



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:02 PM GMT

PDB ID : 4NK4  
Title : Crystal structure of FabI from Candidatus Liberibacter asiaticus  
Authors : Jiang, L.; Gao, Z.Q.; Dong, Y.H.  
Deposited on : 2013-11-12  
Resolution : 1.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

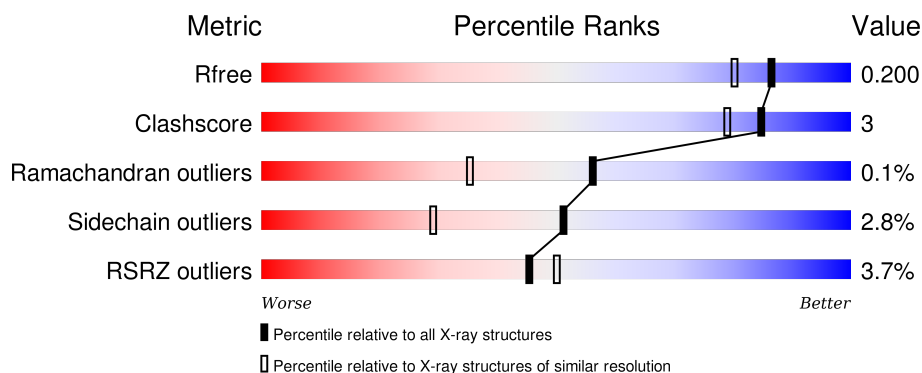
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	301	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>14%</div> </div> </div>
1	B	301	<div> <div></div> <div> <div>80%</div> <div>6%</div> <div>14%</div> </div> </div>
1	C	301	<div> <div>%</div> <div> <div>80%</div> <div>5%</div> <div>14%</div> </div> </div>
1	D	301	<div> <div>6%</div> <div> <div>77%</div> <div>7%</div> <div>14%</div> </div> </div>
1	E	301	<div> <div>4%</div> <div> <div>78%</div> <div>7%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	301	

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	PEG	A	300	-	-	-	X
2	PEG	B	300	-	-	-	X
2	PEG	B	301	-	-	-	X
2	PEG	C	300	-	-	-	X
2	PEG	E	300	-	-	-	X
2	PEG	E	301	-	-	-	X
2	PEG	F	300	-	-	-	X
2	PEG	F	301	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13342 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1973	1247	340	371	15			
1	B	258	Total	C	N	O	S	0	0	0
			1973	1247	340	371	15			
1	C	258	Total	C	N	O	S	0	0	0
			1973	1247	340	371	15			
1	D	258	Total	C	N	O	S	0	0	0
			1973	1247	340	371	15			
1	E	258	Total	C	N	O	S	0	0	0
			1973	1247	340	371	15			
1	F	257	Total	C	N	O	S	0	0	0
			1965	1242	339	370	14			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	EXPRESSION TAG	UNP M4Q2P0
A	-32	GLY	-	EXPRESSION TAG	UNP M4Q2P0
A	-31	SER	-	EXPRESSION TAG	UNP M4Q2P0
A	-30	SER	-	EXPRESSION TAG	UNP M4Q2P0
A	-29	HIS	-	EXPRESSION TAG	UNP M4Q2P0
A	-28	HIS	-	EXPRESSION TAG	UNP M4Q2P0
A	-27	HIS	-	EXPRESSION TAG	UNP M4Q2P0
A	-26	HIS	-	EXPRESSION TAG	UNP M4Q2P0
A	-25	HIS	-	EXPRESSION TAG	UNP M4Q2P0
A	-24	HIS	-	EXPRESSION TAG	UNP M4Q2P0
A	-23	SER	-	EXPRESSION TAG	UNP M4Q2P0
A	-22	SER	-	EXPRESSION TAG	UNP M4Q2P0
A	-21	GLY	-	EXPRESSION TAG	UNP M4Q2P0
A	-20	GLU	-	EXPRESSION TAG	UNP M4Q2P0
A	-19	ASN	-	EXPRESSION TAG	UNP M4Q2P0
A	-18	LEU	-	EXPRESSION TAG	UNP M4Q2P0
A	-17	TYR	-	EXPRESSION TAG	UNP M4Q2P0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	PHE	-	EXPRESSION TAG	UNP M4Q2P0
A	-15	GLU	-	EXPRESSION TAG	UNP M4Q2P0
A	-14	GLY	-	EXPRESSION TAG	UNP M4Q2P0
A	-13	SER	-	EXPRESSION TAG	UNP M4Q2P0
A	-12	HIS	-	EXPRESSION TAG	UNP M4Q2P0
A	-11	MET	-	EXPRESSION TAG	UNP M4Q2P0
A	-10	ALA	-	EXPRESSION TAG	UNP M4Q2P0
A	-9	SER	-	EXPRESSION TAG	UNP M4Q2P0
A	-8	MET	-	EXPRESSION TAG	UNP M4Q2P0
A	-7	THR	-	EXPRESSION TAG	UNP M4Q2P0
A	-6	GLY	-	EXPRESSION TAG	UNP M4Q2P0
A	-5	GLY	-	EXPRESSION TAG	UNP M4Q2P0
A	-4	GLN	-	EXPRESSION TAG	UNP M4Q2P0
A	-3	GLN	-	EXPRESSION TAG	UNP M4Q2P0
A	-2	MET	-	EXPRESSION TAG	UNP M4Q2P0
A	-1	GLY	-	EXPRESSION TAG	UNP M4Q2P0
A	0	ARG	-	EXPRESSION TAG	UNP M4Q2P0
B	-33	MET	-	EXPRESSION TAG	UNP M4Q2P0
B	-32	GLY	-	EXPRESSION TAG	UNP M4Q2P0
B	-31	SER	-	EXPRESSION TAG	UNP M4Q2P0
B	-30	SER	-	EXPRESSION TAG	UNP M4Q2P0
B	-29	HIS	-	EXPRESSION TAG	UNP M4Q2P0
B	-28	HIS	-	EXPRESSION TAG	UNP M4Q2P0
B	-27	HIS	-	EXPRESSION TAG	UNP M4Q2P0
B	-26	HIS	-	EXPRESSION TAG	UNP M4Q2P0
B	-25	HIS	-	EXPRESSION TAG	UNP M4Q2P0
B	-24	HIS	-	EXPRESSION TAG	UNP M4Q2P0
B	-23	SER	-	EXPRESSION TAG	UNP M4Q2P0
B	-22	SER	-	EXPRESSION TAG	UNP M4Q2P0
B	-21	GLY	-	EXPRESSION TAG	UNP M4Q2P0
B	-20	GLU	-	EXPRESSION TAG	UNP M4Q2P0
B	-19	ASN	-	EXPRESSION TAG	UNP M4Q2P0
B	-18	LEU	-	EXPRESSION TAG	UNP M4Q2P0
B	-17	TYR	-	EXPRESSION TAG	UNP M4Q2P0
B	-16	PHE	-	EXPRESSION TAG	UNP M4Q2P0
B	-15	GLU	-	EXPRESSION TAG	UNP M4Q2P0
B	-14	GLY	-	EXPRESSION TAG	UNP M4Q2P0
B	-13	SER	-	EXPRESSION TAG	UNP M4Q2P0
B	-12	HIS	-	EXPRESSION TAG	UNP M4Q2P0
B	-11	MET	-	EXPRESSION TAG	UNP M4Q2P0
B	-10	ALA	-	EXPRESSION TAG	UNP M4Q2P0
B	-9	SER	-	EXPRESSION TAG	UNP M4Q2P0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	EXPRESSION TAG	UNP M4Q2P0
B	-7	THR	-	EXPRESSION TAG	UNP M4Q2P0
B	-6	GLY	-	EXPRESSION TAG	UNP M4Q2P0
B	-5	GLY	-	EXPRESSION TAG	UNP M4Q2P0
B	-4	GLN	-	EXPRESSION TAG	UNP M4Q2P0
B	-3	GLN	-	EXPRESSION TAG	UNP M4Q2P0
B	-2	MET	-	EXPRESSION TAG	UNP M4Q2P0
B	-1	GLY	-	EXPRESSION TAG	UNP M4Q2P0
B	0	ARG	-	EXPRESSION TAG	UNP M4Q2P0
C	-33	MET	-	EXPRESSION TAG	UNP M4Q2P0
C	-32	GLY	-	EXPRESSION TAG	UNP M4Q2P0
C	-31	SER	-	EXPRESSION TAG	UNP M4Q2P0
C	-30	SER	-	EXPRESSION TAG	UNP M4Q2P0
C	-29	HIS	-	EXPRESSION TAG	UNP M4Q2P0
C	-28	HIS	-	EXPRESSION TAG	UNP M4Q2P0
C	-27	HIS	-	EXPRESSION TAG	UNP M4Q2P0
C	-26	HIS	-	EXPRESSION TAG	UNP M4Q2P0
C	-25	HIS	-	EXPRESSION TAG	UNP M4Q2P0
C	-24	HIS	-	EXPRESSION TAG	UNP M4Q2P0
C	-23	SER	-	EXPRESSION TAG	UNP M4Q2P0
C	-22	SER	-	EXPRESSION TAG	UNP M4Q2P0
C	-21	GLY	-	EXPRESSION TAG	UNP M4Q2P0
C	-20	GLU	-	EXPRESSION TAG	UNP M4Q2P0
C	-19	ASN	-	EXPRESSION TAG	UNP M4Q2P0
C	-18	LEU	-	EXPRESSION TAG	UNP M4Q2P0
C	-17	TYR	-	EXPRESSION TAG	UNP M4Q2P0
C	-16	PHE	-	EXPRESSION TAG	UNP M4Q2P0
C	-15	GLU	-	EXPRESSION TAG	UNP M4Q2P0
C	-14	GLY	-	EXPRESSION TAG	UNP M4Q2P0
C	-13	SER	-	EXPRESSION TAG	UNP M4Q2P0
C	-12	HIS	-	EXPRESSION TAG	UNP M4Q2P0
C	-11	MET	-	EXPRESSION TAG	UNP M4Q2P0
C	-10	ALA	-	EXPRESSION TAG	UNP M4Q2P0
C	-9	SER	-	EXPRESSION TAG	UNP M4Q2P0
C	-8	MET	-	EXPRESSION TAG	UNP M4Q2P0
C	-7	THR	-	EXPRESSION TAG	UNP M4Q2P0
C	-6	GLY	-	EXPRESSION TAG	UNP M4Q2P0
C	-5	GLY	-	EXPRESSION TAG	UNP M4Q2P0
C	-4	GLN	-	EXPRESSION TAG	UNP M4Q2P0
C	-3	GLN	-	EXPRESSION TAG	UNP M4Q2P0
C	-2	MET	-	EXPRESSION TAG	UNP M4Q2P0
C	-1	GLY	-	EXPRESSION TAG	UNP M4Q2P0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ARG	-	EXPRESSION TAG	UNP M4Q2P0
D	-33	MET	-	EXPRESSION TAG	UNP M4Q2P0
D	-32	GLY	-	EXPRESSION TAG	UNP M4Q2P0
D	-31	SER	-	EXPRESSION TAG	UNP M4Q2P0
D	-30	SER	-	EXPRESSION TAG	UNP M4Q2P0
D	-29	HIS	-	EXPRESSION TAG	UNP M4Q2P0
D	-28	HIS	-	EXPRESSION TAG	UNP M4Q2P0
D	-27	HIS	-	EXPRESSION TAG	UNP M4Q2P0
D	-26	HIS	-	EXPRESSION TAG	UNP M4Q2P0
D	-25	HIS	-	EXPRESSION TAG	UNP M4Q2P0
D	-24	HIS	-	EXPRESSION TAG	UNP M4Q2P0
D	-23	SER	-	EXPRESSION TAG	UNP M4Q2P0
D	-22	SER	-	EXPRESSION TAG	UNP M4Q2P0
D	-21	GLY	-	EXPRESSION TAG	UNP M4Q2P0
D	-20	GLU	-	EXPRESSION TAG	UNP M4Q2P0
D	-19	ASN	-	EXPRESSION TAG	UNP M4Q2P0
D	-18	LEU	-	EXPRESSION TAG	UNP M4Q2P0
D	-17	TYR	-	EXPRESSION TAG	UNP M4Q2P0
D	-16	PHE	-	EXPRESSION TAG	UNP M4Q2P0
D	-15	GLU	-	EXPRESSION TAG	UNP M4Q2P0
D	-14	GLY	-	EXPRESSION TAG	UNP M4Q2P0
D	-13	SER	-	EXPRESSION TAG	UNP M4Q2P0
D	-12	HIS	-	EXPRESSION TAG	UNP M4Q2P0
D	-11	MET	-	EXPRESSION TAG	UNP M4Q2P0
D	-10	ALA	-	EXPRESSION TAG	UNP M4Q2P0
D	-9	SER	-	EXPRESSION TAG	UNP M4Q2P0
D	-8	MET	-	EXPRESSION TAG	UNP M4Q2P0
D	-7	THR	-	EXPRESSION TAG	UNP M4Q2P0
D	-6	GLY	-	EXPRESSION TAG	UNP M4Q2P0
D	-5	GLY	-	EXPRESSION TAG	UNP M4Q2P0
D	-4	GLN	-	EXPRESSION TAG	UNP M4Q2P0
D	-3	GLN	-	EXPRESSION TAG	UNP M4Q2P0
D	-2	MET	-	EXPRESSION TAG	UNP M4Q2P0
D	-1	GLY	-	EXPRESSION TAG	UNP M4Q2P0
D	0	ARG	-	EXPRESSION TAG	UNP M4Q2P0
E	-33	MET	-	EXPRESSION TAG	UNP M4Q2P0
E	-32	GLY	-	EXPRESSION TAG	UNP M4Q2P0
E	-31	SER	-	EXPRESSION TAG	UNP M4Q2P0
E	-30	SER	-	EXPRESSION TAG	UNP M4Q2P0
E	-29	HIS	-	EXPRESSION TAG	UNP M4Q2P0
E	-28	HIS	-	EXPRESSION TAG	UNP M4Q2P0
E	-27	HIS	-	EXPRESSION TAG	UNP M4Q2P0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-26	HIS	-	EXPRESSION TAG	UNP M4Q2P0
E	-25	HIS	-	EXPRESSION TAG	UNP M4Q2P0
E	-24	HIS	-	EXPRESSION TAG	UNP M4Q2P0
E	-23	SER	-	EXPRESSION TAG	UNP M4Q2P0
E	-22	SER	-	EXPRESSION TAG	UNP M4Q2P0
E	-21	GLY	-	EXPRESSION TAG	UNP M4Q2P0
E	-20	GLU	-	EXPRESSION TAG	UNP M4Q2P0
E	-19	ASN	-	EXPRESSION TAG	UNP M4Q2P0
E	-18	LEU	-	EXPRESSION TAG	UNP M4Q2P0
E	-17	TYR	-	EXPRESSION TAG	UNP M4Q2P0
E	-16	PHE	-	EXPRESSION TAG	UNP M4Q2P0
E	-15	GLU	-	EXPRESSION TAG	UNP M4Q2P0
E	-14	GLY	-	EXPRESSION TAG	UNP M4Q2P0
E	-13	SER	-	EXPRESSION TAG	UNP M4Q2P0
E	-12	HIS	-	EXPRESSION TAG	UNP M4Q2P0
E	-11	MET	-	EXPRESSION TAG	UNP M4Q2P0
E	-10	ALA	-	EXPRESSION TAG	UNP M4Q2P0
E	-9	SER	-	EXPRESSION TAG	UNP M4Q2P0
E	-8	MET	-	EXPRESSION TAG	UNP M4Q2P0
E	-7	THR	-	EXPRESSION TAG	UNP M4Q2P0
E	-6	GLY	-	EXPRESSION TAG	UNP M4Q2P0
E	-5	GLY	-	EXPRESSION TAG	UNP M4Q2P0
E	-4	GLN	-	EXPRESSION TAG	UNP M4Q2P0
E	-3	GLN	-	EXPRESSION TAG	UNP M4Q2P0
E	-2	MET	-	EXPRESSION TAG	UNP M4Q2P0
E	-1	GLY	-	EXPRESSION TAG	UNP M4Q2P0
E	0	ARG	-	EXPRESSION TAG	UNP M4Q2P0
F	-33	MET	-	EXPRESSION TAG	UNP M4Q2P0
F	-32	GLY	-	EXPRESSION TAG	UNP M4Q2P0
F	-31	SER	-	EXPRESSION TAG	UNP M4Q2P0
F	-30	SER	-	EXPRESSION TAG	UNP M4Q2P0
F	-29	HIS	-	EXPRESSION TAG	UNP M4Q2P0
F	-28	HIS	-	EXPRESSION TAG	UNP M4Q2P0
F	-27	HIS	-	EXPRESSION TAG	UNP M4Q2P0
F	-26	HIS	-	EXPRESSION TAG	UNP M4Q2P0
F	-25	HIS	-	EXPRESSION TAG	UNP M4Q2P0
F	-24	HIS	-	EXPRESSION TAG	UNP M4Q2P0
F	-23	SER	-	EXPRESSION TAG	UNP M4Q2P0
F	-22	SER	-	EXPRESSION TAG	UNP M4Q2P0
F	-21	GLY	-	EXPRESSION TAG	UNP M4Q2P0
F	-20	GLU	-	EXPRESSION TAG	UNP M4Q2P0
F	-19	ASN	-	EXPRESSION TAG	UNP M4Q2P0

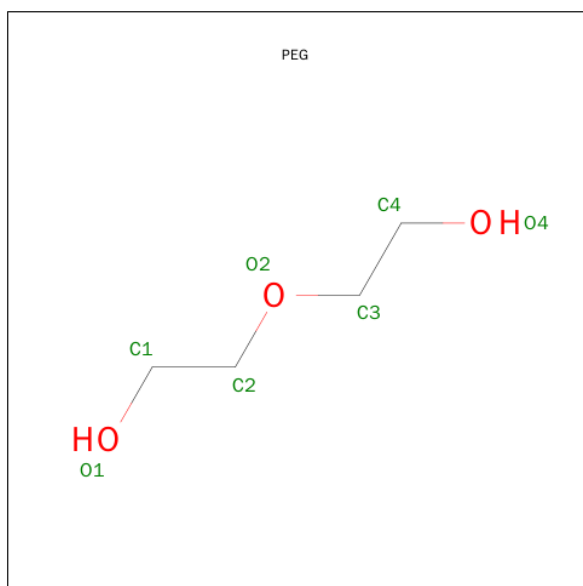
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	LEU	-	EXPRESSION TAG	UNP M4Q2P0
F	-17	TYR	-	EXPRESSION TAG	UNP M4Q2P0
F	-16	PHE	-	EXPRESSION TAG	UNP M4Q2P0
F	-15	GLU	-	EXPRESSION TAG	UNP M4Q2P0
F	-14	GLY	-	EXPRESSION TAG	UNP M4Q2P0
F	-13	SER	-	EXPRESSION TAG	UNP M4Q2P0
F	-12	HIS	-	EXPRESSION TAG	UNP M4Q2P0
F	-11	MET	-	EXPRESSION TAG	UNP M4Q2P0
F	-10	ALA	-	EXPRESSION TAG	UNP M4Q2P0
F	-9	SER	-	EXPRESSION TAG	UNP M4Q2P0
F	-8	MET	-	EXPRESSION TAG	UNP M4Q2P0
F	-7	THR	-	EXPRESSION TAG	UNP M4Q2P0
F	-6	GLY	-	EXPRESSION TAG	UNP M4Q2P0
F	-5	GLY	-	EXPRESSION TAG	UNP M4Q2P0
F	-4	GLN	-	EXPRESSION TAG	UNP M4Q2P0
F	-3	GLN	-	EXPRESSION TAG	UNP M4Q2P0
F	-2	MET	-	EXPRESSION TAG	UNP M4Q2P0
F	-1	GLY	-	EXPRESSION TAG	UNP M4Q2P0
F	0	ARG	-	EXPRESSION TAG	UNP M4Q2P0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		

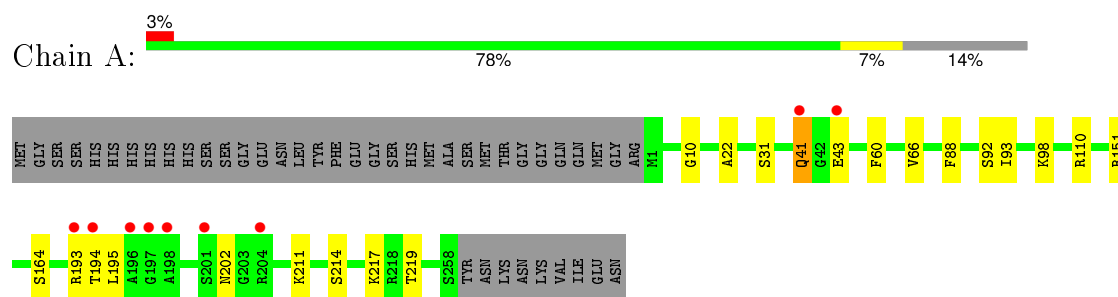
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	276	Total	O	0	0
			276	276		
3	B	291	Total	O	0	0
			291	291		
3	C	246	Total	O	0	0
			246	246		
3	D	187	Total	O	0	0
			187	187		
3	E	241	Total	O	0	0
			241	241		
3	F	201	Total	O	0	0
			201	201		

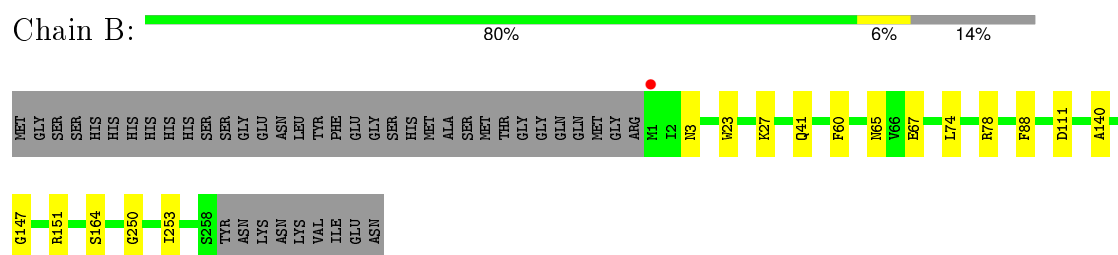
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

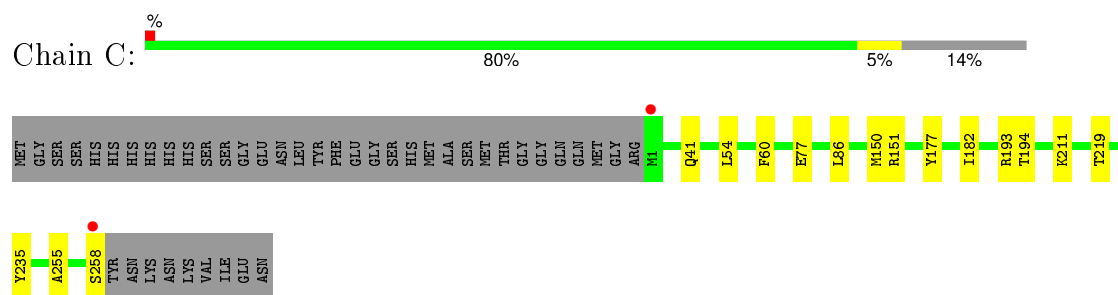
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



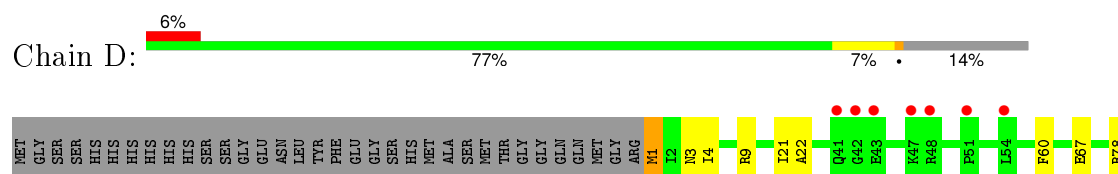
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

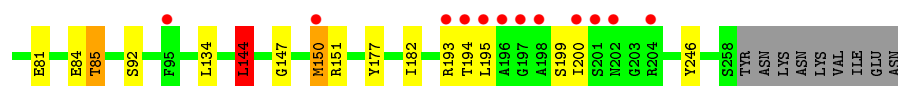


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

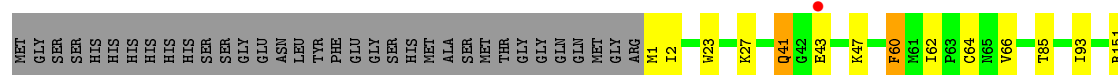
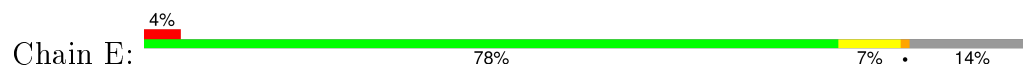


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

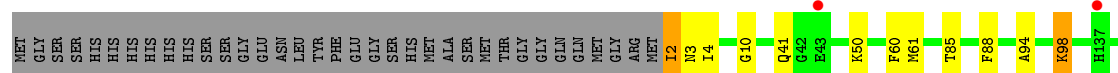
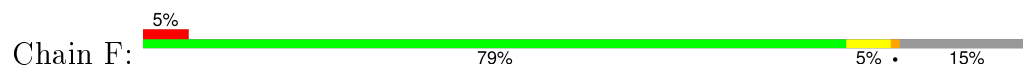




- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.49 Å   203.49 Å   81.76 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	43.19 – 1.70 44.06 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.19-1.70) 99.7 (44.06-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 1.70 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.174 , 0.201 0.174 , 0.200	Depositor DCC
$R_{free}$ test set	10619 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.5	EDS
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 211634 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/2012	0.58	0/2723
1	B	0.40	0/2012	0.60	0/2723
1	C	0.36	0/2012	0.57	0/2723
1	D	0.35	0/2012	0.56	1/2723 (0.0%)
1	E	0.35	0/2012	0.56	0/2723
1	F	0.36	0/2004	0.56	0/2713
All	All	0.37	0/12064	0.57	1/16328 (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	D	144	LEU	CA-CB-CG	-6.45	100.47	115.30

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	A	1973	0	1973	13	0
1	B	1973	0	1973	14	0
1	C	1973	0	1973	6	0
1	D	1973	0	1973	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1973	0	1973	17	0
1	F	1965	0	1961	11	0
2	A	7	0	10	1	0
2	B	14	0	20	3	0
2	C	14	0	20	1	0
2	D	7	0	10	0	0
2	E	14	0	20	1	0
2	F	14	0	20	3	0
3	A	276	0	0	2	1
3	B	291	0	0	5	1
3	C	246	0	0	1	1
3	D	187	0	0	2	1
3	E	241	0	0	2	0
3	F	201	0	0	0	0
All	All	13342	0	11926	70	2

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 (70) 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:D:9:ARG:HH21	1:D:85:THR:HG22	1.50	0.76
1:B:41:GLN:HE22	1:B:65:ASN:HA	1.52	0.73
1:B:41:GLN:NE2	3:B:658:HOH:O	2.21	0.71
1:D:1:MET:N	3:D:579:HOH:O	2.24	0.71
1:C:255:ALA:HB2	1:E:151:ARG:HB3	1.71	0.70
1:B:147:GLY:HA3	2:B:301:PEG:H22	1.73	0.70
1:F:94:ALA:HB2	2:F:300:PEG:H21	1.75	0.69
1:C:151:ARG:HB3	1:E:255:ALA:HB2	1.76	0.68
1:B:78:ARG:NH1	3:B:604:HOH:O	2.28	0.67
1:B:78:ARG:NH1	3:B:608:HOH:O	2.28	0.67
1:E:195:LEU:O	3:E:559:HOH:O	2.13	0.67
1:A:211:LYS:HB2	1:A:219:THR:HG23	1.79	0.65
1:B:3:ASN:OD1	3:B:544:HOH:O	2.14	0.64
1:E:41:GLN:HG3	1:E:64:CYS:O	2.01	0.61
1:D:151:ARG:HB3	1:F:255:ALA:HB2	1.84	0.58
1:B:78:ARG:NE	3:B:645:HOH:O	2.35	0.57
1:E:195:LEU:HB3	3:E:596:HOH:O	2.04	0.57
1:A:202:ASN:N	1:A:202:ASN:OD1	2.37	0.57
1:E:211:LYS:HB2	1:E:219:THR:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:CZ	2:A:300:PEG:H41	2.36	0.55
1:E:191:PRO:HA	2:E:300:PEG:H41	1.89	0.55
1:A:193:ARG:NH2	3:A:448:HOH:O	2.40	0.54
1:E:66:VAL:HG21	1:E:93:ILE:HG21	1.89	0.53
1:E:192:VAL:HG11	1:E:222:LEU:HD13	1.91	0.53
1:F:2:ILE:HG22	1:F:4:ILE:HG23	1.91	0.53
1:C:211:LYS:HB2	1:C:219:THR:HG23	1.90	0.53
1:E:200:ILE:HG12	1:E:201:SER:H	1.76	0.50
1:D:147:GLY:HA2	1:D:150:MET:HE3	1.94	0.50
1:B:147:GLY:CA	2:B:301:PEG:H22	2.40	0.49
1:F:94:ALA:CB	2:F:300:PEG:H21	2.41	0.48
1:D:199:SER:HB2	1:D:200:ILE:HG22	1.96	0.48
1:F:10:GLY:HA3	1:F:88:PHE:CE1	2.49	0.47
1:D:147:GLY:HA2	1:D:150:MET:CE	2.44	0.47
1:B:151:ARG:CZ	2:B:301:PEG:H12	2.44	0.47
1:E:43:GLU:HG2	1:E:47:LYS:HE3	1.97	0.47
2:C:300:PEG:H11	3:C:453:HOH:O	2.15	0.46
1:A:164:SER:HG	1:B:164:SER:HG	1.62	0.46
1:A:31:SER:O	3:A:517:HOH:O	2.21	0.46
1:E:200:ILE:HG12	1:E:201:SER:N	2.31	0.45
1:E:23:TRP:NE1	1:E:27:LYS:HD2	2.31	0.45
1:D:21:ILE:HG21	1:D:144:LEU:HD22	1.98	0.44
1:A:10:GLY:HA3	1:A:88:PHE:CE1	2.51	0.44
1:D:78:ARG:O	1:D:81:GLU:HG2	2.18	0.44
1:D:150:MET:H	1:D:150:MET:HG2	1.64	0.44
1:C:193:ARG:HG3	1:C:194:THR:HG23	1.99	0.44
1:B:23:TRP:NE1	1:B:27:LYS:HD2	2.32	0.44
1:D:22:ALA:HB2	1:D:92:SER:HB3	2.01	0.43
1:D:193:ARG:O	1:D:194:THR:OG1	2.32	0.43
1:B:88:PHE:HA	1:B:140:ALA:O	2.19	0.42
1:F:213:ASN:OD1	1:F:257:PRO:HB3	2.20	0.42
3:D:436:HOH:O	1:E:1:MET:HB3	2.19	0.42
1:A:41:GLN:HB2	1:A:41:GLN:HE21	1.69	0.42
1:D:177:TYR:HB3	1:D:182:ILE:HB	2.02	0.42
1:A:193:ARG:O	1:A:194:THR:OG1	2.31	0.41
1:B:250:GLY:O	1:B:253:ILE:HG12	2.20	0.41
1:E:60:PHE:CE1	1:E:62:ILE:HD11	2.55	0.41
1:C:235:TYR:OH	1:F:2:ILE:HD11	2.21	0.41
1:F:50:LYS:HA	1:F:61:MET:SD	2.61	0.41
1:D:193:ARG:H	1:D:193:ARG:HG3	1.68	0.41
1:A:66:VAL:HG11	1:A:93:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:NH1	1:B:67:GLU:O	2.54	0.41
1:D:150:MET:HE3	1:D:246:TYR:OH	2.21	0.41
1:F:98:LYS:HD3	1:F:98:LYS:HA	1.77	0.41
1:F:246:TYR:HH	2:F:301:PEG:HO1	1.62	0.41
1:A:214:SER:O	1:A:217:LYS:HE2	2.21	0.41
1:D:4:ILE:HG22	1:E:1:MET:HE3	2.02	0.40
1:D:3:ASN:OD1	1:E:1:MET:HA	2.21	0.40
1:A:22:ALA:HB2	1:A:92:SER:HB3	2.04	0.40
1:C:177:TYR:HB3	1:C:182:ILE:HB	2.03	0.40
1:F:211:LYS:HB2	1:F:219:THR:HG23	2.02	0.40

All (2) 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)
3:B:645:HOH:O	3:D:541:HOH:O[3_565]	2.12	0.08
3:A:523:HOH:O	3:C:566:HOH:O[3_565]	2.18	0.02

## 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	256/301 (85%)	249 (97%)	7 (3%)	0	100	100
1	B	256/301 (85%)	249 (97%)	7 (3%)	0	100	100
1	C	256/301 (85%)	248 (97%)	8 (3%)	0	100	100
1	D	256/301 (85%)	247 (96%)	9 (4%)	0	100	100
1	E	256/301 (85%)	246 (96%)	9 (4%)	1 (0%)	39	20
1	F	255/301 (85%)	245 (96%)	10 (4%)	0	100	100
All	All	1535/1806 (85%)	1484 (97%)	50 (3%)	1 (0%)	56	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	ILE

### 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	213/249 (86%)	208 (98%)	5 (2%)	58	37
1	B	213/249 (86%)	210 (99%)	3 (1%)	74	59
1	C	213/249 (86%)	206 (97%)	7 (3%)	45	22
1	D	213/249 (86%)	204 (96%)	9 (4%)	36	14
1	E	213/249 (86%)	207 (97%)	6 (3%)	51	29
1	F	212/249 (85%)	206 (97%)	6 (3%)	51	29
All	All	1277/1494 (86%)	1241 (97%)	36 (3%)	51	29

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	43	GLU
1	A	60	PHE
1	A	98	LYS
1	A	195	LEU
1	B	60	PHE
1	B	74	LEU
1	B	111	ASP
1	C	41	GLN
1	C	54	LEU
1	C	60	PHE
1	C	77	GLU
1	C	86	LEU
1	C	150	MET
1	C	258	SER
1	D	1	MET

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Mol	Chain	Res	Type
1	D	60	PHE
1	D	67	GLU
1	D	84	GLU
1	D	85	THR
1	D	134	LEU
1	D	144	LEU
1	D	150	MET
1	D	195	LEU
1	E	41	GLN
1	E	60	PHE
1	E	85	THR
1	E	195	LEU
1	E	199	SER
1	E	222	LEU
1	F	2	ILE
1	F	3	ASN
1	F	41	GLN
1	F	60	PHE
1	F	85	THR
1	F	98	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	ASN
1	B	41	GLN
1	C	133	GLN
1	F	41	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	PEG	A	300	-	6,6,6	0.60	0	5,5,5	0.77	0
2	PEG	B	300	-	6,6,6	0.60	0	5,5,5	0.76	0
2	PEG	B	301	-	6,6,6	0.62	0	5,5,5	0.90	0
2	PEG	C	300	-	6,6,6	0.63	0	5,5,5	0.60	0
2	PEG	C	301	-	6,6,6	0.61	0	5,5,5	0.50	0
2	PEG	D	301	-	6,6,6	0.60	0	5,5,5	0.63	0
2	PEG	E	300	-	6,6,6	0.54	0	5,5,5	0.81	0
2	PEG	E	301	-	6,6,6	0.58	0	5,5,5	0.62	0
2	PEG	F	300	-	6,6,6	0.76	0	5,5,5	0.70	0
2	PEG	F	301	-	6,6,6	0.59	0	5,5,5	0.59	0

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	PEG	A	300	-	-	0/4/4/4	0/0/0/0
2	PEG	B	300	-	-	0/4/4/4	0/0/0/0
2	PEG	B	301	-	-	0/4/4/4	0/0/0/0
2	PEG	C	300	-	-	0/4/4/4	0/0/0/0
2	PEG	C	301	-	-	0/4/4/4	0/0/0/0
2	PEG	D	301	-	-	0/4/4/4	0/0/0/0
2	PEG	E	300	-	-	0/4/4/4	0/0/0/0
2	PEG	E	301	-	-	0/4/4/4	0/0/0/0
2	PEG	F	300	-	-	0/4/4/4	0/0/0/0
2	PEG	F	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	PEG	1	0
2	B	301	PEG	3	0
2	C	300	PEG	1	0
2	E	300	PEG	1	0
2	F	300	PEG	2	0
2	F	301	PEG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	258/301 (85%)	-0.17	9 (3%)	48	52	9, 16, 35, 46	0
1	B	258/301 (85%)	-0.34	1 (0%)	93	94	10, 14, 25, 39	0
1	C	258/301 (85%)	-0.19	2 (0%)	87	90	12, 18, 36, 54	0
1	D	258/301 (85%)	0.23	19 (7%)	17	19	13, 23, 45, 64	0
1	E	258/301 (85%)	-0.09	13 (5%)	32	35	13, 19, 41, 61	0
1	F	257/301 (85%)	0.11	14 (5%)	29	31	12, 19, 40, 62	0
All	All	1547/1806 (85%)	-0.08	58 (3%)	45	50	9, 18, 38, 64	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	198	ALA	10.7
1	F	194	THR	8.1
1	F	196	ALA	7.8
1	D	195	LEU	7.3
1	D	198	ALA	7.2
1	E	196	ALA	6.8
1	D	201	SER	6.7
1	D	193	ARG	6.6
1	E	198	ALA	6.3
1	D	194	THR	6.2
1	F	195	LEU	6.1
1	D	196	ALA	6.1
1	F	197	GLY	6.0
1	F	193	ARG	5.7
1	F	204	ARG	5.7
1	E	194	THR	5.4
1	A	193	ARG	5.3
1	F	200	ILE	5.1
1	A	194	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	4.7
1	E	193	ARG	4.6
1	E	204	ARG	4.5
1	D	197	GLY	4.4
1	A	198	ALA	4.1
1	F	199	SER	4.1
1	F	201	SER	4.0
1	E	195	LEU	3.8
1	E	199	SER	3.8
1	D	202	ASN	3.7
1	D	54	LEU	3.6
1	E	197	GLY	3.6
1	A	197	GLY	3.6
1	D	43	GLU	3.5
1	C	258	SER	3.5
1	D	204	ARG	3.5
1	A	196	ALA	3.5
1	D	47	LYS	3.3
1	E	200	ILE	3.3
1	D	42	GLY	3.3
1	E	201	SER	3.3
1	F	192	VAL	3.3
1	D	150	MET	3.2
1	B	1	MET	2.7
1	F	137	HIS	2.6
1	D	200	ILE	2.6
1	D	51	PRO	2.6
1	A	204	ARG	2.5
1	A	43	GLU	2.4
1	D	48	ARG	2.3
1	D	95	PHE	2.3
1	F	43	GLU	2.3
1	A	41	GLN	2.2
1	E	43	GLU	2.1
1	E	202	ASN	2.1
1	D	41	GLN	2.1
1	F	202	ASN	2.1
1	A	201	SER	2.0
1	E	212	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PEG	F	300	7/7	0.89	0.26	9.56	26,29,32,33	0
2	PEG	F	301	7/7	0.79	0.24	4.89	30,32,35,38	0
2	PEG	C	300	7/7	0.87	0.19	4.56	27,29,36,38	0
2	PEG	E	301	7/7	0.85	0.19	4.17	27,30,35,35	0
2	PEG	B	300	7/7	0.89	0.14	3.41	21,23,31,31	0
2	PEG	A	300	7/7	0.92	0.16	2.78	23,28,32,34	0
2	PEG	B	301	7/7	0.84	0.15	2.77	18,25,29,34	0
2	PEG	E	300	7/7	0.71	0.32	2.09	28,34,39,40	0
2	PEG	D	301	7/7	0.88	0.17	1.40	27,31,34,39	0
2	PEG	C	301	7/7	0.95	0.09	-0.42	27,28,31,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.