

Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 07:06 pm GMT

PDB ID	:	5I7F
Title	:	Crystal structure of B. pseudomallei FabI in complex with NAD and PT405
Authors	:	Eltschkner, S.; Tonge, P.J.; Kisker, C.
Deposited on	:	2016-02-17
Resolution	:	2.70 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
M1	•	1.025 107 1.0.4 CCD (411 - (2020)
Mogui	÷	1.8.4, CSD assume (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069(2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain		
1	А	276	86%	7%	7%
1	В	276	86%	7%	7%
1	С	276	88%	5%	7%
1	D	276	87%	7%	7%
1	Е	276	89%	•	7%
1	F	276	89%	•	7%
1	G	276	86%	7%	7%



Mol	Chain	Length	Quality of chain		
1	Н	276	84%	9%	7%
1	Ι	276	90%	•	7%
1	J	276	88%	5%	7%
1	K	276	89%	•	7%
1	L	276	86%	7%	7%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 46664 atoms, of which 22715 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.

Mol	Chain	Residues			Atoms	5			ZeroOcc	AltConf	Trace
1	р	257	Total	С	Н	Ν	0	S	0	0	0
1	D	207	3754	1218	1842	325	363	6	0	0	0
1	F	257	Total	С	Η	Ν	0	S	0	1	0
1	E	207	3765	1221	1848	325	365	6	0	1	0
1	ц	257	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
1	11	237	3759	1218	1847	325	363	6	0	0	0
1	С	257	Total	С	Η	Ν	0	S	0	0	0
1		201	3754	1218	1842	325	363	6	0	0	0
1	Δ	257	Total	С	Η	Ν	0	S	0	0	0
1	Л	201	3759	1218	1847	325	363	6		0	0
1	F	257	Total	С	Η	Ν	0	S	19	1	0
1	Ľ	201	3777	1223	1859	326	363	6		1	0
1	G	257	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	1	0
1	ŭ	201	3766	1221	1849	325	365	6	0	I	0
1	Л	257	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	D	201	3759	1218	1847	325	363	6	0	0	0
1	т	257	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0
1	T	201	3772	1218	1860	325	363	6	0	0	0
1	K	257	Total	С	Η	Ν	0	\mathbf{S}	0	1	0
1	17	201	3771	1223	1853	326	363	6	0	T	0
1	т	257	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
		201	3774	1218	1862	325	363	6		U	U
1	T	257	Total	C	Н	Ν	0	S	10	1	0
	J	201	3809	1223	1891	326	363	6			

• Molecule 1 is a protein called Enoyl-[acyl-carrier-protein] reductase [NADH].

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	264	LYS	-	expression tag	UNP A0A069B9A4
В	265	LEU	-	expression tag	UNP A0A069B9A4
В	266	ALA	-	expression tag	UNP A0A069B9A4
В	267	ALA	-	expression tag	UNP A0A069B9A4
В	268	ALA	-	expression tag	UNP A0A069B9A4



Chain	Residue	Modelled	Actual	Comment	Reference	
В	269	LEU	-	expression tag	UNP A0A069B9A4	
В	270	GLU	_	expression tag	UNP A0A069B9A4	
В	271	HIS	-	expression tag	UNP A0A069B9A4	
В	272	HIS	_	expression tag	UNP A0A069B9A4	
В	273	HIS	-	expression tag	UNP A0A069B9A4	
В	274	HIS	-	expression tag	UNP A0A069B9A4	
В	275	HIS	-	expression tag	UNP A0A069B9A4	
В	276	HIS	-	expression tag	UNP A0A069B9A4	
Е	264	LYS	-	expression tag	UNP A0A069B9A4	
Е	265	LEU	-	expression tag	UNP A0A069B9A4	
Е	266	ALA	-	expression tag	UNP A0A069B9A4	
Е	267	ALA	-	expression tag	UNP A0A069B9A4	
Е	268	ALA	-	expression tag	UNP A0A069B9A4	
Е	269	LEU	-	expression tag	UNP A0A069B9A4	
Е	270	GLU	-	expression tag	UNP A0A069B9A4	
Е	271	HIS	-	expression tag	UNP A0A069B9A4	
Е	272	HIS	-	expression tag	UNP A0A069B9A4	
Е	273	HIS	-	expression tag	UNP A0A069B9A4	
Е	274	HIS	-	expression tag	UNP A0A069B9A4	
Е	275	HIS	-	expression tag	UNP A0A069B9A4	
Е	276	HIS	-	expression tag	UNP A0A069B9A4	
Н	264	LYS	-	expression tag	UNP A0A069B9A4	
Н	265	LEU	-	expression tag	UNP A0A069B9A4	
Н	266	ALA	-	expression tag	UNP A0A069B9A4	
Н	267	ALA	-	expression tag	UNP A0A069B9A4	
Н	268	ALA	-	expression tag	UNP A0A069B9A4	
Н	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	
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	



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



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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

• Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).





Mol	Chain	Residues		Α	Aton	ıs			ZeroOcc	AltConf				
0	D	1	Total	С	Η	Ν	0	Р	0	0				
	D	1	71	21	27	7	14	2	0	0				
0	F	1	Total	С	Η	Ν	0	Р	0	0				
	E	1	71	21	27	7	14	2	0	0				
9	Ц	1	Total	С	Η	Ν	Ο	Р	0	0				
	11	1	71	21	27	7	14	2	0	0				
2	С	1	Total	С	Η	Ν	Ο	Р	0	0				
2	U	1	71	21	27	7	14	2	0	0				
2	Δ	1	Total	С	Η	Ν	Ο	Р	0	0				
2	11	1	71	21	27	7	14	2	0	0				
2	F	1	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0				
	1	Ĩ	71	21	27	7	14	2		0				
2	G	1	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0				
	u	Ĩ	71	21	27	7	14	2	0	0				
2	Л	1	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0				
	D	Ĩ	71	21	27	7	14	2	0	0				
2	T	1	Total	С	Η	Ν	Ο	Р	0	0				
	1	Ŧ	71	21	27	7	14	2	0	0				
2	K	1	Total	С	Η	Ν	Ο	Р	0	0				
	11	1	71	21	27	7	14	2	0	0				
2	T.	1	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0				
	Ľ	L			L	L	71	21	27	7	14	2	0	0
2	I	1	Total	\mathbf{C}	Η	Ν	Ο	Р	0	0				
	J	1	71	21	27	7	14	2	0					

• Molecule 3 is 5-ethyl-4-fluoro-2-(2-fluorophenoxy) phenol (three-letter code: 68O) (formula: $\rm C_{14}H_{12}F_2O_2).$





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
9	D	1	Total	С	F	Η	0	0	0	
3	D	1	30	14	2	12	2	0	0	
9	Б	1	Total	С	F	Η	0	0	0	
5	E	1	30	14	2	12	2	0	0	
2	ц	1	Total	С	F	Η	Ο	0	0	
0	11	1	30	14	2	12	2	0	0	
2	C	1	Total	С	F	Η	Ο	0	0	
5	U	1	30	14	2	12	2	0	0	
3	Λ	1	Total	С	F	Η	Ο	0	0	
0	Л	1	30	14	2	12	2	0	U	
3	F	1	Total	С	F	Η	Ο	0	0	
0	Ľ	T	30	14	2	12	2	0	0	
3	C	1	Total	С	F	Η	Ο	0	0	
0	G	T	30	14	2	12	2	0	0	
3	л	1	Total	С	F	Η	Ο	0	0	
0	D	1	30	14	2	12	2	0	0	
3	Т	1	Total	\mathbf{C}	F	Η	Ο	0	0	
0	T	1	30	14	2	12	2	0	0	
3	K	1	Total	С	F	Η	Ο	0	0	
0	IX	T	30	14	2	12	2	0	0	
3	L	1	Total	$\overline{\mathbf{C}}$	F	Η	0	0	0	
J		1	30	14	2	12	2	0		
3	T	1	Total	$\overline{\mathbf{C}}$	F	Η	0	0	0	
J	บ	T	30	14	2	12	2	0		

• Molecule 4 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	20	TotalO2020	0	0
4	Е	22	Total O 22 22	0	0
4	Н	17	Total O 17 17	0	0
4	С	13	Total O 13 13	0	0
4	А	22	TotalO2222	0	0
4	F	24	Total O 24 24	0	0
4	G	23	TotalO2323	0	0
4	D	32	$\begin{array}{cc} \text{Total} & \text{O} \\ 32 & 32 \end{array}$	0	0
4	Ι	10	Total O 10 10	0	0
4	Κ	18	Total O 18 18	0	0
4	L	12	$\begin{array}{cc} \text{Total} & \text{O} \\ 12 & 12 \end{array}$	0	0
4	J	20	$\begin{array}{cc} \text{Total} & O \\ 20 & 20 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain B:	86%	7%	7%	
MET [11] [11] [11] [11] [11] [11] [11] [11	D64 F75 F75 B63 K79 B63 B63 B63 B64 B64 B63 B63 B63 B63 B63 B63 B133 F133 F133 F133 F133 F133 F133 F13	ALA LEU GLU HIS	HIS HIS HIS	HIS
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]			
Chain E:	89%	•	7%	
MET G2 L11 819 A25 F37	R55 198 198 198 198 198 198 198 198 198 198			
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]			
Chain H:	84%	9%	7%	
MET G2 L11 L15 A25 K26 K26	R43 F75 F75 K79 B83 B83 A101 F124 F124 F124 F124 F125 F133 F133 F133 F133 F133 F133 F133 F13	M258 ALA GLY LEU	GLU GLU LYS LEU	ALA ALA ALA I FII
GLU HIS HIS HIS HIS HIS				
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]			
Chain C:	88%	5%	7%	
MET G2 L11 A25 R30 V40	D64 764 83 83 83 83 83 83 83 83 83 84 84 84 84 84 84 84 84 84 84 84 84 84			
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]			
Chain A:	86%	7%	7%	
MET G2 S19 X26 X26 K26 K26 K26 K41 C41 D42	R43 P64 P64 P64 P128 P128 P128 P128 P128 P128 P128 P128	ALA ALA ALA LEU	GLU HIS HIS	HIS HIS HIS
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]			



Chain F:	89%	• 7%	
MET G2 R1 L11 S19 S19	A25 V40 V40 D64 D64 D138 L132 L177 L132 ALA ALA ALA ALA ALA ALA ALA ALA ALA AL		
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]		
Chain G:	86%	7% 7%	
MET 62 119 1110 1111 111 111 111 111 111 111 1	R47 R47 R47 R58 B83 B83 B83 B83 B83 F19 F124 F124 F124 F125 F125 F125 F195 R195 R195 R195 R195 R195 R195 R195 R	ALA ALA ALA LEU GLU HIS HIS HIS	HIS
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]		
Chain D:	87%	7% 7%	
MET G2 D5 R47 K79 K79 B3	L88 188 188 188 125 125 125 125 125 125 125 125	HIS HIS HIS HIS	
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]		
Chain I:	90%	• 7%	
MET G2 F44 F44 L88 L88 D137	L141 L177 L177 L177 L177 L177 L177 L177		
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]		
Chain K:	89%	• 7%	
MET G2 819 813 042 083	L132 L132 L132 L177 L177 L177 L177 L177 L177 L177 L17		
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]		
Chain L:	86%	7% 7%	
MET G 2 K 26 K 26 R 30 R 30	R43 K79 K79 L88 L88 L88 L98 L98 L141 L141 L141 L141 L141 L141 L141 R156 R156 R156 R156 R156 R1221 L222 L223 L222 L222 L222 L222 L222	ALA LEU GLU HIS HIS HIS HIS	HIS
• Molecule 1:	Enoyl-[acyl-carrier-protein] reductase [NADH]		
Chain J:	88%	5% 7%	
MET C2 S19 K26 K26 I48	V60 V60 V83 V156 V156 V156 V182 V182 V182 V182 V182 V182 V182 V182	HIS HIS HIS	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants	138.43Å 109.78Å 269.80Å	Depositor
a, b, c, α , β , γ	90.00° 104.51° 90.00°	Depositor
Bosolution(A)	47.17 - 2.70	Depositor
Resolution (A)	48.99 - 2.70	EDS
% Data completeness	94.4 (47.17-2.70)	Depositor
(in resolution range)	94.6 (48.99-2.70)	EDS
R _{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.96 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
P. P.	0.192 , 0.223	Depositor
n, n_{free}	0.445 , 0.464	DCC
R_{free} test set	4941 reflections (4.86%)	wwPDB-VP
Wilson B-factor $(Å^2)$	115.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.37, 29.0	EDS
L-test for $twinning^2$	$ < L >=0.57, < L^2>=0.47$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	46664	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	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 52.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, $68\mathrm{O}$

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).

Mal	Chain	Bond lengths		Bo	ond angles
		RMSZ = # Z > 5		RMSZ	# Z > 5
1	А	0.36	2/1945~(0.1%)	0.68	2/2631~(0.1%)
1	В	0.27	0/1945	0.45	0/2631
1	С	0.26	0/1945	0.46	0/2631
1	D	0.28	0/1945	0.46	0/2631
1	Ε	0.28	0/1953	0.46	0/2642
1	F	0.28	0/1954	0.47	0/2642
1	G	0.27	0/1953	0.46	0/2642
1	Н	0.27	0/1945	0.47	0/2631
1	Ι	0.26	0/1945	0.45	0/2631
1	J	0.28	0/1954	0.47	0/2642
1	Κ	0.29	0/1954	0.49	0/2642
1	L	0.27	0/1945	0.48	0/2631
All	All	0.28	2/23383~(0.0%)	0.49	2/31627~(0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	43	ARG	CZ-NH2	-6.43	1.24	1.33
1	А	43	ARG	CD-NE	-5.42	1.37	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	43	ARG	NE-CZ-NH2	-18.27	111.17	120.30
1	А	43	ARG	NE-CZ-NH1	16.36	128.48	120.30

There are no chirality outliers.

There are no planarity outliers.



5.2 Too-close contacts (i)

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	А	1912	1847	1919	15	0
1	В	1912	1842	1919	17	0
1	С	1912	1842	1919	7	0
1	D	1912	1847	1919	10	0
1	Е	1917	1848	1923	7	0
1	F	1918	1859	1932	6	0
1	G	1917	1849	1923	10	0
1	Н	1912	1847	1919	15	0
1	Ι	1912	1860	1919	4	0
1	J	1918	1891	1932	12	0
1	K	1918	1853	1932	7	0
1	L	1912	1862	1919	14	0
2	А	44	27	26	3	0
2	В	44	27	26	3	0
2	С	44	27	26	1	0
2	D	44	27	26	0	0
2	Ε	44	27	26	1	0
2	F	44	27	26	1	0
2	G	44	27	26	2	0
2	Н	44	27	26	1	0
2	Ι	44	27	26	2	0
2	J	44	27	26	1	0
2	K	44	27	26	2	0
2	L	44	27	26	1	0
3	А	18	12	0	1	0
3	В	18	12	0	0	0
3	С	18	12	0	0	0
3	D	18	12	0	0	0
3	E	18	12	0	0	0
3	F	18	12	0	0	0
3	G	18	12	0	0	0
3	Н	18	12	0	0	0
3	Ι	18	12	0	0	0
3	J	18	12	0	1	0
3	K	18	12	0	0	0
3	L	18	12	0	1	0
4	A	$2\overline{2}$	0	0	0	0



Mol	Chain	Non-H	${ m H(model)}$	H(added)	Clashes	Symm-Clashes		
4	В	20	0	0	1	0		
4	С	13	0	0	0	0		
4	D	32	0	0	0	0		
4	Е	22	0	0	0	0		
4	F	24	0	0	0	0		
4	G	23	0	0	0	0		
4	Н	17	0	0	0	0		
4	Ι	10	0	0	0	0		
4	J	20	0	0	1	0		
4	Κ	18	0	0	0	0		
4	L	12	0	0	0	0		
All	All	23949	22715	23387	120	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 3.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:101:ALA:HB1	1:L:201:LYS:HD2	1.50	0.91
1:H:101:ALA:HB1	1:H:201:LYS:HD2	1.56	0.87
1:G:97:ARG:NH1	1:L:138:ASP:OD2	2.15	0.79
1:C:30:ARG:NH2	1:C:227:ASN:OD1	2.18	0.76
1:A:101:ALA:HB1	1:A:201:LYS:HD2	1.67	0.76
1:B:202:SER:HB3	1:B:205:LYS:HD2	1.68	0.75
1:H:79:LYS:NZ	1:H:83:ASP:O	2.23	0.72
1:C:79:LYS:NZ	1:C:83:ASP:O	2.25	0.69
1:G:79:LYS:NZ	1:G:83:ASP:O	2.27	0.67
1:L:101:ALA:CB	1:L:201:LYS:HD2	2.24	0.65
1:D:95:ALA:HB2	1:D:159:MET:HE2	1.80	0.64
1:B:11:LEU:HD23	1:B:89:VAL:HB	1.80	0.63
1:D:79:LYS:NZ	1:D:83:ASP:O	2.32	0.63
1:D:155:ASN:ND2	1:D:201:LYS:O	2.32	0.62
2:I:301:NAD:O1N	2:I:301:NAD:H2N	1.99	0.62
1:B:97:ARG:NE	4:B:401:HOH:O	2.33	0.60
1:J:193:LYS:NZ	4:J:401:HOH:O	2.34	0.60
2:B:301:NAD:O1N	2:B:301:NAD:H2N	2.02	0.59
1:B:194:THR:HG21	2:B:301:NAD:O2N	2.04	0.58
1:A:194:THR:HG21	2:A:301:NAD:O2N	2.04	0.57
1:K:19:SER:OG	2:K:301:NAD:O1A	2.19	0.57
1:B:106:ASP:OD2	1:L:26:LYS:NZ	2.38	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:195:LEU:HG	1:J:83:ASP:OD2	2.06	0.56
1:C:11:LEU:HD23	1:C:89:VAL:HB	1.88	0.56
2:A:301:NAD:O1N	2:A:301:NAD:H2N	2.05	0.56
1:A:102:GLY:H	1:A:201:LYS:HD3	1.70	0.55
1:H:101:ALA:CB	1:H:201:LYS:HD2	2.33	0.55
1:F:19:SER:OG	2:F:301:NAD:O1A	2.21	0.55
1:H:202:SER:HB2	1:H:205:LYS:HD2	1.88	0.55
1:E:19:SER:OG	2:E:301:NAD:O1A	2.26	0.53
1:B:79:LYS:NZ	1:B:83:ASP:O	2.40	0.53
1:D:2:GLY:N	1:D:5:ASP:OD2	2.42	0.52
1:A:95:ALA:HB2	1:A:159:MET:CE	2.40	0.51
1:H:221:THR:HB	1:H:223:GLU:OE1	2.11	0.51
1:B:19:SER:OG	2:B:301:NAD:O1A	2.20	0.50
1:B:40:VAL:HG23	1:B:64:ASP:HB2	1.94	0.50
1:K:42:ASP:N	1:K:42:ASP:OD1	2.44	0.50
1:L:196:ALA:HB2	2:L:301:NAD:O2A	2.12	0.50
1:G:9:ILE:HG22	1:G:11:LEU:HD12	1.94	0.50
1:G:88:LEU:HB3	1:G:141:LEU:HD22	1.94	0.49
1:I:194:THR:HG21	2:I:301:NAD:O2N	2.12	0.49
1:J:156:TYR:OH	3:J:302:68O:OAB	2.23	0.49
1:K:138:ASP:N	1:K:138:ASP:OD1	2.45	0.49
1:L:88:LEU:HB3	1:L:141:LEU:HD22	1.94	0.49
1:J:8:ARG:HH12	1:J:83:ASP:HB3	1.76	0.49
1:L:221:THR:HB	1:L:223:GLU:OE1	2.14	0.48
1:C:11:LEU:HD13	1:C:25:ALA:HB2	1.96	0.47
1:G:47:ARG:CZ	1:L:79:LYS:HE2	2.44	0.47
1:F:11:LEU:CD2	1:F:25:ALA:HB2	2.45	0.47
1:J:151:ARG:NH2	1:J:252:ASN:O	2.47	0.47
1:H:88:LEU:HB3	1:H:141:LEU:HD22	1.96	0.47
1:F:8:ARG:HH22	1:F:83:ASP:H	1.63	0.47
1:G:192:ILE:HD11	1:G:220:VAL:HG23	1.97	0.47
1:B:16:SER:HB2	1:J:83:ASP:OD1	2.14	0.47
1:D:88:LEU:HB3	1:D:141:LEU:HD22	1.97	0.47
1:H:195:LEU:O	1:H:198:SER:OG	2.28	0.47
1:H:196:ALA:HB2	2:H:301:NAD:O2A	2.15	0.47
1:A:40:VAL:HG23	1:A:64:ASP:HB2	1.98	0.46
1:C:40:VAL:HG23	1:C:64:ASP:HB2	1.98	0.46
1:J:48:ILE:HG23	1:J:60:VAL:HG11	1.96	0.46
1:K:196:ALA:HB2	2:K:301:NAD:O2A	2.15	0.46
1:L:156:TYR:OH	3:L:302:68O:OAB	2.26	0.46
1:B:16:SER:CB	1:J:83:ASP:OD1	2.64	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:26:LYS:NZ	1:A:223:GLU:OE2	2.49	0.46
2:G:301:NAD:H2N	2:G:301:NAD:O1N	2.16	0.46
1:E:25:ALA:HB1	1:E:55:PHE:CE2	2.51	0.46
1:J:19:SER:OG	2:J:301:NAD:O1A	2.18	0.45
1:D:151:ARG:NH2	1:D:252:ASN:O	2.46	0.45
1:H:26:LYS:NZ	1:H:223:GLU:HG3	2.30	0.45
1:D:132:LEU:HD13	1:D:177:LEU:HD22	1.98	0.45
1:H:192:ILE:HD11	1:H:220:VAL:HG23	1.99	0.45
1:B:11:LEU:HD23	1:B:89:VAL:CB	2.46	0.45
1:G:34:GLU:HG2	1:G:82:TRP:HZ2	1.81	0.45
1:B:202:SER:HB3	1:B:205:LYS:CD	2.44	0.44
1:C:196:ALA:HB2	2:C:301:NAD:O2A	2.17	0.44
1:A:101:ALA:CB	1:A:201:LYS:HD2	2.43	0.44
1:A:42:ASP:O	1:A:43:ARG:HB3	2.18	0.44
1:G:196:ALA:HB2	2:G:301:NAD:O2A	2.17	0.44
1:I:88:LEU:HB3	1:I:141:LEU:HD22	1.99	0.44
1:F:40:VAL:HG23	1:F:64:ASP:HB2	1.99	0.44
1:F:132:LEU:HD13	1:F:177:LEU:HD22	2.01	0.43
1:E:88:LEU:HB3	1:E:141:LEU:HD22	1.99	0.43
1:B:11:LEU:HD23	1:B:89:VAL:CG2	2.48	0.43
1:A:26:LYS:NZ	1:A:223:GLU:HG3	2.34	0.43
1:J:221:THR:HB	1:J:223:GLU:OE1	2.19	0.43
1:H:11:LEU:CD2	1:H:25:ALA:HB2	2.49	0.42
1:A:64:ASP:OD1	2:A:301:NAD:N6A	2.49	0.42
1:L:30:ARG:NH2	1:L:227:ASN:OD1	2.46	0.42
1:A:201:LYS:HB3	1:A:201:LYS:HE3	1.86	0.42
1:B:11:LEU:CD2	1:B:89:VAL:HG21	2.49	0.42
1:C:88:LEU:HB3	1:C:141:LEU:HD22	2.00	0.42
1:A:88:LEU:HB3	1:A:141:LEU:HD22	2.02	0.42
1:H:75:PHE:CZ	1:H:131:ALA:HB2	2.55	0.41
1:K:8:ARG:HH12	1:K:83:ASP:HB3	1.85	0.41
1:L:101:ALA:HA	1:L:201:LYS:HD3	2.01	0.41
1:E:37:PHE:HZ	1:E:55:PHE:HD2	1.68	0.41
1:E:124:PHE:HB3	1:E:125:PRO:CD	2.50	0.41
1:I:40:VAL:O	1:I:44:PHE:HD2	2.03	0.41
1:L:124:PHE:HB3	1:L:125:PRO:CD	2.49	0.41
1:G:194:THR:O	1:G:197:ALA:HB3	2.20	0.41
1:K:132:LEU:HD13	1:K:177:LEU:HD22	2.01	0.41
1:K:206:ILE:HG12	1:L:258:MET:SD	2.61	0.41
1:H:15:LEU:HD23	1:H:195:LEU:HD12	2.02	0.41
1:B:132:LEU:N	1:B:133:PRO:CD	2.84	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:223:GLU:OE1	1:J:223:GLU:N	2.47	0.41
1:B:75:PHE:CZ	1:B:131:ALA:HB2	2.56	0.41
1:A:209:PHE:CG	1:D:258:MET:HG2	2.56	0.41
1:D:95:ALA:HB2	1:D:159:MET:CE	2.49	0.41
1:L:138:ASP:OD1	1:L:138:ASP:N	2.50	0.41
1:E:37:PHE:CZ	1:E:55:PHE:HD2	2.39	0.41
1:A:124:PHE:HB3	1:A:125:PRO:CD	2.51	0.41
1:A:200:ILE:HD12	3:A:302:68O:CAN	2.50	0.41
1:H:124:PHE:HB3	1:H:125:PRO:CD	2.51	0.41
1:D:124:PHE:HB3	1:D:125:PRO:CD	2.51	0.41
1:F:138:ASP:N	1:F:138:ASP:OD1	2.53	0.40
1:I:177:LEU:HB3	1:I:182:VAL:HB	2.03	0.40
1:E:11:LEU:HD13	1:E:25:ALA:HB2	2.04	0.40
1:J:177:LEU:HB3	1:J:182:VAL:HB	2.03	0.40
1:H:132:LEU:HB3	1:H:133:PRO:HD3	2.04	0.40
1:G:124:PHE:HB3	1:G:125:PRO:CD	2.52	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	Perce	ntiles
1	А	255/276~(92%)	241 (94%)	13 (5%)	1 (0%)	34	60
1	В	255/276~(92%)	243 (95%)	12 (5%)	0	100	100
1	С	255/276~(92%)	241 (94%)	14 (6%)	0	100	100
1	D	255/276~(92%)	244 (96%)	11 (4%)	0	100	100
1	Е	256/276~(93%)	244 (95%)	12 (5%)	0	100	100
1	F	256/276~(93%)	243 (95%)	13 (5%)	0	100	100
1	G	256/276~(93%)	242 (94%)	13 (5%)	1 (0%)	34	60



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Н	255/276~(92%)	243~(95%)	12 (5%)	0	100 100
1	Ι	255/276~(92%)	243~(95%)	12~(5%)	0	100 100
1	J	256/276~(93%)	245~(96%)	11 (4%)	0	100 100
1	Κ	256/276~(93%)	245~(96%)	11 (4%)	0	100 100
1	L	255/276~(92%)	243~(95%)	12 (5%)	0	100 100
All	All	3065/3312~(92%)	2917 (95%)	146 (5%)	2~(0%)	51 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	202	SER
1	А	202	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	195/209~(93%)	193~(99%)	2(1%)	76	91
1	В	195/209~(93%)	194 (100%)	1 (0%)	88	96
1	С	195/209~(93%)	194 (100%)	1 (0%)	88	96
1	D	195/209~(93%)	194 (100%)	1 (0%)	88	96
1	Ε	196/209~(94%)	195 (100%)	1 (0%)	88	96
1	F	196/209~(94%)	194 (99%)	2(1%)	76	91
1	G	196/209~(94%)	194 (99%)	2(1%)	76	91
1	Η	195/209~(93%)	194 (100%)	1 (0%)	88	96
1	Ι	195/209~(93%)	194 (100%)	1 (0%)	88	96
1	J	196/209~(94%)	193~(98%)	3(2%)	65	86
1	Κ	196/209~(94%)	194 (99%)	2(1%)	76	91
1	L	195/209~(93%)	191 (98%)	4 (2%)	53	80
All	All	2345/2508~(94%)	2324 (99%)	21 (1%)	78	92



Mol	Chain	\mathbf{Res}	Type
1	В	136	SER
1	Е	136	SER
1	Н	43	ARG
1	С	258	MET
1	А	19	SER
1	А	136	SER
1	F	18	ARG
1	F	208	ASP
1	G	43	ARG
1	G	176	SER
1	D	47	ARG
1	Ι	137	ASP
1	Κ	42	ASP
1	Κ	258	MET
1	L	8	ARG
1	L	29	LYS
1	L	43	ARG
1	L	180	LYS
1	J	8	ARG
1	J	26	LYS
1	J	97	ARG

All (21) residues with a non-rotameric sidechain are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

24 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).

Mal	Type	Chain	Bos	Link	Bo	Bond lengths		Bond angles		
	Type	Unam	Ites		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	68O	Н	302	-	19,19,19	1.26	1(5%)	$25,\!26,\!26$	1.31	3 (12%)
2	NAD	L	301	-	42,48,48	0.83	2 (4%)	50,73,73	1.37	3 (6%)
3	68O	F	302	-	19,19,19	1.22	1 (5%)	25,26,26	1.32	3 (12%)
3	68O	L	302	-	19,19,19	1.20	1 (5%)	25,26,26	1.32	3 (12%)
3	68O	Е	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.27	3 (12%)
2	NAD	В	301	-	42,48,48	0.87	2 (4%)	50,73,73	1.43	3 (6%)
3	68O	D	302	-	19,19,19	1.37	2 (10%)	25,26,26	1.35	5 (20%)
3	68O	Ι	302	-	19,19,19	1.21	1 (5%)	25,26,26	1.29	3 (12%)
2	NAD	J	301	-	42,48,48	0.94	2 (4%)	50,73,73	1.40	2 (4%)
2	NAD	Ι	301	-	42,48,48	0.86	2 (4%)	50,73,73	1.38	2 (4%)
3	68O	А	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.28	3 (12%)
2	NAD	F	301	-	42,48,48	0.93	2 (4%)	50,73,73	1.34	3 (6%)
2	NAD	А	301	-	42,48,48	0.88	2 (4%)	50,73,73	1.40	4 (8%)
2	NAD	G	301	-	42,48,48	0.82	2 (4%)	50,73,73	1.41	4 (8%)
3	68O	G	302	-	19,19,19	1.25	1 (5%)	25,26,26	1.33	3 (12%)
2	NAD	С	301	-	42,48,48	0.94	2 (4%)	50,73,73	1.35	3 (6%)
2	NAD	Е	301	-	42,48,48	0.94	2 (4%)	50,73,73	1.33	3 (6%)
3	68O	J	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.20	3 (12%)
3	68O	С	302	-	19,19,19	1.33	2 (10%)	25,26,26	1.25	3 (12%)
3	68O	В	302	-	19,19,19	1.25	1 (5%)	25,26,26	1.26	3 (12%)
3	68O	K	302	-	19,19,19	1.23	1 (5%)	25,26,26	1.52	6 (24%)
2	NAD	D	301	-	42,48,48	0.88	2 (4%)	50,73,73	1.37	3 (6%)
2	NAD	Н	301	-	42,48,48	0.96	2 (4%)	50,73,73	1.40	2 (4%)
2	NAD	K	301	-	42,48,48	0.92	2 (4%)	50,73,73	1.34	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	68O	Н	302	-	-	0/6/6/6	0/2/2/2
2	NAD	L	301	-	-	5/26/62/62	0/5/5/5
3	68O	F	302	-	-	0/6/6/6	0/2/2/2
3	68O	L	302	-	-	0/6/6/6	0/2/2/2
3	68O	Е	302	-	-	0/6/6/6	0/2/2/2
2	NAD	В	301	-	-	6/26/62/62	0/5/5/5
3	68O	D	302	-	-	0/6/6/6	0/2/2/2
3	68O	Ι	302	-	-	0/6/6/6	0/2/2/2
2	NAD	J	301	-	-	14/26/62/62	0/5/5/5
2	NAD	Ι	301	-	-	4/26/62/62	0/5/5/5
3	68O	А	302	-	-	0/6/6/6	0/2/2/2
2	NAD	F	301	-	-	7/26/62/62	0/5/5/5
2	NAD	А	301	-	-	5/26/62/62	0/5/5/5
2	NAD	G	301	-	-	4/26/62/62	0/5/5/5
3	68O	G	302	-	-	0/6/6/6	0/2/2/2
2	NAD	С	301	-	-	7/26/62/62	0/5/5/5
2	NAD	Е	301	-	-	6/26/62/62	0/5/5/5
3	68O	J	302	-	-	0/6/6/6	0/2/2/2
3	68O	С	302	-	-	0/6/6/6	0/2/2/2
3	68O	В	302	-	-	0/6/6/6	0/2/2/2
3	68O	K	302	-	-	2/6/6/6	0/2/2/2
2	NAD	D	301	-	-	6/26/62/62	0/5/5/5
2	NAD	Н	301	-	-	6/26/62/62	0/5/5/5
2	NAD	K	301	-	-	7/26/62/62	0/5/5/5

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.

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	68O	CAK-CAP	-4.64	1.39	1.51
3	Ι	302	68O	CAK-CAP	-4.51	1.39	1.51
3	D	302	68O	CAK-CAP	-4.50	1.39	1.51
3	Н	302	68O	CAK-CAP	-4.48	1.39	1.51
3	А	302	68O	CAK-CAP	-4.45	1.39	1.51
3	В	302	68O	CAK-CAP	-4.42	1.39	1.51
3	L	302	68O	CAK-CAP	-4.41	1.39	1.51
3	J	302	68O	CAK-CAP	-4.36	1.39	1.51
3	F	302	68O	CAK-CAP	-4.30	1.39	1.51



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Е	302	68O	CAK-CAP	-4.18	1.40	1.51
3	Κ	302	68O	CAK-CAP	-4.15	1.40	1.51
3	С	302	68O	CAK-CAP	-4.12	1.40	1.51
2	Κ	301	NAD	C2N-N1N	4.04	1.39	1.35
2	J	301	NAD	C2N-N1N	4.02	1.39	1.35
2	D	301	NAD	C2N-N1N	3.92	1.39	1.35
2	А	301	NAD	C2N-N1N	3.91	1.39	1.35
2	Н	301	NAD	O4D-C1D	-3.83	1.35	1.41
2	С	301	NAD	C2N-N1N	3.77	1.39	1.35
2	Е	301	NAD	C2N-N1N	3.66	1.39	1.35
2	Ι	301	NAD	C2N-N1N	3.66	1.39	1.35
2	В	301	NAD	C2N-N1N	3.65	1.39	1.35
2	Н	301	NAD	C2N-N1N	3.57	1.39	1.35
2	F	301	NAD	O4D-C1D	-3.52	1.36	1.41
2	L	301	NAD	C2N-N1N	3.46	1.39	1.35
2	F	301	NAD	C2N-N1N	3.45	1.39	1.35
2	С	301	NAD	O4D-C1D	-3.30	1.36	1.41
2	Е	301	NAD	O4D-C1D	-3.26	1.36	1.41
2	G	301	NAD	C2N-N1N	3.22	1.38	1.35
2	J	301	NAD	O4D-C1D	-3.03	1.36	1.41
3	С	302	68O	FAC-CAN	-2.83	1.28	1.35
2	Κ	301	NAD	O4D-C1D	-2.72	1.37	1.41
2	В	301	NAD	O4D-C1D	-2.67	1.37	1.41
3	D	302	680	FAC-CAN	-2.66	1.28	1.35
2	A	301	NAD	O4D-C1D	-2.28	1.37	1.41
2	Ι	301	NAD	O4D-C1D	-2.26	1.37	1.41
2	G	301	NAD	O4D-C1D	-2.18	1.38	1.41
2	L	301	NAD	O4D-C1D	-2.16	1.38	1.41
2	D	301	NAD	O4D-C1D	-2.11	1.38	1.41

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All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	301	NAD	PN-O3-PA	8.27	161.22	132.83
2	Н	301	NAD	PN-O3-PA	8.08	160.57	132.83
2	J	301	NAD	PN-O3-PA	8.04	160.41	132.83
2	G	301	NAD	PN-O3-PA	7.87	159.84	132.83
2	Ι	301	NAD	PN-O3-PA	7.79	159.55	132.83
2	А	301	NAD	PN-O3-PA	7.74	159.39	132.83
2	С	301	NAD	PN-O3-PA	7.69	159.20	132.83
2	L	301	NAD	PN-O3-PA	7.64	159.05	132.83
2	Е	301	NAD	PN-O3-PA	7.61	158.95	132.83



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	Κ	301	NAD	PN-O3-PA	7.48	158.51	132.83
2	D	301	NAD	PN-O3-PA	7.47	158.45	132.83
2	F	301	NAD	PN-O3-PA	7.40	158.21	132.83
3	Κ	302	68O	FAC-CAN-CAP	3.25	123.27	117.96
3	G	302	68O	CAI-CAP-CAN	3.02	120.10	116.58
3	Κ	302	68O	CAJ-CAN-CAP	-3.01	120.04	123.98
3	Ι	302	68O	CAI-CAP-CAN	2.90	119.96	116.58
3	В	302	68O	CAI-CAP-CAN	2.86	119.91	116.58
3	L	302	68O	CAJ-CAN-CAP	-2.86	120.23	123.98
3	Н	302	68O	CAI-CAP-CAN	2.85	119.90	116.58
3	L	302	68O	CAI-CAP-CAN	2.83	119.88	116.58
2	G	301	NAD	C3D-C2D-C1D	-2.81	96.75	100.98
3	А	302	68O	CAI-CAP-CAN	2.81	119.84	116.58
3	D	302	68O	CAI-CAP-CAN	2.79	119.83	116.58
3	F	302	68O	CAI-CAP-CAN	2.79	119.82	116.58
3	Κ	302	68O	CAQ-OAL-CAR	-2.75	111.48	118.04
3	В	302	68O	CAJ-CAN-CAP	-2.73	120.40	123.98
3	Ι	302	68O	CAJ-CAN-CAP	-2.70	120.44	123.98
3	Н	302	68O	CAJ-CAN-CAP	-2.68	120.46	123.98
3	G	302	68O	CAJ-CAN-CAP	-2.68	120.46	123.98
3	J	302	68O	CAJ-CAN-CAP	-2.64	120.51	123.98
3	J	302	68O	CAI-CAP-CAN	2.60	119.60	116.58
3	А	302	68O	CAJ-CAN-CAP	-2.59	120.58	123.98
3	F	302	68O	CAJ-CAN-CAP	-2.57	120.61	123.98
3	Е	302	68O	CAJ-CAN-CAP	-2.55	120.63	123.98
2	Ε	301	NAD	O4D-C1D-C2D	-2.52	103.24	106.93
3	А	302	68O	OAL-CAR-CAO	-2.44	114.22	119.26
3	С	302	68O	CAI-CAP-CAN	2.43	119.41	116.58
2	F	301	NAD	O4D-C1D-C2D	-2.39	103.43	106.93
2	В	301	NAD	O4D-C1D-C2D	-2.38	103.44	106.93
3	L	302	68O	OAL-CAR-CAO	-2.37	114.37	119.26
3	Ε	302	68O	CAI-CAP-CAN	2.33	119.29	116.58
2	Ε	301	NAD	C5A-C6A-N6A	2.33	123.89	120.35
2	F	301	NAD	C5A-C6A-N6A	2.32	123.88	120.35
3	K	$30\overline{2}$	68O	CAK-CAP-CAI	-2.32	114.85	119.60
3	В	302	68O	OAL-CAR-CAO	-2.32	114.48	119.26
2	D	301	NAD	C5A-C6A-N6A	2.32	123.87	120.35
3	C	$30\overline{2}$	68O	CAJ-CAN-CAP	-2.30	$120.9\overline{7}$	123.98
2	D	$30\overline{1}$	NAD	C3D-C2D-C1D	-2.29	97.52	100.98
3	Ι	302	68O	OAL-CAR-CAO	-2.29	114.54	119.26
2	K	$30\overline{1}$	NAD	C5A-C6A-N6A	$2.2\overline{9}$	$123.8\overline{3}$	120.35
2	А	301	NAD	C5A-C6A-N6A	2.28	123.82	120.35

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
2	С	301	NAD	C5A-C6A-N6A	2.27	123.80	120.35
2	Н	301	NAD	C5A-C6A-N6A	2.25	123.78	120.35
2	В	301	NAD	C5A-C6A-N6A	2.25	123.78	120.35
2	Ι	301	NAD	C5A-C6A-N6A	2.25	123.77	120.35
2	G	301	NAD	C5A-C6A-N6A	2.24	123.76	120.35
2	L	301	NAD	C5A-C6A-N6A	2.23	123.73	120.35
2	J	301	NAD	C5A-C6A-N6A	2.21	123.71	120.35
3	G	302	68O	OAL-CAR-CAO	-2.19	114.75	119.26
3	F	302	68O	OAL-CAR-CAO	-2.18	114.76	119.26
3	Н	302	68O	OAL-CAR-CAO	-2.18	114.77	119.26
3	С	302	68O	OAL-CAR-CAO	-2.16	114.81	119.26
2	С	301	NAD	O4D-C1D-C2D	-2.14	103.80	106.93
2	А	301	NAD	C3D-C2D-C1D	-2.13	97.77	100.98
3	D	302	68O	OAL-CAR-CAO	-2.13	114.87	119.26
3	D	302	68O	CAJ-CAN-CAP	-2.13	121.19	123.98
3	D	302	68O	CAM-CAI-CAP	-2.12	118.52	121.55
3	Е	302	68O	OAL-CAR-CAO	-2.12	114.89	119.26
2	L	301	NAD	C3D-C2D-C1D	-2.12	97.79	100.98
3	K	302	68O	CAI-CAP-CAN	2.09	119.01	116.58
2	А	301	NAD	O4D-C1D-C2D	-2.06	103.91	106.93
3	D	302	680	CAG-CAO-CAR	-2.06	119.84	122.12
2	G	301	NAD	O4D-C1D-C2D	-2.04	103.94	106.93
3	K	302	680	OAL-CAR-CAO	-2.02	115.09	119.26
3	J	302	680	OAL-CAR-CAO	-2.02	115.09	119.26

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	301	NAD	C5B-O5B-PA-O2A
2	Е	301	NAD	C5D-O5D-PN-O2N
2	Н	301	NAD	PN-O3-PA-O5B
2	Н	301	NAD	C5D-O5D-PN-O2N
2	С	301	NAD	C5B-O5B-PA-O2A
2	С	301	NAD	C5D-O5D-PN-O1N
2	С	301	NAD	C5D-O5D-PN-O2N
2	А	301	NAD	C5B-O5B-PA-O2A
2	F	301	NAD	PN-O3-PA-O5B
2	F	301	NAD	C5D-O5D-PN-O1N
2	F	301	NAD	C5D-O5D-PN-O2N
2	F	301	NAD	O4D-C1D-N1N-C2N
2	D	301	NAD	C5B-O5B-PA-O2A



Mol	Chain	Res	Type	Atoms
2	K	301	NAD	C5D-O5D-PN-O2N
2	K	301	NAD	O4D-C1D-N1N-C2N
2	J	301	NAD	C5D-O5D-PN-O2N
2	J	301	NAD	O4D-C1D-N1N-C2N
2	J	301	NAD	O4D-C1D-N1N-C6N
3	K	302	68O	CAA-CAK-CAP-CAI
3	K	302	68O	CAA-CAK-CAP-CAN
2	В	301	NAD	O4D-C4D-C5D-O5D
2	В	301	NAD	C3D-C4D-C5D-O5D
2	J	301	NAD	O4B-C4B-C5B-O5B
2	J	301	NAD	C3B-C4B-C5B-O5B
2	Ι	301	NAD	O4D-C4D-C5D-O5D
2	Ι	301	NAD	C3D-C4D-C5D-O5D
2	G	301	NAD	C3D-C4D-C5D-O5D
2	L	301	NAD	C3D-C4D-C5D-O5D
2	В	301	NAD	PA-O3-PN-O5D
2	Е	301	NAD	PN-O3-PA-O5B
2	С	301	NAD	PN-O3-PA-O5B
2	J	301	NAD	C4B-C5B-O5B-PA
2	Е	301	NAD	C5D-O5D-PN-O3
2	Н	301	NAD	C5D-O5D-PN-O3
2	С	301	NAD	C5D-O5D-PN-O3
2	F	301	NAD	C5D-O5D-PN-O3
2	K	301	NAD	C5D-O5D-PN-O3
2	J	301	NAD	C5B-O5B-PA-O3
2	J	301	NAD	C5D-O5D-PN-O3
2	А	301	NAD	C3D-C4D-C5D-O5D
2	L	301	NAD	PA-O3-PN-O1N
2	В	301	NAD	C5B-O5B-PA-O1A
2	Е	301	NAD	C5D-O5D-PN-O1N
2	Н	301	NAD	C5B-O5B-PA-O1A
2	Н	301	NAD	C5D-O5D-PN-O1N
2	С	301	NAD	C5B-O5B-PA-O1A
2	А	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5B-O5B-PA-O1A
2	Ι	301	NAD	C5B-O5B-PA-O1A
2	K	301	NAD	C5D-O5D-PN-O1N
2	J	301	NAD	C5B-O5B-PA-O1A
2	J	301	NAD	C5B-O5B-PA-O2A
2	J	301	NAD	C5D-O5D-PN-O1N
2	D	301	NAD	C3D-C4D-C5D-O5D
2	G	301	NAD	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	L	301	NAD	O4D-C4D-C5D-O5D
2	J	301	NAD	PA-O3-PN-O2N
2	F	301	NAD	O4B-C4B-C5B-O5B
2	Κ	301	NAD	O4B-C4B-C5B-O5B
2	L	301	NAD	O4B-C4B-C5B-O5B
2	L	301	NAD	PA-O3-PN-O2N
2	С	301	NAD	O4B-C4B-C5B-O5B
2	А	301	NAD	O4D-C4D-C5D-O5D
2	Н	301	NAD	O4B-C4B-C5B-O5B
2	А	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	C5B-O5B-PA-O3
2	J	301	NAD	C2D-C1D-N1N-C6N
2	В	301	NAD	O4B-C4B-C5B-O5B
2	Е	301	NAD	O4B-C4B-C5B-O5B
2	G	301	NAD	O4B-C4B-C5B-O5B
2	Ι	301	NAD	O4B-C4B-C5B-O5B
2	K	301	NAD	PA-O3-PN-O2N
2	J	301	NAD	PA-O3-PN-O1N
2	Е	301	NAD	C5B-O5B-PA-O1A
2	F	301	NAD	C5B-O5B-PA-O1A
2	G	301	NAD	C5B-O5B-PA-O1A
2	К	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	O4D-C4D-C5D-O5D

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There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	301	NAD	1	0
3	L	302	68O	1	0
2	В	301	NAD	3	0
2	J	301	NAD	1	0
2	Ι	301	NAD	2	0
3	А	302	68O	1	0
2	F	301	NAD	1	0
2	А	301	NAD	3	0
2	G	301	NAD	2	0
2	С	301	NAD	1	0
2	Е	301	NAD	1	0
3	J	302	68O	1	0
2	Н	301	NAD	1	0



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Κ	301	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







W O R L D W I D E PROTEIN DATA BANK



















































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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









































6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

