



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:22 PM UTC

PDB ID : 4ALN / pdb_00004aln
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

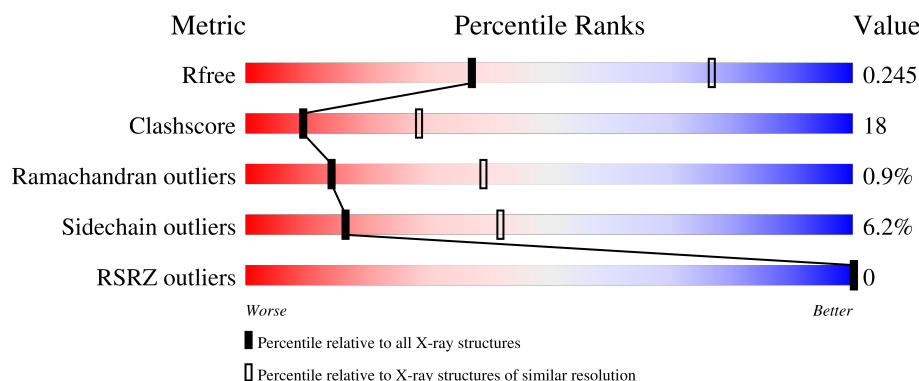
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (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 $\leq 5\%$. 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	282	
1	B	282	
1	C	282	
1	D	282	
1	E	282	

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Mol	Chain	Length	Quality of chain
1	F	282	
1	G	282	
1	H	282	
1	I	282	
1	J	282	
1	K	282	
1	L	282	

2 Entry composition

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

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
2	A	25	Total O 25 25	0	0
2	B	26	Total O 26 26	0	0
2	C	27	Total O 27 27	0	0
2	D	30	Total O 30 30	0	0
2	E	22	Total O 22 22	0	0
2	F	26	Total O 26 26	0	0

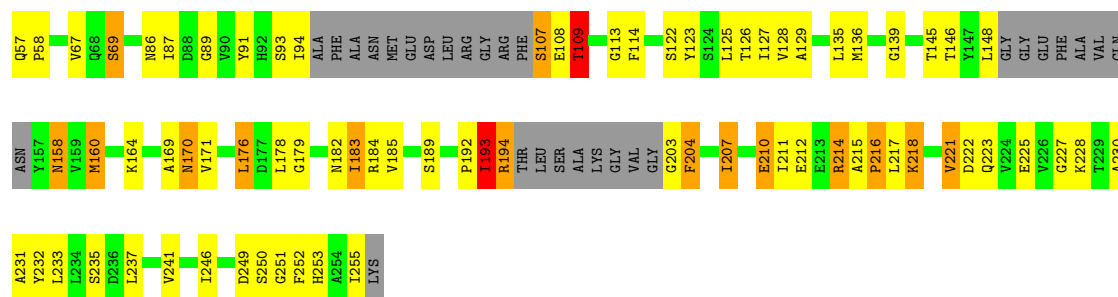
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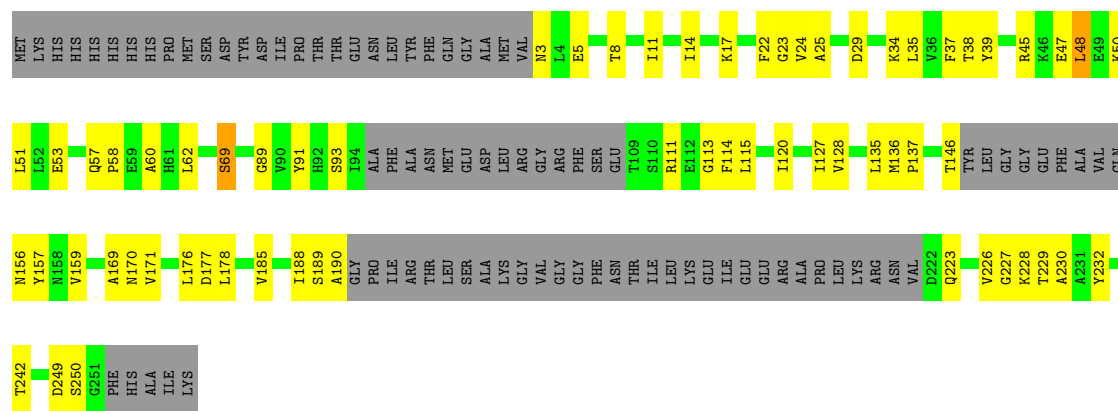
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	21	Total 21	O 21	0	0
2	H	22	Total 22	O 22	0	0
2	I	10	Total 10	O 10	0	0
2	J	7	Total 7	O 7	0	0
2	K	11	Total 11	O 11	0	0
2	L	23	Total 23	O 23	0	0

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.

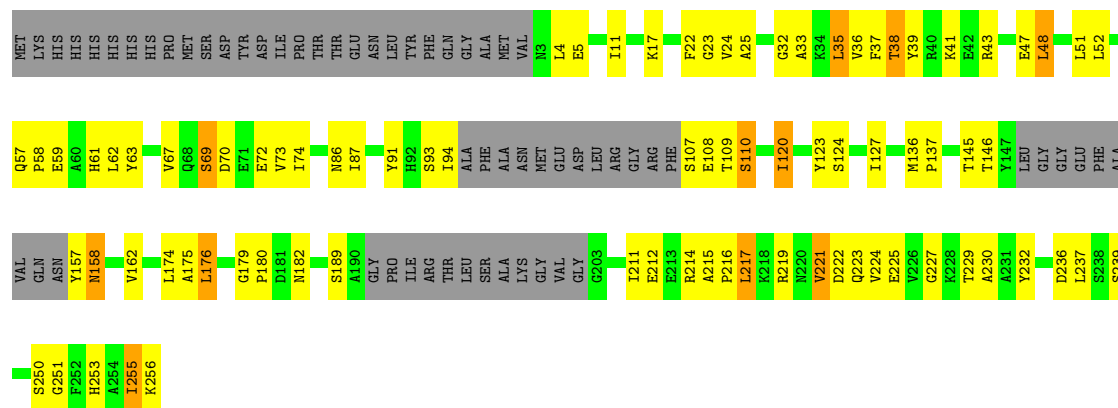
MET	LYS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	PRO	PRO	MET	SER	ASP	THR	TRP	ASP	ILE	LEU	PRO	THR	THR	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ALA	VAL	MET	MET	N3	R3	E5	T8	I11	R18	G23	V24	Q30	L31	G32	A33	K34	L35	T38	Y39	R45	L48	L51	L52	L55	R56
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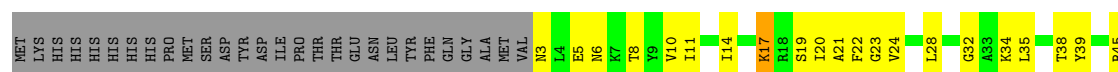
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

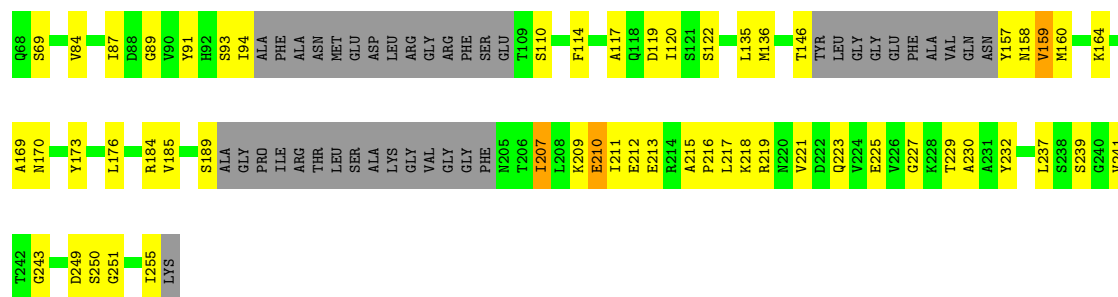


• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

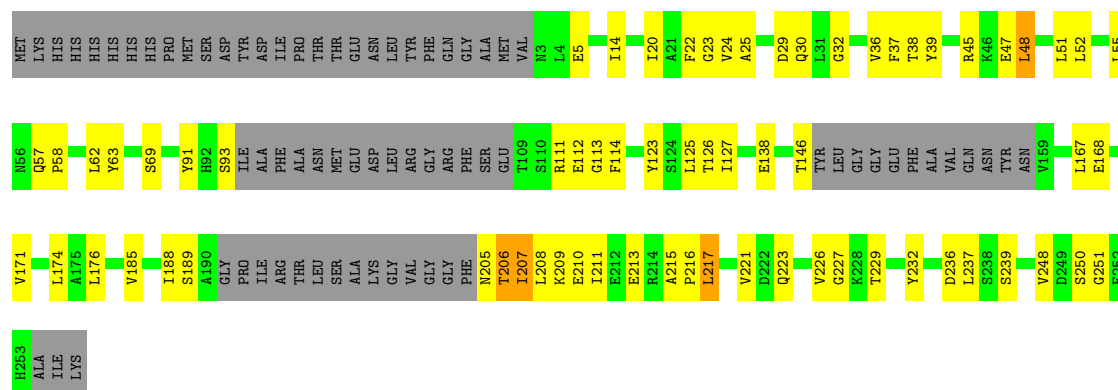


• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

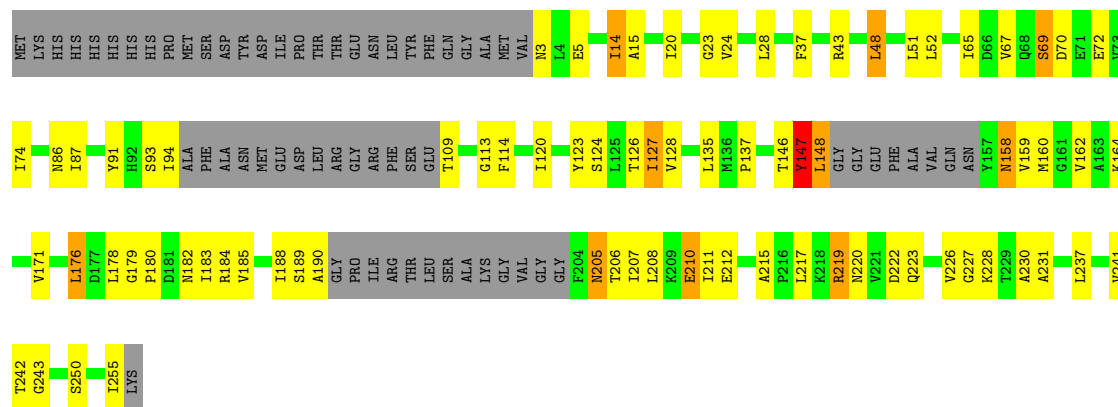




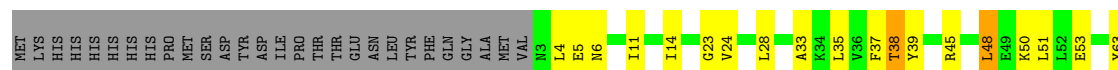
- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]

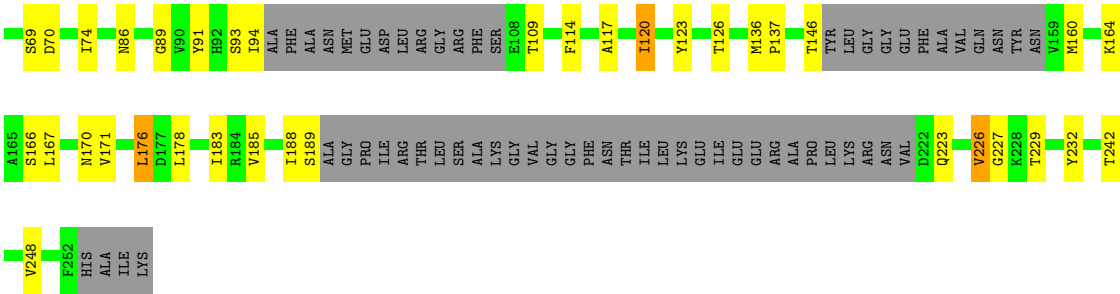


- Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE [NADPH]



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





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.36 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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	0.97	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	1.00	4/1790 (0.2%)	1.06	5/2414 (0.2%)
1	B	1.02	1/1712 (0.1%)	1.10	2/2307 (0.1%)
1	C	0.96	0/1760	1.11	4/2372 (0.2%)
1	D	1.01	0/1507	1.10	5/2031 (0.2%)
1	E	0.95	0/1730	1.06	2/2330 (0.1%)
1	F	1.05	1/1576 (0.1%)	1.08	2/2125 (0.1%)
1	G	0.94	0/1731	1.12	7/2333 (0.3%)
1	H	0.97	1/1719 (0.1%)	1.13	9/2318 (0.4%)
1	I	0.72	0/1672	1.04	3/2253 (0.1%)
1	J	0.74	0/1635	0.99	1/2202 (0.0%)
1	K	0.79	0/1710	1.04	4/2305 (0.2%)
1	L	0.77	1/1494 (0.1%)	0.98	1/2012 (0.0%)
All	All	0.92	8/20036 (0.0%)	1.07	45/27002 (0.2%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	ALA	CA-CB	-6.10	1.44	1.53
1	A	190	ALA	CA-CB	-5.55	1.44	1.53
1	A	226	VAL	CA-CB	-5.46	1.48	1.54
1	F	10	VAL	CA-CB	-5.36	1.47	1.54
1	A	162	VAL	CA-CB	-5.27	1.47	1.54

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	191	GLY	CA-C-N	8.16	130.04	119.84
1	H	191	GLY	C-N-CA	8.16	130.04	119.84
1	I	159	VAL	CB-CA-C	-7.33	103.12	111.55
1	D	120	ILE	N-CA-C	7.08	117.21	110.42
1	G	230	ALA	N-CA-C	-7.00	103.65	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1769	0	1779	70	0
1	B	1693	0	1716	73	0
1	C	1739	0	1754	85	0
1	D	1492	0	1497	56	0
1	E	1710	0	1722	63	0
1	F	1558	0	1558	61	0
1	G	1710	0	1723	76	0
1	H	1699	0	1713	66	0
1	I	1654	0	1672	53	0
1	J	1618	0	1635	52	0
1	K	1690	0	1706	54	0
1	L	1479	0	1486	44	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	1	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	712	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 18.

The worst 5 of 712 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CE	1.87	1.05
1:I:221:VAL:HG21	1:I:249:ASP:HA	1.37	1.04

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%)	9	29
1	B	212/282 (75%)	188 (89%)	23 (11%)	1 (0%)	24	52
1	C	217/282 (77%)	190 (88%)	21 (10%)	6 (3%)	4	16
1	D	187/282 (66%)	162 (87%)	25 (13%)	0	100	100
1	E	213/282 (76%)	188 (88%)	23 (11%)	2 (1%)	14	39
1	F	195/282 (69%)	176 (90%)	19 (10%)	0	100	100
1	G	213/282 (76%)	182 (85%)	29 (14%)	2 (1%)	14	39
1	H	212/282 (75%)	181 (85%)	26 (12%)	5 (2%)	4	18
1	I	206/282 (73%)	189 (92%)	17 (8%)	0	100	100
1	J	202/282 (72%)	175 (87%)	26 (13%)	1 (0%)	24	52
1	K	210/282 (74%)	179 (85%)	29 (14%)	2 (1%)	12	37
1	L	185/282 (66%)	170 (92%)	15 (8%)	0	100	100
All	All	2473/3384 (73%)	2179 (88%)	272 (11%)	22 (1%)	14	39

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	221	VAL

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

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	191/234 (82%)	178 (93%)	13 (7%)	14	39
1	B	183/234 (78%)	169 (92%)	14 (8%)	12	35
1	C	188/234 (80%)	169 (90%)	19 (10%)	7	24
1	D	162/234 (69%)	154 (95%)	8 (5%)	22	50
1	E	185/234 (79%)	174 (94%)	11 (6%)	18	44
1	F	168/234 (72%)	160 (95%)	8 (5%)	23	50
1	G	184/234 (79%)	173 (94%)	11 (6%)	17	43
1	H	184/234 (79%)	175 (95%)	9 (5%)	22	50
1	I	180/234 (77%)	172 (96%)	8 (4%)	25	53
1	J	176/234 (75%)	168 (96%)	8 (4%)	24	52
1	K	183/234 (78%)	164 (90%)	19 (10%)	7	23
1	L	161/234 (69%)	157 (98%)	4 (2%)	42	65
All	All	2145/2808 (76%)	2013 (94%)	132 (6%)	16	42

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	127	ILE
1	K	159	VAL
1	L	69	SER
1	D	69	SER
1	D	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	130	HIS
1	L	92	HIS
1	F	92	HIS
1	J	92	HIS
1	F	56	ASN

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 oligosaccharides 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%)	-1.57	0 100 100	32, 57, 102, 114	0
1	B	220/282 (78%)	-1.58	0 100 100	30, 51, 94, 104	0
1	C	225/282 (79%)	-1.55	0 100 100	33, 57, 98, 109	0
1	D	195/282 (69%)	-1.60	0 100 100	32, 49, 82, 102	0
1	E	221/282 (78%)	-1.54	0 100 100	36, 60, 109, 127	0
1	F	203/282 (71%)	-1.57	0 100 100	33, 51, 87, 101	0
1	G	221/282 (78%)	-1.49	0 100 100	33, 59, 110, 123	0
1	H	220/282 (78%)	-1.57	0 100 100	33, 55, 102, 137	0
1	I	214/282 (75%)	-1.45	0 100 100	55, 79, 118, 128	0
1	J	210/282 (74%)	-1.51	0 100 100	53, 72, 124, 143	0
1	K	218/282 (77%)	-1.48	0 100 100	51, 79, 125, 131	0
1	L	193/282 (68%)	-1.50	0 100 100	48, 69, 107, 122	0
All	All	2569/3384 (75%)	-1.54	0 100 100	30, 63, 111, 143	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.