wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 08:15 am GMT

PDB ID	:	4ALN
Title	:	Crystal structure of S. aureus FabI (P32)
Authors	:	Schiebel, J.; Kisker, C.
Deposited on	:	2012-03-04
Resolution	:	3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

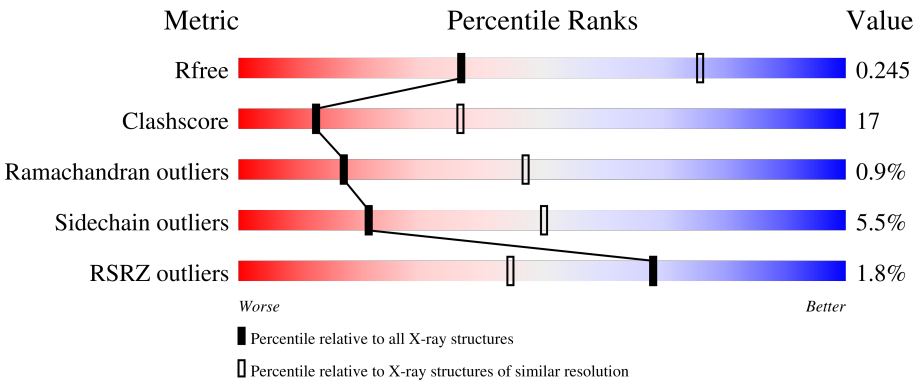
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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% 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	282	% 55% 24% • 19%
1	B	282	46% 29% • 22%
1	C	282	49% 26% 5% 20%
1	D	282	49% 20% • 31%
1	E	282	51% 24% • 22%

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Mol	Chain	Length	Quality of chain
1	F	282	49% 20% • 28%
1	G	282	53% 23% • 22%
1	H	282	2% 48% 28% • 22%
1	I	282	4% 51% 22% • 24%
1	J	282	5% 51% 21% • 26%
1	K	282	2% 52% 22% • • 23%
1	L	282	50% 18% • 32%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20061 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 [NADPH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	229	1769	1114	305	347	3	0	0	0
1	B	220	1693	1067	293	330	3	0	0	0
1	C	225	1739	1098	298	340	3	0	0	0
1	D	195	1492	937	254	298	3	0	0	0
1	E	221	1710	1079	292	336	3	0	0	0
1	F	203	1558	982	265	308	3	0	0	0
1	G	221	1710	1083	291	333	3	0	0	0
1	H	220	1699	1072	290	334	3	0	0	0
1	I	214	1654	1042	284	325	3	0	0	0
1	J	210	1618	1017	279	319	3	0	0	0
1	K	218	1690	1069	288	330	3	0	0	0
1	L	193	1479	931	250	295	3	0	0	0

There are 325 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP Q7A6D8
A	-24	LYS	-	expression tag	UNP Q7A6D8
A	-23	HIS	-	expression tag	UNP Q7A6D8
A	-22	HIS	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	HIS	-	expression tag	UNP Q7A6D8
A	-20	HIS	-	expression tag	UNP Q7A6D8
A	-19	HIS	-	expression tag	UNP Q7A6D8
A	-18	HIS	-	expression tag	UNP Q7A6D8
A	-17	PRO	-	expression tag	UNP Q7A6D8
A	-16	MET	-	expression tag	UNP Q7A6D8
A	-15	SER	-	expression tag	UNP Q7A6D8
A	-14	ASP	-	expression tag	UNP Q7A6D8
A	-13	TYR	-	expression tag	UNP Q7A6D8
A	-12	ASP	-	expression tag	UNP Q7A6D8
A	-11	ILE	-	expression tag	UNP Q7A6D8
A	-10	PRO	-	expression tag	UNP Q7A6D8
A	-9	THR	-	expression tag	UNP Q7A6D8
A	-8	THR	-	expression tag	UNP Q7A6D8
A	-7	GLU	-	expression tag	UNP Q7A6D8
A	-6	ASN	-	expression tag	UNP Q7A6D8
A	-5	LEU	-	expression tag	UNP Q7A6D8
A	-4	TYR	-	expression tag	UNP Q7A6D8
A	-3	PHE	-	expression tag	UNP Q7A6D8
A	-2	GLN	-	expression tag	UNP Q7A6D8
A	-1	GLY	-	expression tag	UNP Q7A6D8
A	0	ALA	-	expression tag	UNP Q7A6D8
B	-25	MET	-	expression tag	UNP Q7A6D8
B	-24	LYS	-	expression tag	UNP Q7A6D8
B	-23	HIS	-	expression tag	UNP Q7A6D8
B	-22	HIS	-	expression tag	UNP Q7A6D8
B	-21	HIS	-	expression tag	UNP Q7A6D8
B	-20	HIS	-	expression tag	UNP Q7A6D8
B	-19	HIS	-	expression tag	UNP Q7A6D8
B	-18	HIS	-	expression tag	UNP Q7A6D8
B	-17	PRO	-	expression tag	UNP Q7A6D8
B	-16	MET	-	expression tag	UNP Q7A6D8
B	-15	SER	-	expression tag	UNP Q7A6D8
B	-14	ASP	-	expression tag	UNP Q7A6D8
B	-13	TYR	-	expression tag	UNP Q7A6D8
B	-12	ASP	-	expression tag	UNP Q7A6D8
B	-11	ILE	-	expression tag	UNP Q7A6D8
B	-10	PRO	-	expression tag	UNP Q7A6D8
B	-9	THR	-	expression tag	UNP Q7A6D8
B	-8	THR	-	expression tag	UNP Q7A6D8
B	-7	GLU	-	expression tag	UNP Q7A6D8
B	-6	ASN	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP Q7A6D8
B	-4	TYR	-	expression tag	UNP Q7A6D8
B	-3	PHE	-	expression tag	UNP Q7A6D8
B	-2	GLN	-	expression tag	UNP Q7A6D8
B	-1	GLY	-	expression tag	UNP Q7A6D8
B	0	ALA	-	expression tag	UNP Q7A6D8
C	-25	MET	-	expression tag	UNP Q7A6D8
C	-24	LYS	-	expression tag	UNP Q7A6D8
C	-23	HIS	-	expression tag	UNP Q7A6D8
C	-22	HIS	-	expression tag	UNP Q7A6D8
C	-21	HIS	-	expression tag	UNP Q7A6D8
C	-20	HIS	-	expression tag	UNP Q7A6D8
C	-19	HIS	-	expression tag	UNP Q7A6D8
C	-18	HIS	-	expression tag	UNP Q7A6D8
C	-17	PRO	-	expression tag	UNP Q7A6D8
C	-16	MET	-	expression tag	UNP Q7A6D8
C	-15	SER	-	expression tag	UNP Q7A6D8
C	-14	ASP	-	expression tag	UNP Q7A6D8
C	-13	TYR	-	expression tag	UNP Q7A6D8
C	-12	ASP	-	expression tag	UNP Q7A6D8
C	-11	ILE	-	expression tag	UNP Q7A6D8
C	-10	PRO	-	expression tag	UNP Q7A6D8
C	-9	THR	-	expression tag	UNP Q7A6D8
C	-8	THR	-	expression tag	UNP Q7A6D8
C	-7	GLU	-	expression tag	UNP Q7A6D8
C	-6	ASN	-	expression tag	UNP Q7A6D8
C	-5	LEU	-	expression tag	UNP Q7A6D8
C	-4	TYR	-	expression tag	UNP Q7A6D8
C	-3	PHE	-	expression tag	UNP Q7A6D8
C	-2	GLN	-	expression tag	UNP Q7A6D8
C	-1	GLY	-	expression tag	UNP Q7A6D8
C	0	ALA	-	expression tag	UNP Q7A6D8
D	-25	MET	-	expression tag	UNP Q7A6D8
D	-24	LYS	-	expression tag	UNP Q7A6D8
D	-23	HIS	-	expression tag	UNP Q7A6D8
D	-22	HIS	-	expression tag	UNP Q7A6D8
D	-21	HIS	-	expression tag	UNP Q7A6D8
D	-20	HIS	-	expression tag	UNP Q7A6D8
D	-19	HIS	-	expression tag	UNP Q7A6D8
D	-18	HIS	-	expression tag	UNP Q7A6D8
D	-17	PRO	-	expression tag	UNP Q7A6D8
D	-16	MET	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP Q7A6D8
D	-14	ASP	-	expression tag	UNP Q7A6D8
D	-13	TYR	-	expression tag	UNP Q7A6D8
D	-12	ASP	-	expression tag	UNP Q7A6D8
D	-11	ILE	-	expression tag	UNP Q7A6D8
D	-10	PRO	-	expression tag	UNP Q7A6D8
D	-9	THR	-	expression tag	UNP Q7A6D8
D	-8	THR	-	expression tag	UNP Q7A6D8
D	-7	GLU	-	expression tag	UNP Q7A6D8
D	-6	ASN	-	expression tag	UNP Q7A6D8
D	-5	LEU	-	expression tag	UNP Q7A6D8
D	-4	TYR	-	expression tag	UNP Q7A6D8
D	-3	PHE	-	expression tag	UNP Q7A6D8
D	-2	GLN	-	expression tag	UNP Q7A6D8
D	-1	GLY	-	expression tag	UNP Q7A6D8
D	0	ALA	-	expression tag	UNP Q7A6D8
E	-25	MET	-	expression tag	UNP Q7A6D8
E	-24	LYS	-	expression tag	UNP Q7A6D8
E	-23	HIS	-	expression tag	UNP Q7A6D8
E	-22	HIS	-	expression tag	UNP Q7A6D8
E	-21	HIS	-	expression tag	UNP Q7A6D8
E	-20	HIS	-	expression tag	UNP Q7A6D8
E	-19	HIS	-	expression tag	UNP Q7A6D8
E	-18	HIS	-	expression tag	UNP Q7A6D8
E	-17	PRO	-	expression tag	UNP Q7A6D8
E	-16	MET	-	expression tag	UNP Q7A6D8
E	-15	SER	-	expression tag	UNP Q7A6D8
E	-14	ASP	-	expression tag	UNP Q7A6D8
E	-13	TYR	-	expression tag	UNP Q7A6D8
E	-12	ASP	-	expression tag	UNP Q7A6D8
E	-11	ILE	-	expression tag	UNP Q7A6D8
E	-10	PRO	-	expression tag	UNP Q7A6D8
E	-9	THR	-	expression tag	UNP Q7A6D8
E	-8	THR	-	expression tag	UNP Q7A6D8
E	-7	GLU	-	expression tag	UNP Q7A6D8
E	-6	ASN	-	expression tag	UNP Q7A6D8
E	-5	LEU	-	expression tag	UNP Q7A6D8
E	-4	TYR	-	expression tag	UNP Q7A6D8
E	-3	PHE	-	expression tag	UNP Q7A6D8
E	-2	GLN	-	expression tag	UNP Q7A6D8
E	-1	GLY	-	expression tag	UNP Q7A6D8
E	0	ALA	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-25	MET	-	expression tag	UNP Q7A6D8
F	-24	LYS	-	expression tag	UNP Q7A6D8
F	-23	HIS	-	expression tag	UNP Q7A6D8
F	-22	HIS	-	expression tag	UNP Q7A6D8
F	-21	HIS	-	expression tag	UNP Q7A6D8
F	-20	HIS	-	expression tag	UNP Q7A6D8
F	-19	HIS	-	expression tag	UNP Q7A6D8
F	-18	HIS	-	expression tag	UNP Q7A6D8
F	-17	PRO	-	expression tag	UNP Q7A6D8
F	-16	MET	-	expression tag	UNP Q7A6D8
F	-15	SER	-	expression tag	UNP Q7A6D8
F	-14	ASP	-	expression tag	UNP Q7A6D8
F	-13	TYR	-	expression tag	UNP Q7A6D8
F	-12	ASP	-	expression tag	UNP Q7A6D8
F	-11	ILE	-	expression tag	UNP Q7A6D8
F	-10	PRO	-	expression tag	UNP Q7A6D8
F	-9	THR	-	expression tag	UNP Q7A6D8
F	-8	THR	-	expression tag	UNP Q7A6D8
F	-7	GLU	-	expression tag	UNP Q7A6D8
F	-6	ASN	-	expression tag	UNP Q7A6D8
F	-5	LEU	-	expression tag	UNP Q7A6D8
F	-4	TYR	-	expression tag	UNP Q7A6D8
F	-3	PHE	-	expression tag	UNP Q7A6D8
F	-2	GLN	-	expression tag	UNP Q7A6D8
F	-1	GLY	-	expression tag	UNP Q7A6D8
F	0	ALA	-	expression tag	UNP Q7A6D8
G	-25	MET	-	expression tag	UNP Q7A6D8
G	-24	LYS	-	expression tag	UNP Q7A6D8
G	-23	HIS	-	expression tag	UNP Q7A6D8
G	-22	HIS	-	expression tag	UNP Q7A6D8
G	-21	HIS	-	expression tag	UNP Q7A6D8
G	-20	HIS	-	expression tag	UNP Q7A6D8
G	-19	HIS	-	expression tag	UNP Q7A6D8
G	-18	HIS	-	expression tag	UNP Q7A6D8
G	-17	PRO	-	expression tag	UNP Q7A6D8
G	-16	MET	-	expression tag	UNP Q7A6D8
G	-15	SER	-	expression tag	UNP Q7A6D8
G	-14	ASP	-	expression tag	UNP Q7A6D8
G	-13	TYR	-	expression tag	UNP Q7A6D8
G	-12	ASP	-	expression tag	UNP Q7A6D8
G	-11	ILE	-	expression tag	UNP Q7A6D8
G	-10	PRO	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	THR	-	expression tag	UNP Q7A6D8
G	-8	THR	-	expression tag	UNP Q7A6D8
G	-7	GLU	-	expression tag	UNP Q7A6D8
G	-6	ASN	-	expression tag	UNP Q7A6D8
G	-5	LEU	-	expression tag	UNP Q7A6D8
G	-4	TYR	-	expression tag	UNP Q7A6D8
G	-3	PHE	-	expression tag	UNP Q7A6D8
G	-2	GLN	-	expression tag	UNP Q7A6D8
G	-1	GLY	-	expression tag	UNP Q7A6D8
G	0	ALA	-	expression tag	UNP Q7A6D8
H	-25	MET	-	expression tag	UNP Q7A6D8
H	-24	LYS	-	expression tag	UNP Q7A6D8
H	-23	HIS	-	expression tag	UNP Q7A6D8
H	-22	HIS	-	expression tag	UNP Q7A6D8
H	-21	HIS	-	expression tag	UNP Q7A6D8
H	-20	HIS	-	expression tag	UNP Q7A6D8
H	-19	HIS	-	expression tag	UNP Q7A6D8
H	-18	HIS	-	expression tag	UNP Q7A6D8
H	-17	PRO	-	expression tag	UNP Q7A6D8
H	-16	MET	-	expression tag	UNP Q7A6D8
H	-15	SER	-	expression tag	UNP Q7A6D8
H	-14	ASP	-	expression tag	UNP Q7A6D8
H	-13	TYR	-	expression tag	UNP Q7A6D8
H	-12	ASP	-	expression tag	UNP Q7A6D8
H	-11	ILE	-	expression tag	UNP Q7A6D8
H	-10	PRO	-	expression tag	UNP Q7A6D8
H	-9	THR	-	expression tag	UNP Q7A6D8
H	-8	THR	-	expression tag	UNP Q7A6D8
H	-7	GLU	-	expression tag	UNP Q7A6D8
H	-6	ASN	-	expression tag	UNP Q7A6D8
H	-5	LEU	-	expression tag	UNP Q7A6D8
H	-4	TYR	-	expression tag	UNP Q7A6D8
H	-3	PHE	-	expression tag	UNP Q7A6D8
H	-2	GLN	-	expression tag	UNP Q7A6D8
H	-1	GLY	-	expression tag	UNP Q7A6D8
H	0	ALA	-	expression tag	UNP Q7A6D8
H	1	MET	-	expression tag	UNP Q7A6D8
I	-25	MET	-	expression tag	UNP Q7A6D8
I	-24	LYS	-	expression tag	UNP Q7A6D8
I	-23	HIS	-	expression tag	UNP Q7A6D8
I	-22	HIS	-	expression tag	UNP Q7A6D8
I	-21	HIS	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-20	HIS	-	expression tag	UNP Q7A6D8
I	-19	HIS	-	expression tag	UNP Q7A6D8
I	-18	HIS	-	expression tag	UNP Q7A6D8
I	-17	PRO	-	expression tag	UNP Q7A6D8
I	-16	MET	-	expression tag	UNP Q7A6D8
I	-15	SER	-	expression tag	UNP Q7A6D8
I	-14	ASP	-	expression tag	UNP Q7A6D8
I	-13	TYR	-	expression tag	UNP Q7A6D8
I	-12	ASP	-	expression tag	UNP Q7A6D8
I	-11	ILE	-	expression tag	UNP Q7A6D8
I	-10	PRO	-	expression tag	UNP Q7A6D8
I	-9	THR	-	expression tag	UNP Q7A6D8
I	-8	THR	-	expression tag	UNP Q7A6D8
I	-7	GLU	-	expression tag	UNP Q7A6D8
I	-6	ASN	-	expression tag	UNP Q7A6D8
I	-5	LEU	-	expression tag	UNP Q7A6D8
I	-4	TYR	-	expression tag	UNP Q7A6D8
I	-3	PHE	-	expression tag	UNP Q7A6D8
I	-2	GLN	-	expression tag	UNP Q7A6D8
I	-1	GLY	-	expression tag	UNP Q7A6D8
I	0	ALA	-	expression tag	UNP Q7A6D8
J	-25	MET	-	expression tag	UNP Q7A6D8
J	-24	LYS	-	expression tag	UNP Q7A6D8
J	-23	HIS	-	expression tag	UNP Q7A6D8
J	-22	HIS	-	expression tag	UNP Q7A6D8
J	-21	HIS	-	expression tag	UNP Q7A6D8
J	-20	HIS	-	expression tag	UNP Q7A6D8
J	-19	HIS	-	expression tag	UNP Q7A6D8
J	-18	HIS	-	expression tag	UNP Q7A6D8
J	-17	PRO	-	expression tag	UNP Q7A6D8
J	-16	MET	-	expression tag	UNP Q7A6D8
J	-15	SER	-	expression tag	UNP Q7A6D8
J	-14	ASP	-	expression tag	UNP Q7A6D8
J	-13	TYR	-	expression tag	UNP Q7A6D8
J	-12	ASP	-	expression tag	UNP Q7A6D8
J	-11	ILE	-	expression tag	UNP Q7A6D8
J	-10	PRO	-	expression tag	UNP Q7A6D8
J	-9	THR	-	expression tag	UNP Q7A6D8
J	-8	THR	-	expression tag	UNP Q7A6D8
J	-7	GLU	-	expression tag	UNP Q7A6D8
J	-6	ASN	-	expression tag	UNP Q7A6D8
J	-5	LEU	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	TYR	-	expression tag	UNP Q7A6D8
J	-3	PHE	-	expression tag	UNP Q7A6D8
J	-2	GLN	-	expression tag	UNP Q7A6D8
J	-1	GLY	-	expression tag	UNP Q7A6D8
J	0	ALA	-	expression tag	UNP Q7A6D8
K	-25	MET	-	expression tag	UNP Q7A6D8
K	-24	LYS	-	expression tag	UNP Q7A6D8
K	-23	HIS	-	expression tag	UNP Q7A6D8
K	-22	HIS	-	expression tag	UNP Q7A6D8
K	-21	HIS	-	expression tag	UNP Q7A6D8
K	-20	HIS	-	expression tag	UNP Q7A6D8
K	-19	HIS	-	expression tag	UNP Q7A6D8
K	-18	HIS	-	expression tag	UNP Q7A6D8
K	-17	PRO	-	expression tag	UNP Q7A6D8
K	-16	MET	-	expression tag	UNP Q7A6D8
K	-15	SER	-	expression tag	UNP Q7A6D8
K	-14	ASP	-	expression tag	UNP Q7A6D8
K	-13	TYR	-	expression tag	UNP Q7A6D8
K	-12	ASP	-	expression tag	UNP Q7A6D8
K	-11	ILE	-	expression tag	UNP Q7A6D8
K	-10	PRO	-	expression tag	UNP Q7A6D8
K	-9	THR	-	expression tag	UNP Q7A6D8
K	-8	THR	-	expression tag	UNP Q7A6D8
K	-7	GLU	-	expression tag	UNP Q7A6D8
K	-6	ASN	-	expression tag	UNP Q7A6D8
K	-5	LEU	-	expression tag	UNP Q7A6D8
K	-4	TYR	-	expression tag	UNP Q7A6D8
K	-3	PHE	-	expression tag	UNP Q7A6D8
K	-2	GLN	-	expression tag	UNP Q7A6D8
K	-1	GLY	-	expression tag	UNP Q7A6D8
K	0	ALA	-	expression tag	UNP Q7A6D8
L	-25	MET	-	expression tag	UNP Q7A6D8
L	-24	LYS	-	expression tag	UNP Q7A6D8
L	-23	HIS	-	expression tag	UNP Q7A6D8
L	-22	HIS	-	expression tag	UNP Q7A6D8
L	-21	HIS	-	expression tag	UNP Q7A6D8
L	-20	HIS	-	expression tag	UNP Q7A6D8
L	-19	HIS	-	expression tag	UNP Q7A6D8
L	-18	HIS	-	expression tag	UNP Q7A6D8
L	-17	PRO	-	expression tag	UNP Q7A6D8
L	-16	MET	-	expression tag	UNP Q7A6D8
L	-15	SER	-	expression tag	UNP Q7A6D8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-14	ASP	-	expression tag	UNP Q7A6D8
L	-13	TYR	-	expression tag	UNP Q7A6D8
L	-12	ASP	-	expression tag	UNP Q7A6D8
L	-11	ILE	-	expression tag	UNP Q7A6D8
L	-10	PRO	-	expression tag	UNP Q7A6D8
L	-9	THR	-	expression tag	UNP Q7A6D8
L	-8	THR	-	expression tag	UNP Q7A6D8
L	-7	GLU	-	expression tag	UNP Q7A6D8
L	-6	ASN	-	expression tag	UNP Q7A6D8
L	-5	LEU	-	expression tag	UNP Q7A6D8
L	-4	TYR	-	expression tag	UNP Q7A6D8
L	-3	PHE	-	expression tag	UNP Q7A6D8
L	-2	GLN	-	expression tag	UNP Q7A6D8
L	-1	GLY	-	expression tag	UNP Q7A6D8
L	0	ALA	-	expression tag	UNP Q7A6D8
A	2	VAL	LEU	engineered mutation	UNP Q7A6D8
B	2	VAL	LEU	engineered mutation	UNP Q7A6D8
C	2	VAL	LEU	engineered mutation	UNP Q7A6D8
D	2	VAL	LEU	engineered mutation	UNP Q7A6D8
E	2	VAL	LEU	engineered mutation	UNP Q7A6D8
F	2	VAL	LEU	engineered mutation	UNP Q7A6D8
G	2	VAL	LEU	engineered mutation	UNP Q7A6D8
H	2	VAL	LEU	engineered mutation	UNP Q7A6D8
I	2	VAL	LEU	engineered mutation	UNP Q7A6D8
J	2	VAL	LEU	engineered mutation	UNP Q7A6D8
K	2	VAL	LEU	engineered mutation	UNP Q7A6D8
L	2	VAL	LEU	engineered mutation	UNP Q7A6D8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	25	25	25	0	0
			Total	O		
2	B	26	26	26	0	0
			Total	O		
2	C	27	27	27	0	0
			Total	O		
2	D	30	30	30	0	0
			Total	O		
2	E	22	22	22	0	0
			Total	O		
2	F	26	26	26	0	0

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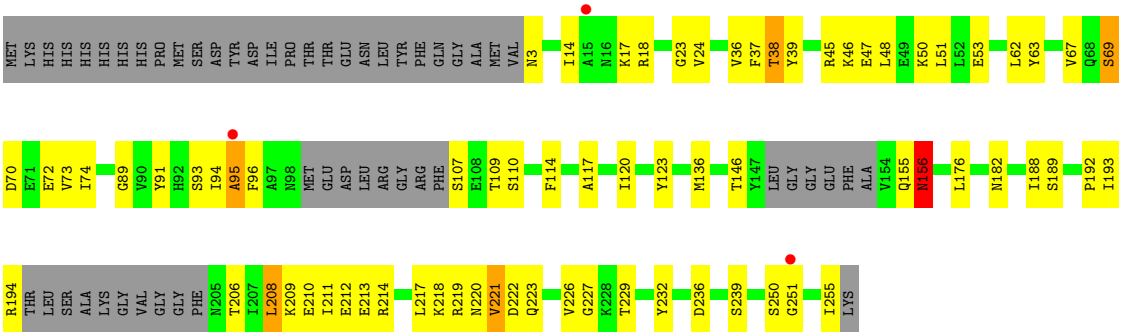
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	G	21	21	21	0	0
			Total	O		
2	H	22	22	22	0	0
			Total	O		
2	I	10	10	10	0	0
			Total	O		
2	J	7	7	7	0	0
			Total	O		
2	K	11	11	11	0	0
			Total	O		
2	L	23	23	23	0	0

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 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.

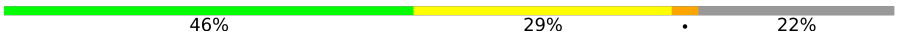
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

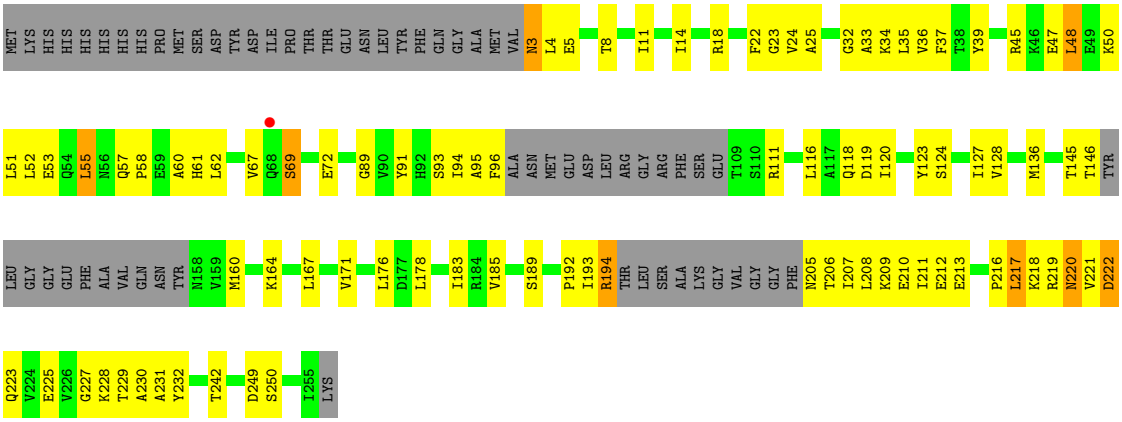
Chain A:



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

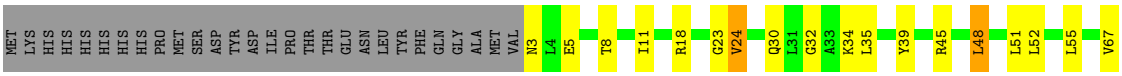
Chain B:

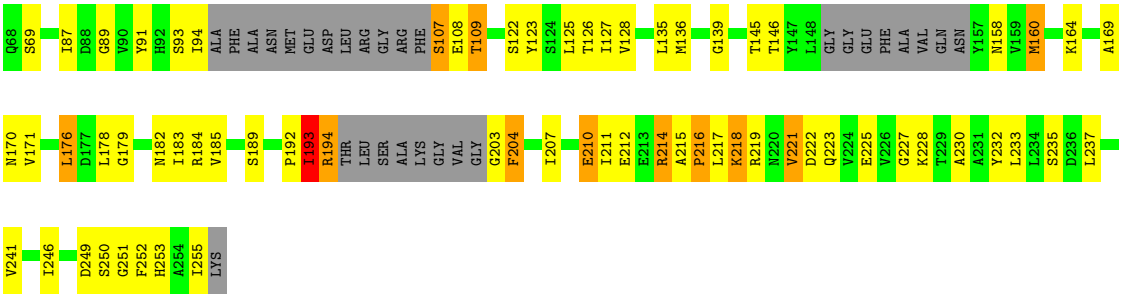




• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

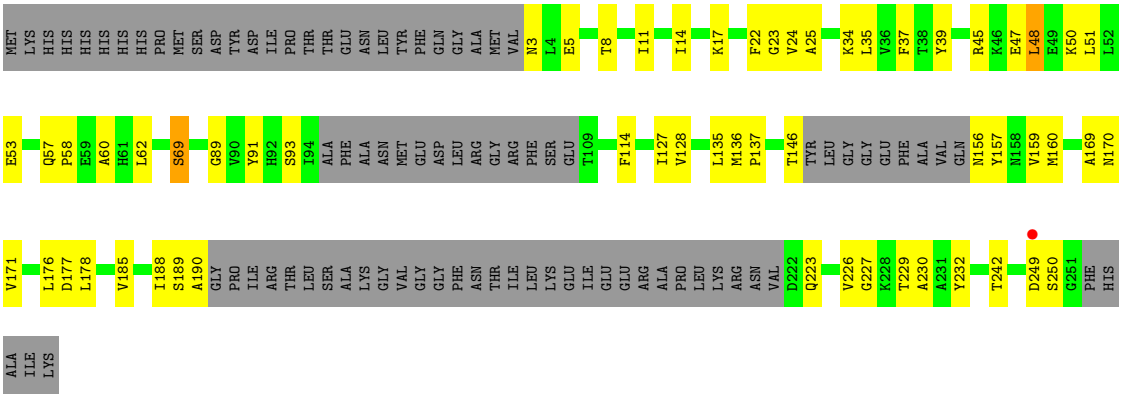
Chain C:





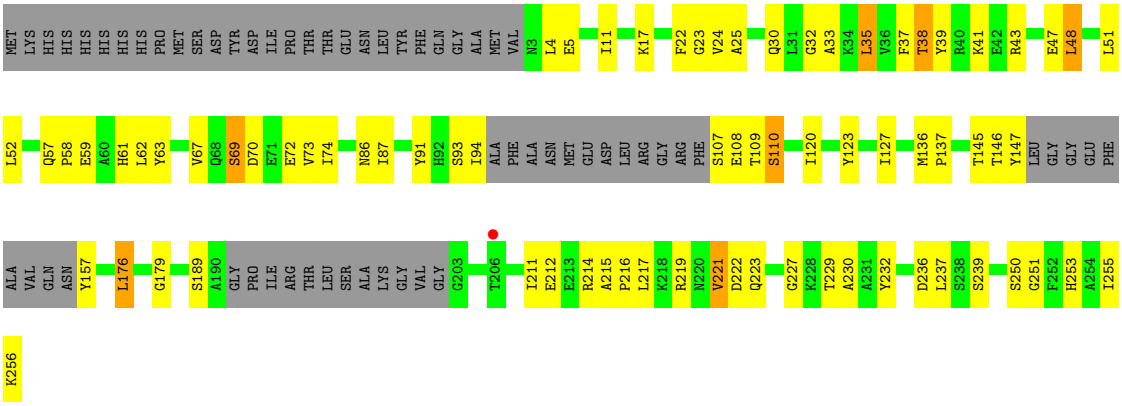
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain D:



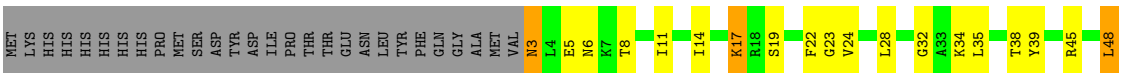
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

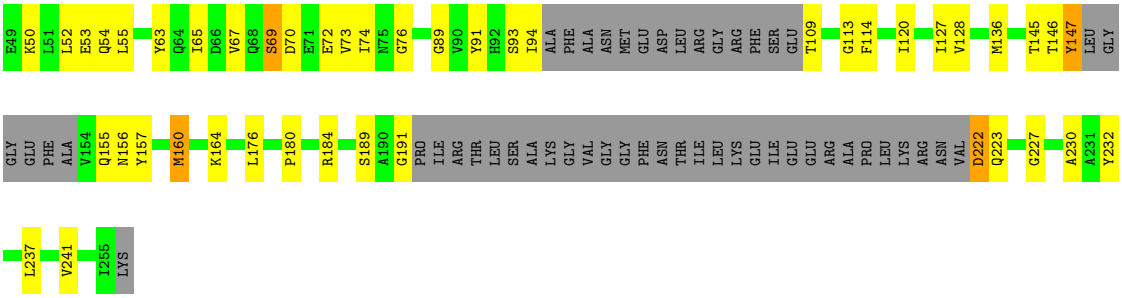
Chain E:



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

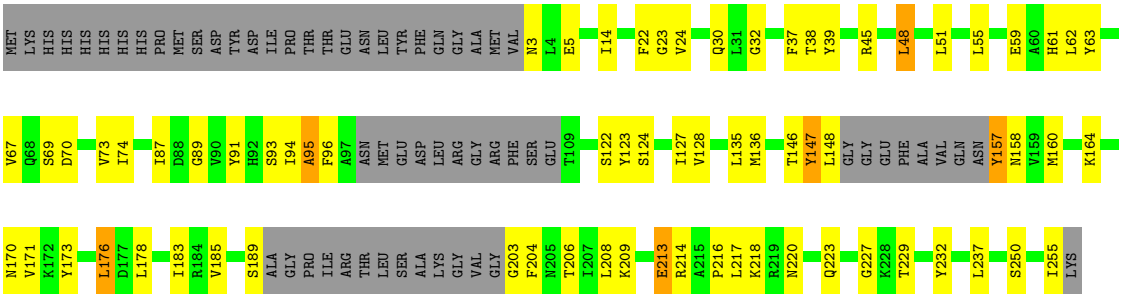
Chain F:





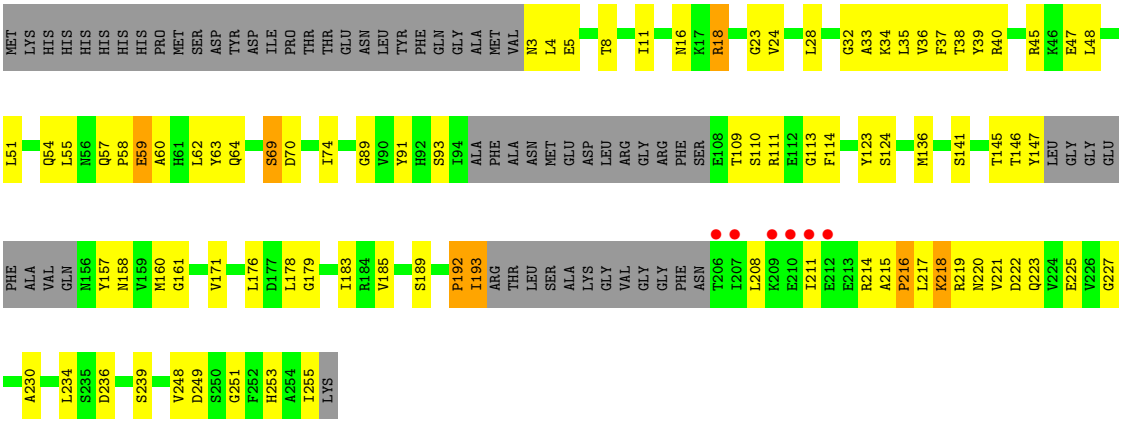
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain G:



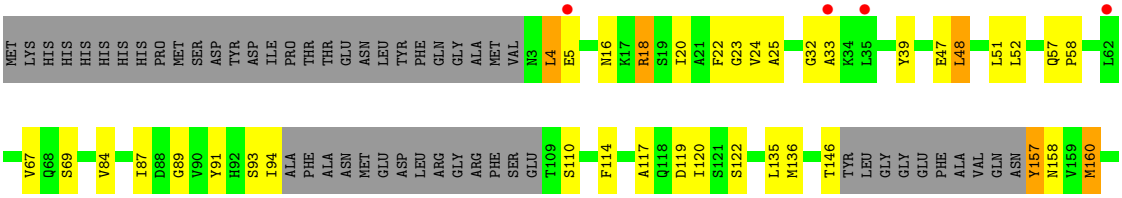
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

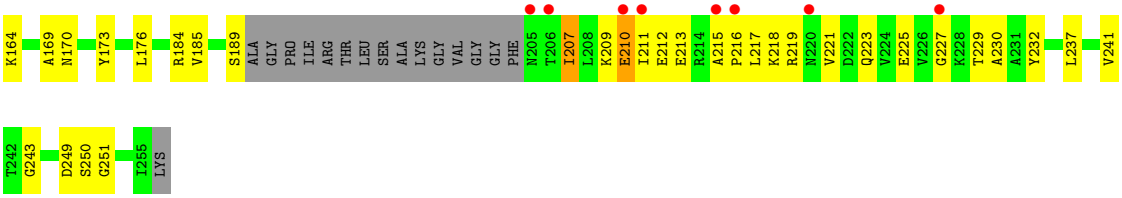
Chain H:



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

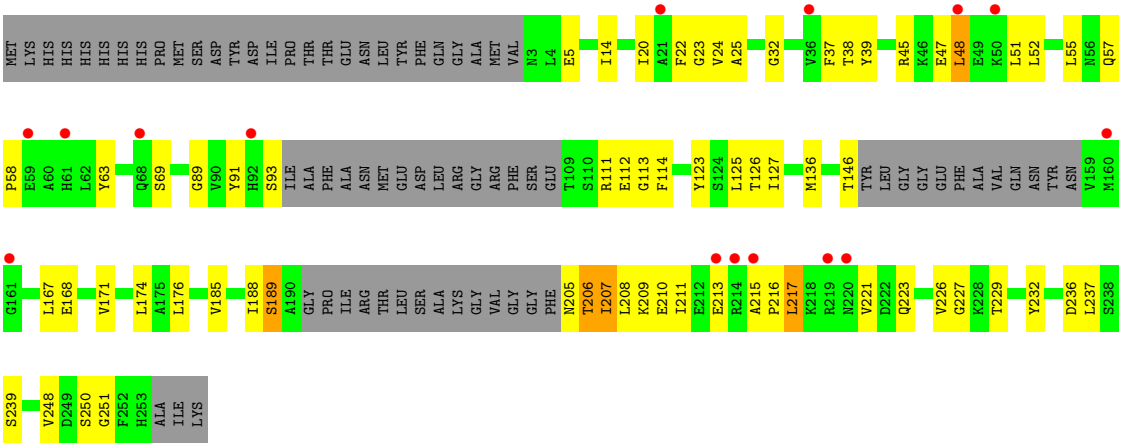
Chain I:





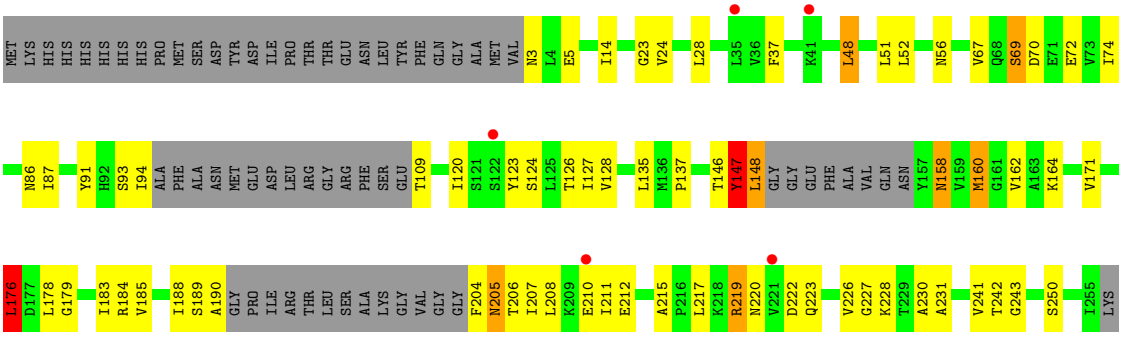
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain J:



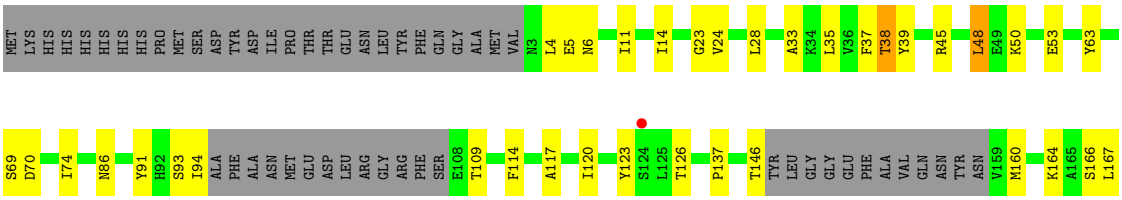
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

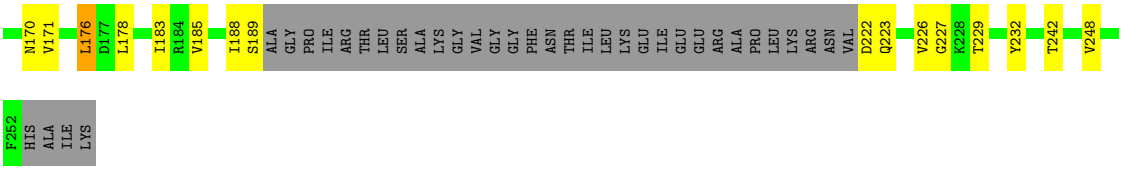
Chain K:



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

Chain L:




F252
HIS
ALA
ILE
LYS
N170
V171
L176
D177
L178
I183
R184
V185
I188
S189
ALA
GLY
PRO
ILE
ARG
THR
LEU
SER
ALA
LYS
GLY
VAL
GLY
GLY
PHE
ASN
THR
ILE
LEU
LYS
GLU
ILE
GLU
GLU
ARG
ALA
PRO
LEU
LYS
ARG
ASN
VAL
D222
Q223
V226
G227
K228
T229
Y232
T242
V248

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	123.78Å 123.78Å 190.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.28 – 3.05 44.28 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.28-3.05) 99.3 (44.28-3.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.203 , 0.246 0.202 , 0.245	Depositor DCC
R_{free} test set	3064 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.328 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
Reported twinning fraction	0.674 for H, K, L 0.326 for K, H, -L	Depositor
Outliers	0 of 61621 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20061	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.78	0/1790	0.76	0/2414
1	B	0.82	0/1712	0.80	1/2307 (0.0%)
1	C	0.77	0/1760	0.82	1/2372 (0.0%)
1	D	0.80	0/1507	0.77	0/2031
1	E	0.75	0/1730	0.76	0/2330
1	F	0.82	0/1576	0.80	0/2125
1	G	0.77	0/1731	0.79	1/2333 (0.0%)
1	H	0.76	0/1719	0.78	2/2318 (0.1%)
1	I	0.60	0/1672	0.71	1/2253 (0.0%)
1	J	0.60	0/1635	0.66	0/2202
1	K	0.62	0/1710	0.71	1/2305 (0.0%)
1	L	0.65	0/1494	0.67	0/2012
All	All	0.73	0/20036	0.75	7/27002 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	176	LEU	CA-CB-CG	-7.93	97.07	115.30
1	H	18	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	K	176	LEU	CA-CB-CG	5.90	128.86	115.30
1	G	176	LEU	CA-CB-CG	-5.48	102.69	115.30
1	H	18	ARG	NE-CZ-NH2	-5.31	117.65	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	A	1769	0	1779	64	0
1	B	1693	0	1716	70	0
1	C	1739	0	1754	78	0
1	D	1492	0	1497	53	0
1	E	1710	0	1722	55	0
1	F	1558	0	1558	54	0
1	G	1710	0	1723	69	0
1	H	1699	0	1713	64	0
1	I	1654	0	1672	53	0
1	J	1618	0	1635	49	0
1	K	1690	0	1706	51	0
1	L	1479	0	1486	41	0
2	A	25	0	0	1	0
2	B	26	0	0	0	0
2	C	27	0	0	1	0
2	D	30	0	0	0	0
2	E	22	0	0	1	0
2	F	26	0	0	3	0
2	G	21	0	0	0	0
2	H	22	0	0	1	0
2	I	10	0	0	2	0
2	J	7	0	0	0	0
2	K	11	0	0	0	0
2	L	23	0	0	0	0
All	All	20061	0	19961	659	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 17.

The worst 5 of 659 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:HH22	1:C:194:ARG:CB	1.57	1.17
1:C:18:ARG:NH2	1:C:194:ARG:HB2	1.63	1.11
1:B:18:ARG:HH22	1:B:194:ARG:HB3	0.97	1.10
1:D:89:GLY:HA2	1:D:136:MET:HE1	1.29	1.10
1:D:89:GLY:HA2	1:D:136:MET:CE	1.87	1.05

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/282 (78%)	199 (90%)	19 (9%)	3 (1%)	11	36
1	B	212/282 (75%)	188 (89%)	23 (11%)	1 (0%)	29	60
1	C	217/282 (77%)	190 (88%)	21 (10%)	6 (3%)	5	21
1	D	187/282 (66%)	162 (87%)	25 (13%)	0	100	100
1	E	213/282 (76%)	188 (88%)	23 (11%)	2 (1%)	17	47
1	F	195/282 (69%)	176 (90%)	19 (10%)	0	100	100
1	G	213/282 (76%)	182 (85%)	29 (14%)	2 (1%)	17	47
1	H	212/282 (75%)	181 (85%)	26 (12%)	5 (2%)	6	23
1	I	206/282 (73%)	189 (92%)	17 (8%)	0	100	100
1	J	202/282 (72%)	175 (87%)	26 (13%)	1 (0%)	29	60
1	K	210/282 (74%)	179 (85%)	29 (14%)	2 (1%)	15	45
1	L	185/282 (66%)	170 (92%)	15 (8%)	0	100	100
All	All	2473/3384 (73%)	2179 (88%)	272 (11%)	22 (1%)	17	47

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	221	VAL
1	G	95	ALA
1	A	95	ALA
1	C	109	THR
1	C	218	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/234 (82%)	179 (94%)	12 (6%)	18	45
1	B	183/234 (78%)	172 (94%)	11 (6%)	19	46
1	C	188/234 (80%)	172 (92%)	16 (8%)	10	34
1	D	162/234 (69%)	154 (95%)	8 (5%)	25	55
1	E	185/234 (79%)	176 (95%)	9 (5%)	25	55
1	F	168/234 (72%)	159 (95%)	9 (5%)	22	51
1	G	184/234 (79%)	174 (95%)	10 (5%)	22	51
1	H	184/234 (79%)	176 (96%)	8 (4%)	29	59
1	I	180/234 (77%)	172 (96%)	8 (4%)	28	58
1	J	176/234 (75%)	169 (96%)	7 (4%)	31	62
1	K	183/234 (78%)	168 (92%)	15 (8%)	11	35
1	L	161/234 (69%)	156 (97%)	5 (3%)	40	68
All	All	2145/2808 (76%)	2027 (94%)	118 (6%)	21	50

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	17	LYS
1	K	206	THR
1	G	147	TYR
1	K	205	ASN
1	K	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	56	ASN
1	G	92	HIS
1	J	92	HIS
1	G	220	ASN
1	B	92	HIS

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)

There are no ligands in this entry.

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)

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	229/282 (81%)	0.12	3 (1%)	77	56	32, 57, 102, 114	0
1	B	220/282 (78%)	0.08	1 (0%)	91	79	30, 51, 94, 104	0
1	C	225/282 (79%)	0.07	0	100	100	33, 57, 98, 109	0
1	D	195/282 (69%)	0.06	1 (0%)	91	79	32, 49, 82, 102	0
1	E	221/282 (78%)	0.13	1 (0%)	91	79	36, 60, 109, 127	0
1	F	203/282 (71%)	0.10	0	100	100	33, 51, 87, 101	0
1	G	221/282 (78%)	0.10	0	100	100	33, 59, 110, 123	0
1	H	220/282 (78%)	0.19	6 (2%)	54	28	33, 55, 102, 137	0
1	I	214/282 (75%)	0.46	12 (5%)	24	10	55, 79, 118, 128	0
1	J	210/282 (74%)	0.37	15 (7%)	16	6	53, 72, 124, 143	0
1	K	218/282 (77%)	0.42	5 (2%)	60	36	51, 79, 125, 131	0
1	L	193/282 (68%)	0.26	1 (0%)	91	79	48, 69, 107, 122	0
All	All	2569/3384 (75%)	0.20	45 (1%)	68	45	30, 63, 111, 143	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	210	GLU	5.3
1	J	214	ARG	4.0
1	H	212	GLU	3.7
1	J	92	HIS	3.6
1	I	206	THR	3.6

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.