NAD	O4D-C1D	-2.68	1.37	1.41
3	H	302	NAD	O4D-C1D	-2.66	1.37	1.41
3	F	302	NAD	O4D-C1D	-2.48	1.37	1.41
3	M	302	NAD	O4D-C1D	-2.45	1.37	1.41
3	A	302	NAD	O4D-C1D	-2.38	1.38	1.41
3	D	302	NAD	O4D-C1D	-2.31	1.38	1.41
3	J	302	NAD	O4D-C1D	-2.09	1.38	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	302	NAD	C4B-O4B-C1B	-5.29	104.14	109.77
3	C	302	NAD	C4B-O4B-C1B	-5.03	104.42	109.77
3	B	302	NAD	C4B-O4B-C1B	-4.96	104.49	109.77
3	D	302	NAD	C4B-O4B-C1B	-4.74	104.73	109.77
3	G	302	NAD	C4B-O4B-C1B	-4.43	105.05	109.77
3	A	302	NAD	C4B-O4B-C1B	-4.22	105.28	109.77
3	I	302	NAD	C4B-O4B-C1B	-3.97	105.54	109.77
3	K	302	NAD	C4B-O4B-C1B	-3.86	105.66	109.77
3	E	302	NAD	C4B-O4B-C1B	-3.42	106.13	109.77
3	L	302	NAD	C4B-O4B-C1B	-3.34	106.21	109.77
3	H	302	NAD	C4B-O4B-C1B	-3.30	106.25	109.77
3	P	302	NAD	C4B-O4B-C1B	-3.29	106.26	109.77
3	F	302	NAD	C4B-O4B-C1B	-3.01	106.57	109.77
3	M	302	NAD	C4B-O4B-C1B	-2.83	106.76	109.77
3	N	302	NAD	O2D-C2D-C1D	-2.78	102.93	111.61
3	N	302	NAD	C4B-O4B-C1B	-2.64	106.96	109.77
3	P	302	NAD	O2D-C2D-C1D	-2.37	104.21	111.61
3	G	302	NAD	O2D-C2D-C1D	-2.12	104.97	111.61
3	M	302	NAD	O2D-C2D-C1D	-2.12	105.00	111.61
2	G	301	TCL	O7-C5-C6	2.01	120.27	116.24
2	L	301	TCL	O7-C5-C6	2.07	120.39	116.24
2	C	301	TCL	O7-C5-C6	2.11	120.47	116.24
2	O	301	TCL	O7-C5-C6	2.17	120.60	116.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	TCL	O7-C5-C6	2.19	120.63	116.24
2	M	301	TCL	C8-C9-CL16	2.23	121.99	119.42
2	K	301	TCL	O7-C5-C6	2.26	120.79	116.24
2	P	301	TCL	O7-C5-C6	2.56	121.38	116.24
3	P	302	NAD	C4D-O4D-C1D	3.40	113.39	109.77

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	301	TCL	2	0
3	A	302	NAD	2	0
2	B	301	TCL	3	0
3	B	302	NAD	1	0
3	C	302	NAD	1	0
2	D	301	TCL	2	0
3	D	302	NAD	3	0
3	E	302	NAD	2	0
2	F	301	TCL	1	0
3	F	302	NAD	1	0
2	G	301	TCL	1	0
3	G	302	NAD	1	0
3	H	302	NAD	4	0
3	I	302	NAD	4	0
2	J	301	TCL	2	0
3	J	302	NAD	4	0
2	K	301	TCL	1	0
3	K	302	NAD	2	0
2	L	301	TCL	1	0
3	L	302	NAD	3	0
2	M	301	TCL	3	0
3	M	302	NAD	8	0
2	N	301	TCL	2	0
3	N	302	NAD	4	0
2	O	301	TCL	2	0
3	O	302	NAD	3	0
2	P	301	TCL	4	0
3	P	302	NAD	6	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	255/276 (92%)	-0.18	1 (0%) 92 91	28, 43, 76, 111	0
1	B	255/276 (92%)	-0.18	2 (0%) 86 83	30, 40, 59, 93	0
1	C	255/276 (92%)	0.08	5 (1%) 65 59	32, 49, 90, 132	0
1	D	255/276 (92%)	-0.16	1 (0%) 92 91	29, 47, 88, 128	0
1	E	255/276 (92%)	-0.11	0 100 100	37, 48, 74, 122	0
1	F	255/276 (92%)	0.07	6 (2%) 59 52	36, 52, 96, 123	0
1	G	255/276 (92%)	-0.14	2 (0%) 86 83	36, 49, 75, 133	0
1	H	255/276 (92%)	0.08	6 (2%) 59 52	39, 54, 94, 139	0
1	I	255/276 (92%)	0.24	9 (3%) 44 36	29, 55, 103, 148	0
1	J	255/276 (92%)	0.32	15 (5%) 23 17	31, 55, 103, 154	0
1	K	255/276 (92%)	-0.12	2 (0%) 86 83	29, 44, 73, 134	0
1	L	255/276 (92%)	-0.02	3 (1%) 79 75	31, 50, 87, 111	0
1	M	255/276 (92%)	1.31	63 (24%) 1 0	47, 82, 135, 165	0
1	N	255/276 (92%)	1.06	50 (19%) 1 0	48, 70, 114, 152	0
1	O	255/276 (92%)	0.33	12 (4%) 32 25	39, 57, 90, 121	0
1	P	255/276 (92%)	1.15	47 (18%) 1 1	46, 80, 128, 193	0
All	All	4080/4416 (92%)	0.23	224 (5%) 26 19	28, 53, 103, 193	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	5	ASP	8.9
1	M	88	LEU	7.1
1	P	200	ILE	7.1
1	J	97	ARG	6.8
1	M	181	GLY	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	45	LYS	6.7
1	M	42	ASP	6.7
1	N	102	GLY	6.4
1	J	200	ILE	5.5
1	M	139	ALA	5.5
1	M	6	GLY	5.4
1	J	41	GLY	5.4
1	M	4	LEU	5.4
1	P	145	SER	5.3
1	O	240	VAL	5.3
1	N	40	VAL	5.2
1	M	2	GLY	5.2
1	P	198	SER	5.1
1	M	199	GLY	5.0
1	M	44	PHE	4.9
1	M	37	PHE	4.7
1	I	59	LEU	4.7
1	P	43	ARG	4.6
1	P	195	LEU	4.5
1	P	203	PHE	4.5
1	M	182	VAL	4.4
1	P	15	LEU	4.4
1	P	206	ILE	4.3
1	N	36	ALA	4.3
1	M	62	PRO	4.2
1	M	40	VAL	4.2
1	M	80	THR	4.2
1	N	95	ALA	4.1
1	N	105	LEU	4.1
1	P	156	TYR	4.0
1	N	117	HIS	4.0
1	N	20	ILE	4.0
1	M	33	ALA	4.0
1	N	73	ALA	4.0
1	N	24	ILE	3.9
1	H	193	LYS	3.9
1	M	141	LEU	3.9
1	N	201	LYS	3.9
1	C	46	ASP	3.8
1	P	219	ASN	3.8
1	N	104	PHE	3.8
1	N	223	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	43	ARG	3.7
1	N	10	LEU	3.7
1	M	82	TRP	3.7
1	P	41	GLY	3.7
1	P	153	ILE	3.7
1	J	42	ASP	3.6
1	M	172	TYR	3.6
1	J	78	LEU	3.5
1	P	207	LEU	3.5
1	M	78	LEU	3.5
1	I	15	LEU	3.5
1	M	127	LEU	3.5
1	N	41	GLY	3.5
1	J	199	GLY	3.5
1	N	220	VAL	3.5
1	M	126	ALA	3.4
1	M	134	MET	3.4
1	N	200	ILE	3.4
1	N	214	SER	3.4
1	M	230	ALA	3.4
1	H	201	LYS	3.3
1	M	118	ASP	3.3
1	N	198	SER	3.3
1	C	42	ASP	3.3
1	M	232	LEU	3.3
1	J	47	ARG	3.3
1	F	108	LEU	3.3
1	J	201	LYS	3.3
1	P	59	LEU	3.3
1	P	146	TYR	3.3
1	L	200	ILE	3.3
1	N	42	ASP	3.3
1	J	40	VAL	3.2
1	M	11	LEU	3.2
1	N	12	THR	3.2
1	K	43	ARG	3.2
1	P	202	SER	3.2
1	I	39	TYR	3.2
1	P	249	SER	3.2
1	M	86	ASP	3.1
1	P	147	LEU	3.1
1	P	217	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	172	TYR	3.1
1	L	97	ARG	3.1
1	F	193	LYS	3.1
1	N	210	VAL	3.1
1	N	88	LEU	3.1
1	N	251	PHE	3.0
1	M	73	ALA	3.0
1	M	133	PRO	3.0
1	C	41	GLY	3.0
1	M	101	ALA	3.0
1	H	199	GLY	3.0
1	M	122	TYR	2.9
1	O	43	ARG	2.9
1	M	56	GLY	2.9
1	N	22	TYR	2.9
1	P	225	VAL	2.9
1	M	242	ALA	2.9
1	M	92	ILE	2.9
1	O	61	PHE	2.9
1	N	65	VAL	2.9
1	M	74	LEU	2.8
1	M	189	ALA	2.8
1	P	191	PRO	2.8
1	P	190	GLY	2.8
1	M	179	ALA	2.8
1	B	43	ARG	2.8
1	N	159	MET	2.8
1	M	184	VAL	2.7
1	N	152	ALA	2.7
1	M	238	SER	2.7
1	N	68	ASP	2.7
1	N	132	LEU	2.7
1	N	254	VAL	2.7
1	J	94	PHE	2.7
1	M	85	LEU	2.7
1	I	48	ILE	2.7
1	N	141	LEU	2.7
1	M	22	TYR	2.7
1	O	242	ALA	2.6
1	P	51	PHE	2.6
1	O	236	LEU	2.6
1	O	42	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	9	ILE	2.6
1	N	215	PRO	2.6
1	A	83	ASP	2.6
1	P	40	VAL	2.6
1	P	78	LEU	2.6
1	N	97	ARG	2.6
1	P	187	ILE	2.5
1	N	150	GLU	2.5
1	M	138	ASP	2.5
1	H	18	ARG	2.5
1	P	221	THR	2.5
1	M	180	LYS	2.5
1	H	200	ILE	2.5
1	O	20	ILE	2.5
1	I	60	VAL	2.5
1	O	237	ALA	2.5
1	P	70	GLN	2.5
1	J	46	ASP	2.5
1	N	145	SER	2.4
1	G	43	ARG	2.4
1	K	97	ARG	2.4
1	P	63	CYS	2.4
1	N	205	LYS	2.4
1	F	18	ARG	2.4
1	M	35	LEU	2.4
1	P	205	LYS	2.4
1	F	97	ARG	2.4
1	M	97	ARG	2.4
1	M	236	LEU	2.4
1	M	142	LEU	2.4
1	N	195	LEU	2.4
1	P	24	ILE	2.4
1	P	141	LEU	2.4
1	N	28	CYS	2.4
1	P	55	PHE	2.4
1	F	200	ILE	2.3
1	N	119	ILE	2.3
1	J	44	PHE	2.3
1	H	40	VAL	2.3
1	P	210	VAL	2.3
1	M	137	ASP	2.3
1	M	119	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	83	ASP	2.3
1	N	146	TYR	2.3
1	J	92	ILE	2.3
1	M	58	GLU	2.3
1	N	113	PHE	2.3
1	N	115	ILE	2.3
1	D	97	ARG	2.2
1	M	237	ALA	2.2
1	F	206	ILE	2.2
1	P	87	GLY	2.2
1	M	136	SER	2.2
1	M	145	SER	2.2
1	B	97	ARG	2.2
1	N	196	ALA	2.2
1	N	55	PHE	2.2
1	P	218	ARG	2.2
1	N	207	LEU	2.2
1	P	144	LEU	2.2
1	C	137	ASP	2.2
1	I	51	PHE	2.2
1	P	22	TYR	2.2
1	L	100	ILE	2.2
1	P	211	GLU	2.2
1	N	38	THR	2.2
1	O	127	LEU	2.2
1	O	128	ALA	2.2
1	M	84	SER	2.1
1	M	135	LEU	2.1
1	M	8	ARG	2.1
1	M	3	PHE	2.1
1	P	213	ASN	2.1
1	M	240	VAL	2.1
1	I	42	ASP	2.1
1	J	128	ALA	2.1
1	G	3	PHE	2.1
1	P	212	SER	2.1
1	M	65	VAL	2.1
1	M	140	SER	2.1
1	I	43	ARG	2.1
1	J	43	ARG	2.1
1	M	129	LYS	2.0
1	P	11	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	220	VAL	2.0
1	P	28	CYS	2.0
1	I	49	THR	2.0
1	P	113	PHE	2.0
1	N	90	HIS	2.0
1	N	206	ILE	2.0
1	O	77	SER	2.0
1	P	94	PHE	2.0
1	P	201	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TCL	K	301	17/17	0.91	0.24	2.17	36,52,94,107	0
2	TCL	I	301	17/17	0.94	0.23	1.02	42,53,80,90	0
2	TCL	B	301	17/17	0.95	0.17	0.64	31,46,68,117	0
2	TCL	M	301	17/17	0.65	0.26	0.62	77,134,158,181	0
2	TCL	E	301	17/17	0.96	0.17	0.59	38,49,79,82	0
2	TCL	D	301	17/17	0.92	0.17	0.40	30,60,91,106	0
2	TCL	A	301	17/17	0.96	0.15	0.03	30,38,82,122	0
2	TCL	J	301	17/17	0.85	0.25	-0.09	80,86,104,133	0
3	NAD	M	302	44/44	0.84	0.23	-0.12	83,110,137,144	0
2	TCL	L	301	17/17	0.92	0.18	-0.18	41,55,72,84	0
2	TCL	F	301	17/17	0.90	0.18	-0.25	67,73,87,88	0
3	NAD	E	302	44/44	0.97	0.16	-0.34	38,46,62,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAD	O	302	44/44	0.95	0.17	-0.40	39,51,72,80	0
3	NAD	G	302	44/44	0.96	0.14	-0.51	37,48,60,68	0
3	NAD	J	302	44/44	0.94	0.18	-0.53	33,53,70,97	0
3	NAD	I	302	44/44	0.95	0.17	-0.55	38,51,66,79	0
3	NAD	H	302	44/44	0.94	0.16	-0.56	42,66,90,103	0
3	NAD	A	302	44/44	0.96	0.14	-0.56	29,40,62,74	0
3	NAD	L	302	44/44	0.95	0.16	-0.59	34,48,64,77	0
2	TCL	H	301	17/17	0.94	0.17	-0.60	44,57,67,221	0
2	TCL	G	301	17/17	0.94	0.16	-0.60	38,48,67,78	0
3	NAD	F	302	44/44	0.93	0.14	-0.62	31,59,76,92	0
2	TCL	O	301	17/17	0.95	0.15	-0.67	39,46,88,98	0
3	NAD	D	302	44/44	0.96	0.13	-0.72	27,39,66,90	0
3	NAD	K	302	44/44	0.97	0.14	-0.75	30,38,60,67	0
2	TCL	P	301	17/17	0.85	0.22	-0.77	64,85,116,170	0
3	NAD	B	302	44/44	0.97	0.14	-0.89	31,38,51,61	0
3	NAD	C	302	44/44	0.96	0.13	-0.93	33,47,70,90	0
2	TCL	C	301	17/17	0.96	0.14	-0.95	33,55,74,95	0
3	NAD	N	302	44/44	0.91	0.19	-1.10	55,78,102,120	0
2	TCL	N	301	17/17	0.94	0.19	-1.42	56,68,74,127	0
3	NAD	P	302	44/44	0.91	0.16	-1.48	47,69,94,112	0

6.5 Other polymers

There are no such residues in this entry.