wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 06:45 PM EDT

PDB ID	:	4NQZ
Title	:	Crystal Structure of the Pseudomonas aeruginosa Enoyl-Acyl Carrier Protein Reductase (FabI) in apo form
Authors	:	Chi, Y.M.; Lee, J.H.; Park, A.K.
Deposited on	:	2013-11-26
Resolution	:	2.60 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:

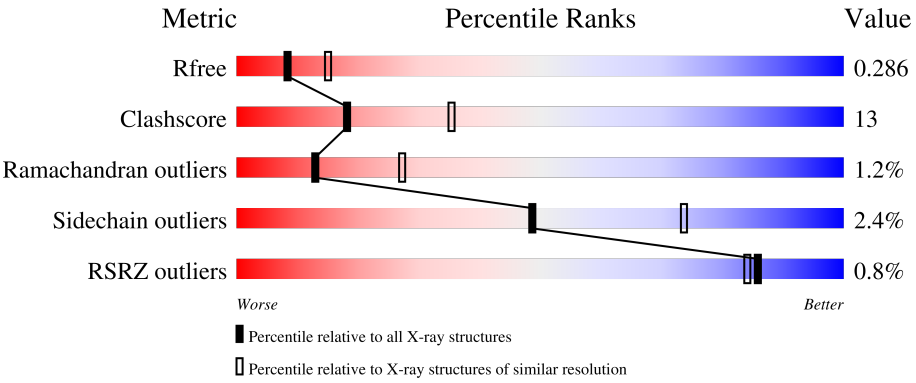
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	273	67% 23% 9%
1	B	273	68% 21% 11%
1	C	273	63% 26% 10%
1	D	273	61% 28% 10%
1	E	273	65% 23% 11%

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Mol	Chain	Length	Quality of chain
1	F	273	61% 27% • 10%
1	G	273	65% 23% • 11%
1	H	273	% 67% 23% 9%
1	I	273	% 65% 23% • 11%
1	J	273	61% 28% 10%
1	K	273	55% 34% 10%
1	L	273	% 61% 27% • 11%
1	M	273	58% 31% 10%
1	N	273	% 65% 24% 11%
1	O	273	3% 56% 33% • 10%
1	P	273	2% 61% 28% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29449 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] FabI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1840	1151	327	351	11			
1	B	243	Total	C	N	O	S	0	0	0
			1797	1125	318	345	9			
1	C	245	Total	C	N	O	S	0	0	0
			1813	1135	320	347	11			
1	D	246	Total	C	N	O	S	0	0	0
			1822	1141	322	348	11			
1	E	244	Total	C	N	O	S	0	0	0
			1805	1130	319	346	10			
1	F	245	Total	C	N	O	S	0	0	0
			1816	1136	323	347	10			
1	G	244	Total	C	N	O	S	0	0	0
			1805	1130	319	346	10			
1	H	248	Total	C	N	O	S	0	0	0
			1844	1153	330	350	11			
1	I	244	Total	C	N	O	S	0	0	0
			1805	1130	319	346	10			
1	J	245	Total	C	N	O	S	0	0	0
			1813	1135	320	347	11			
1	K	246	Total	C	N	O	S	0	0	0
			1824	1141	324	348	11			
1	L	244	Total	C	N	O	S	0	0	0
			1808	1131	322	346	9			
1	M	245	Total	C	N	O	S	0	0	0
			1816	1136	323	347	10			
1	N	244	Total	C	N	O	S	0	0	0
			1811	1133	322	346	10			
1	O	247	Total	C	N	O	S	0	0	0
			1836	1148	329	349	10			
1	P	248	Total	C	N	O	S	0	0	0
			1837	1149	327	350	11			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	LEU	-	expression tag	UNP Q9ZFE4
A	267	GLU	-	expression tag	UNP Q9ZFE4
A	268	HIS	-	expression tag	UNP Q9ZFE4
A	269	HIS	-	expression tag	UNP Q9ZFE4
A	270	HIS	-	expression tag	UNP Q9ZFE4
A	271	HIS	-	expression tag	UNP Q9ZFE4
A	272	HIS	-	expression tag	UNP Q9ZFE4
A	273	HIS	-	expression tag	UNP Q9ZFE4
B	266	LEU	-	expression tag	UNP Q9ZFE4
B	267	GLU	-	expression tag	UNP Q9ZFE4
B	268	HIS	-	expression tag	UNP Q9ZFE4
B	269	HIS	-	expression tag	UNP Q9ZFE4
B	270	HIS	-	expression tag	UNP Q9ZFE4
B	271	HIS	-	expression tag	UNP Q9ZFE4
B	272	HIS	-	expression tag	UNP Q9ZFE4
B	273	HIS	-	expression tag	UNP Q9ZFE4
C	266	LEU	-	expression tag	UNP Q9ZFE4
C	267	GLU	-	expression tag	UNP Q9ZFE4
C	268	HIS	-	expression tag	UNP Q9ZFE4
C	269	HIS	-	expression tag	UNP Q9ZFE4
C	270	HIS	-	expression tag	UNP Q9ZFE4
C	271	HIS	-	expression tag	UNP Q9ZFE4
C	272	HIS	-	expression tag	UNP Q9ZFE4
C	273	HIS	-	expression tag	UNP Q9ZFE4
D	266	LEU	-	expression tag	UNP Q9ZFE4
D	267	GLU	-	expression tag	UNP Q9ZFE4
D	268	HIS	-	expression tag	UNP Q9ZFE4
D	269	HIS	-	expression tag	UNP Q9ZFE4
D	270	HIS	-	expression tag	UNP Q9ZFE4
D	271	HIS	-	expression tag	UNP Q9ZFE4
D	272	HIS	-	expression tag	UNP Q9ZFE4
D	273	HIS	-	expression tag	UNP Q9ZFE4
E	266	LEU	-	expression tag	UNP Q9ZFE4
E	267	GLU	-	expression tag	UNP Q9ZFE4
E	268	HIS	-	expression tag	UNP Q9ZFE4
E	269	HIS	-	expression tag	UNP Q9ZFE4
E	270	HIS	-	expression tag	UNP Q9ZFE4
E	271	HIS	-	expression tag	UNP Q9ZFE4
E	272	HIS	-	expression tag	UNP Q9ZFE4
E	273	HIS	-	expression tag	UNP Q9ZFE4
F	266	LEU	-	expression tag	UNP Q9ZFE4
F	267	GLU	-	expression tag	UNP Q9ZFE4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	268	HIS	-	expression tag	UNP Q9ZFE4
F	269	HIS	-	expression tag	UNP Q9ZFE4
F	270	HIS	-	expression tag	UNP Q9ZFE4
F	271	HIS	-	expression tag	UNP Q9ZFE4
F	272	HIS	-	expression tag	UNP Q9ZFE4
F	273	HIS	-	expression tag	UNP Q9ZFE4
G	266	LEU	-	expression tag	UNP Q9ZFE4
G	267	GLU	-	expression tag	UNP Q9ZFE4
G	268	HIS	-	expression tag	UNP Q9ZFE4
G	269	HIS	-	expression tag	UNP Q9ZFE4
G	270	HIS	-	expression tag	UNP Q9ZFE4
G	271	HIS	-	expression tag	UNP Q9ZFE4
G	272	HIS	-	expression tag	UNP Q9ZFE4
G	273	HIS	-	expression tag	UNP Q9ZFE4
H	266	LEU	-	expression tag	UNP Q9ZFE4
H	267	GLU	-	expression tag	UNP Q9ZFE4
H	268	HIS	-	expression tag	UNP Q9ZFE4
H	269	HIS	-	expression tag	UNP Q9ZFE4
H	270	HIS	-	expression tag	UNP Q9ZFE4
H	271	HIS	-	expression tag	UNP Q9ZFE4
H	272	HIS	-	expression tag	UNP Q9ZFE4
H	273	HIS	-	expression tag	UNP Q9ZFE4
I	266	LEU	-	expression tag	UNP Q9ZFE4
I	267	GLU	-	expression tag	UNP Q9ZFE4
I	268	HIS	-	expression tag	UNP Q9ZFE4
I	269	HIS	-	expression tag	UNP Q9ZFE4
I	270	HIS	-	expression tag	UNP Q9ZFE4
I	271	HIS	-	expression tag	UNP Q9ZFE4
I	272	HIS	-	expression tag	UNP Q9ZFE4
I	273	HIS	-	expression tag	UNP Q9ZFE4
J	266	LEU	-	expression tag	UNP Q9ZFE4
J	267	GLU	-	expression tag	UNP Q9ZFE4
J	268	HIS	-	expression tag	UNP Q9ZFE4
J	269	HIS	-	expression tag	UNP Q9ZFE4
J	270	HIS	-	expression tag	UNP Q9ZFE4
J	271	HIS	-	expression tag	UNP Q9ZFE4
J	272	HIS	-	expression tag	UNP Q9ZFE4
J	273	HIS	-	expression tag	UNP Q9ZFE4
K	266	LEU	-	expression tag	UNP Q9ZFE4
K	267	GLU	-	expression tag	UNP Q9ZFE4
K	268	HIS	-	expression tag	UNP Q9ZFE4
K	269	HIS	-	expression tag	UNP Q9ZFE4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	270	HIS	-	expression tag	UNP Q9ZFE4
K	271	HIS	-	expression tag	UNP Q9ZFE4
K	272	HIS	-	expression tag	UNP Q9ZFE4
K	273	HIS	-	expression tag	UNP Q9ZFE4
L	266	LEU	-	expression tag	UNP Q9ZFE4
L	267	GLU	-	expression tag	UNP Q9ZFE4
L	268	HIS	-	expression tag	UNP Q9ZFE4
L	269	HIS	-	expression tag	UNP Q9ZFE4
L	270	HIS	-	expression tag	UNP Q9ZFE4
L	271	HIS	-	expression tag	UNP Q9ZFE4
L	272	HIS	-	expression tag	UNP Q9ZFE4
L	273	HIS	-	expression tag	UNP Q9ZFE4
M	266	LEU	-	expression tag	UNP Q9ZFE4
M	267	GLU	-	expression tag	UNP Q9ZFE4
M	268	HIS	-	expression tag	UNP Q9ZFE4
M	269	HIS	-	expression tag	UNP Q9ZFE4
M	270	HIS	-	expression tag	UNP Q9ZFE4
M	271	HIS	-	expression tag	UNP Q9ZFE4
M	272	HIS	-	expression tag	UNP Q9ZFE4
M	273	HIS	-	expression tag	UNP Q9ZFE4
N	266	LEU	-	expression tag	UNP Q9ZFE4
N	267	GLU	-	expression tag	UNP Q9ZFE4
N	268	HIS	-	expression tag	UNP Q9ZFE4
N	269	HIS	-	expression tag	UNP Q9ZFE4
N	270	HIS	-	expression tag	UNP Q9ZFE4
N	271	HIS	-	expression tag	UNP Q9ZFE4
N	272	HIS	-	expression tag	UNP Q9ZFE4
N	273	HIS	-	expression tag	UNP Q9ZFE4
O	266	LEU	-	expression tag	UNP Q9ZFE4
O	267	GLU	-	expression tag	UNP Q9ZFE4
O	268	HIS	-	expression tag	UNP Q9ZFE4
O	269	HIS	-	expression tag	UNP Q9ZFE4
O	270	HIS	-	expression tag	UNP Q9ZFE4
O	271	HIS	-	expression tag	UNP Q9ZFE4
O	272	HIS	-	expression tag	UNP Q9ZFE4
O	273	HIS	-	expression tag	UNP Q9ZFE4
P	266	LEU	-	expression tag	UNP Q9ZFE4
P	267	GLU	-	expression tag	UNP Q9ZFE4
P	268	HIS	-	expression tag	UNP Q9ZFE4
P	269	HIS	-	expression tag	UNP Q9ZFE4
P	270	HIS	-	expression tag	UNP Q9ZFE4
P	271	HIS	-	expression tag	UNP Q9ZFE4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	272	HIS	-	expression tag	UNP Q9ZFE4
P	273	HIS	-	expression tag	UNP Q9ZFE4

- Molecule 2 is water.

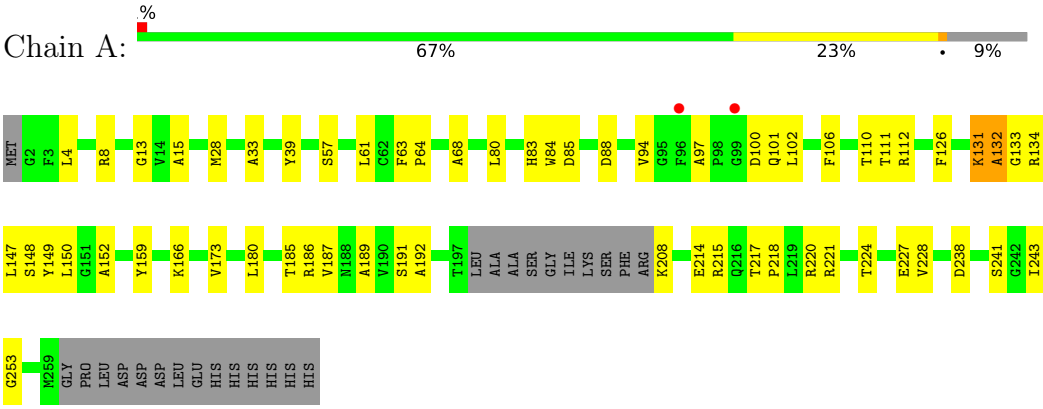
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	27	Total O 27 27	0	0
2	B	24	Total O 24 24	0	0
2	C	33	Total O 33 33	0	0
2	D	24	Total O 24 24	0	0
2	E	22	Total O 22 22	0	0
2	F	26	Total O 26 26	0	0
2	G	23	Total O 23 23	0	0
2	H	32	Total O 32 32	0	0
2	I	23	Total O 23 23	0	0
2	J	16	Total O 16 16	0	0
2	K	20	Total O 20 20	0	0
2	L	16	Total O 16 16	0	0
2	M	16	Total O 16 16	0	0
2	N	22	Total O 22 22	0	0
2	O	13	Total O 13 13	0	0
2	P	20	Total O 20 20	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.

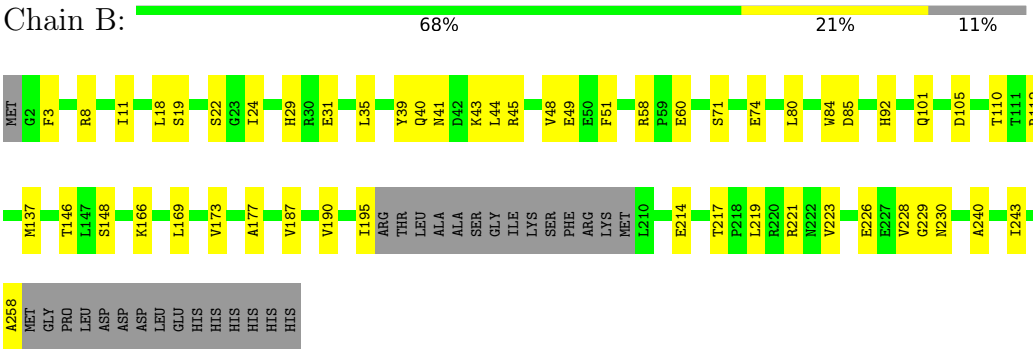
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain A:



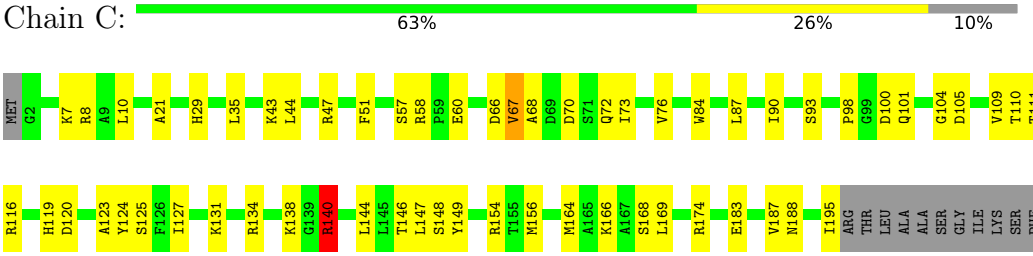
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain B:



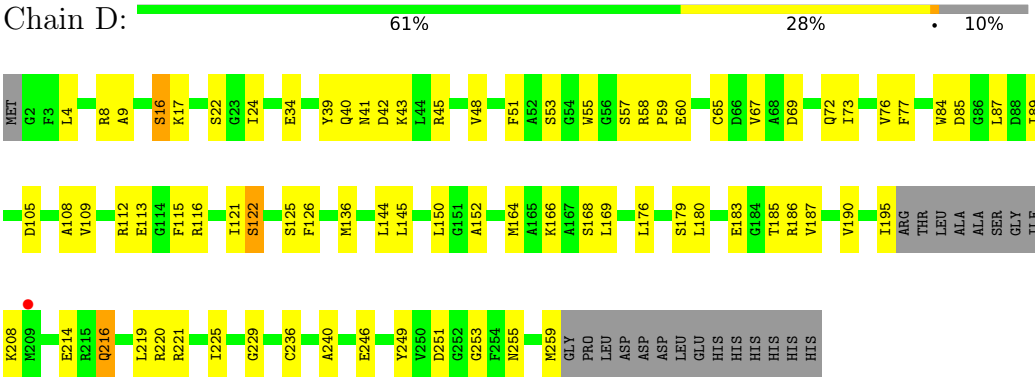
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain C:



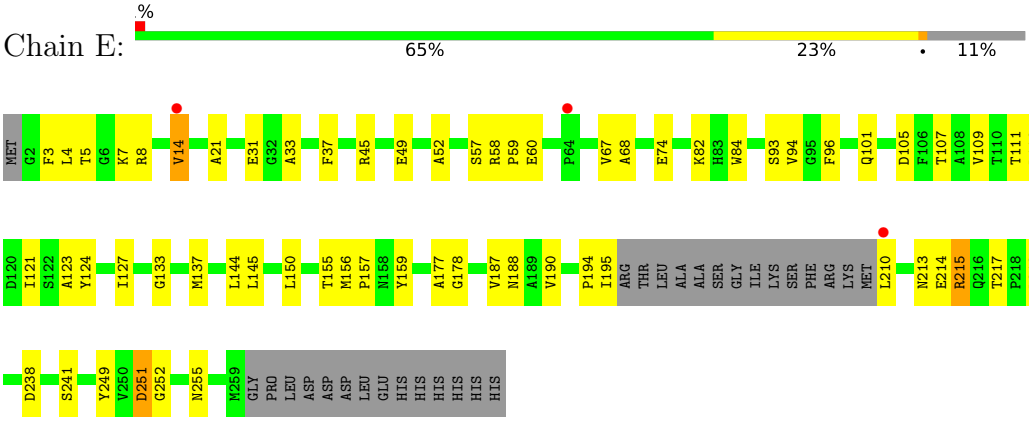
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain D:



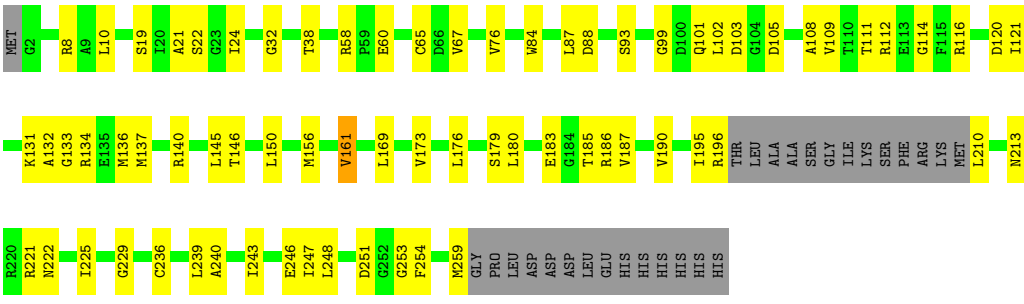
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain E:



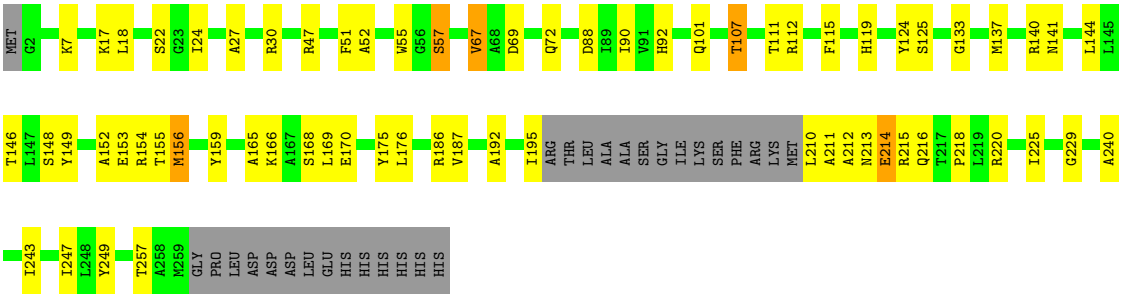
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain F:



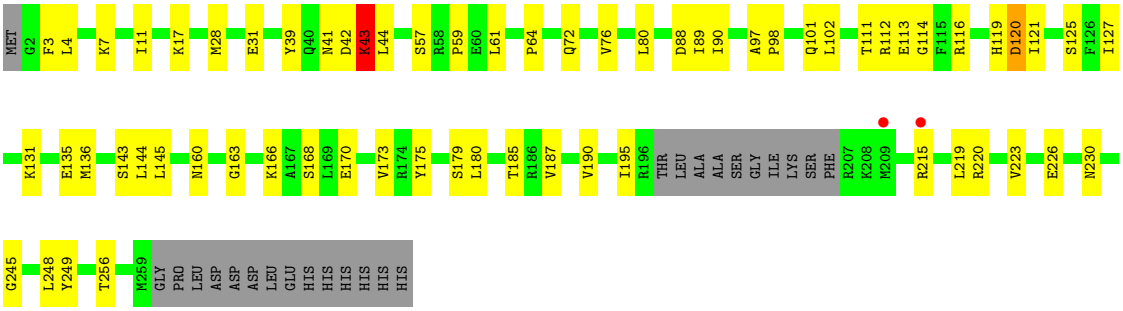
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain G:



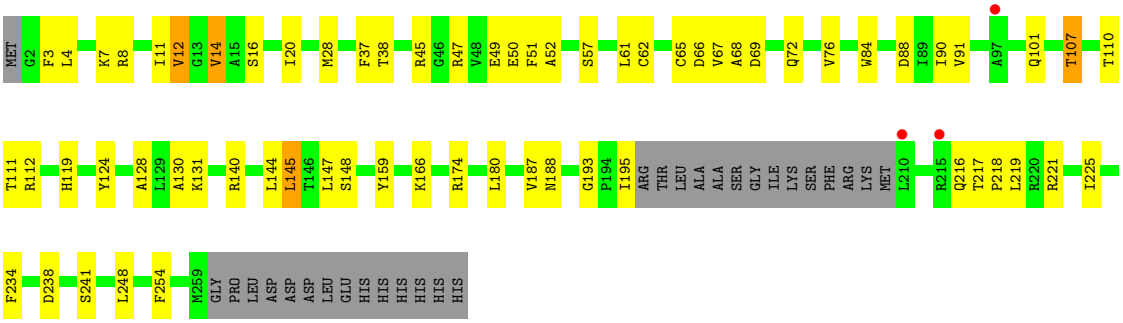
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain H:



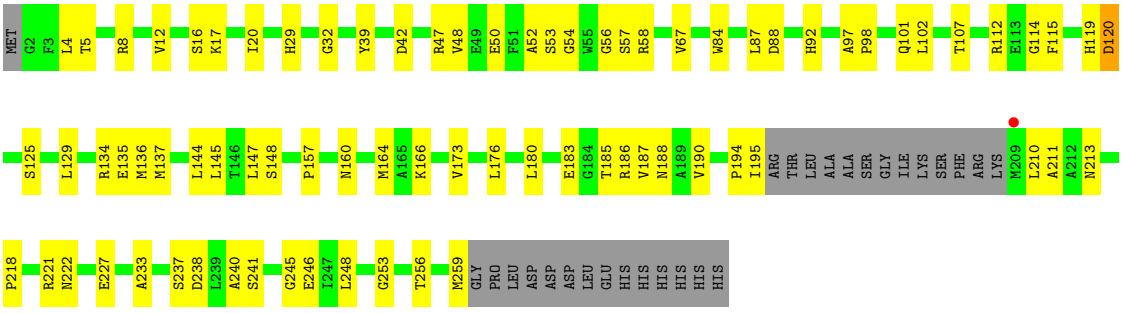
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain I:



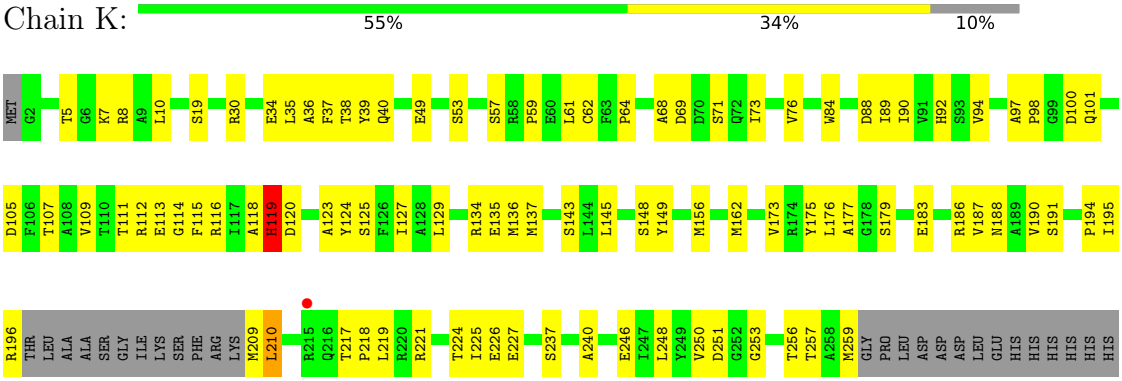
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain J:



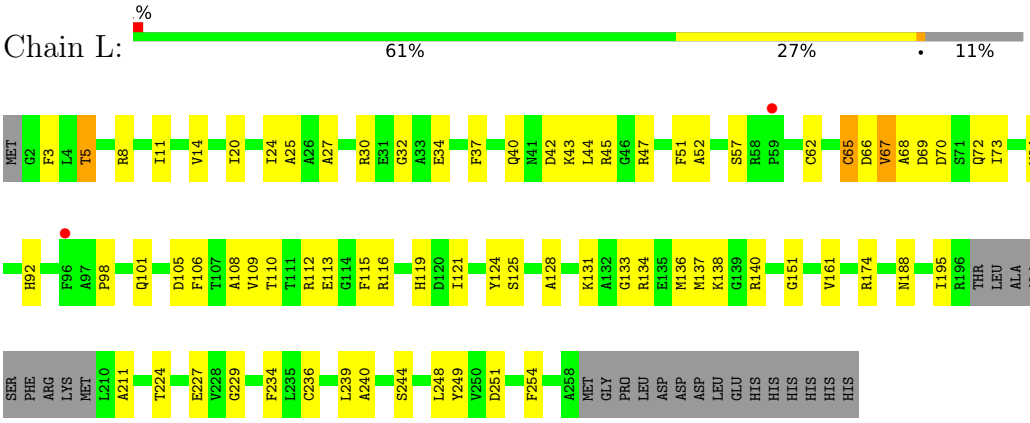
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain K:



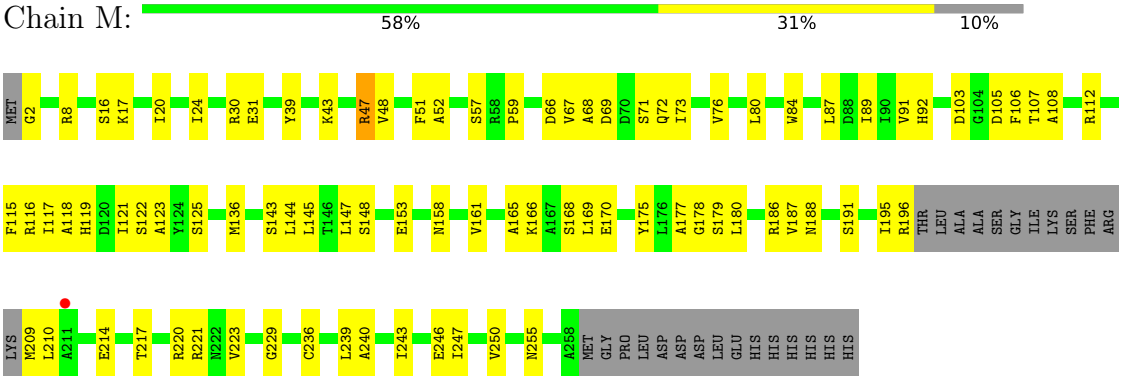
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain L:



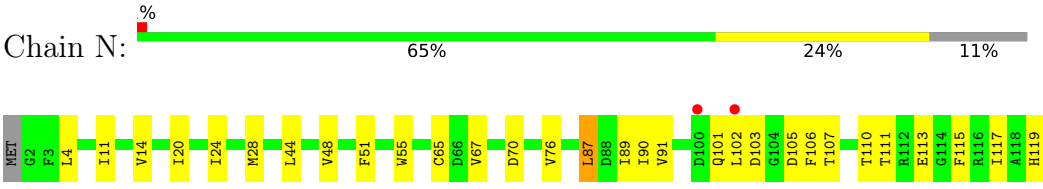
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

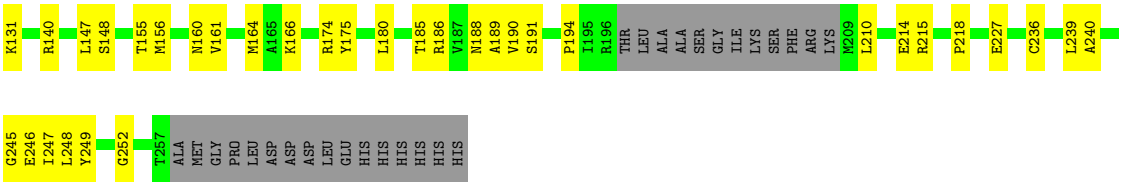
Chain M:



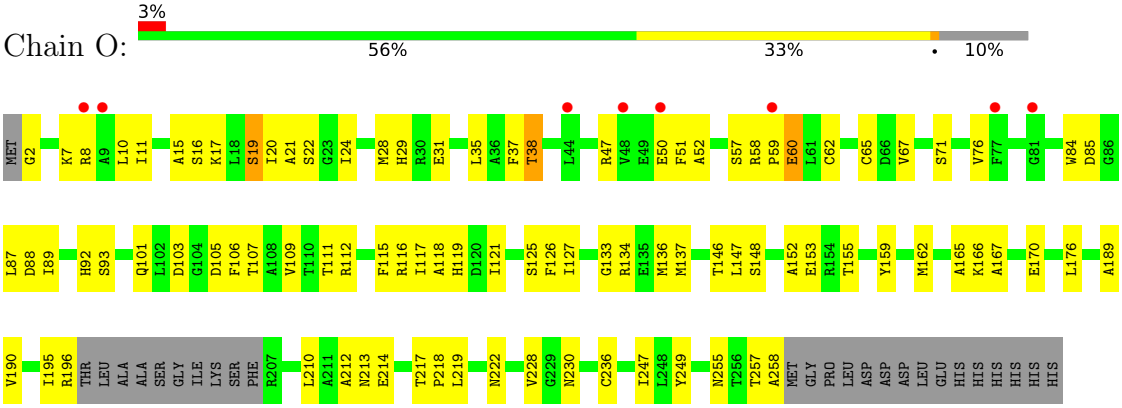
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI

Chain N:

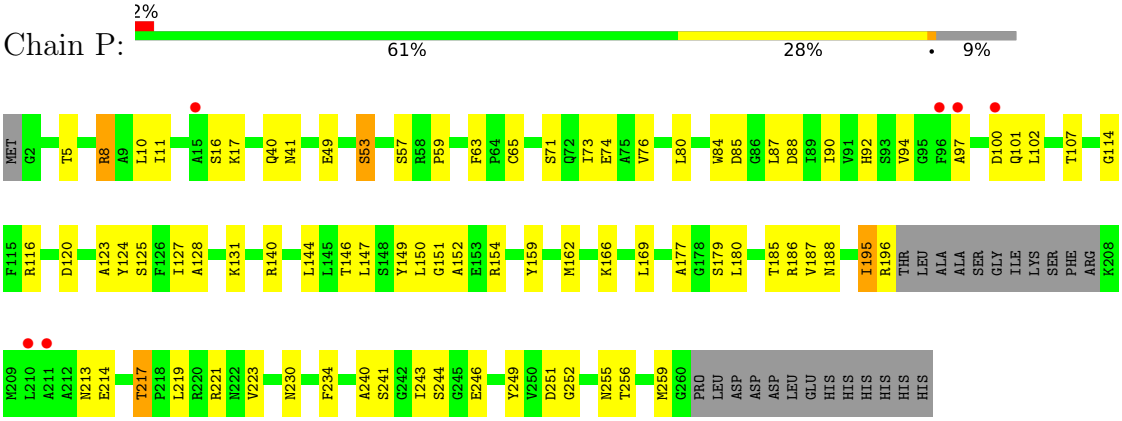




• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH] FabI



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.32Å 155.84Å 129.45Å 90.00° 111.06° 90.00°	Depositor
Resolution (Å)	44.39 – 2.60 48.13 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.7 (44.39-2.60) 84.7 (48.13-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.199 , 0.286 0.202 , 0.286	Depositor DCC
R_{free} test set	5660 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 29.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29449	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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	0.50	0/1869	0.65	0/2520
1	B	0.45	0/1826	0.62	0/2465
1	C	0.50	0/1842	0.66	1/2485 (0.0%)
1	D	0.43	0/1851	0.58	0/2496
1	E	0.42	0/1834	0.58	0/2475
1	F	0.46	0/1845	0.66	0/2489
1	G	0.49	0/1834	0.67	0/2475
1	H	0.47	0/1873	0.66	0/2524
1	I	0.45	0/1834	0.63	0/2475
1	J	0.41	0/1842	0.59	0/2485
1	K	0.47	0/1853	0.65	1/2499 (0.0%)
1	L	0.41	0/1837	0.60	0/2479
1	M	0.43	0/1845	0.60	0/2489
1	N	0.45	0/1840	0.63	1/2482 (0.0%)
1	O	0.41	0/1865	0.60	0/2514
1	P	0.42	0/1866	0.61	1/2515 (0.0%)
All	All	0.45	0/29556	0.63	4/39867 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	195	ILE	C-N-CA	5.56	135.60	121.70
1	K	210	LEU	CA-CB-CG	5.52	128.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	140	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	N	87	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	60	GLU	Peptide

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	1840	0	1820	44	0
1	B	1797	0	1769	36	0
1	C	1813	0	1787	55	0
1	D	1822	0	1800	55	0
1	E	1805	0	1778	51	0
1	F	1816	0	1791	48	0
1	G	1805	0	1778	50	1
1	H	1844	0	1826	47	0
1	I	1805	0	1778	48	1
1	J	1813	0	1787	58	0
1	K	1824	0	1800	69	0
1	L	1808	0	1782	59	0
1	M	1816	0	1791	66	0
1	N	1811	0	1786	56	0
1	O	1836	0	1817	67	0
1	P	1837	0	1816	63	0
2	A	27	0	0	6	0
2	B	24	0	0	1	0
2	C	33	0	0	6	0
2	D	24	0	0	3	0
2	E	22	0	0	3	0
2	F	26	0	0	5	0
2	G	23	0	0	4	0
2	H	32	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	23	0	0	2	0
2	J	16	0	0	2	0
2	K	20	0	0	3	0
2	L	16	0	0	7	0
2	M	16	0	0	1	0
2	N	22	0	0	5	0
2	O	13	0	0	2	0
2	P	20	0	0	6	0
All	All	29449	0	28706	772	1

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 13.

The worst 5 of 772 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:GLN:HE22	1:F:111:THR:H	1.12	0.96
1:G:153:GLU:OE1	1:G:249:TYR:OH	1.88	0.91
1:N:188:ASN:O	2:N:303:HOH:O	1.91	0.88
1:J:241:SER:HB2	1:L:227:GLU:HG2	1.60	0.84
1:O:107:THR:O	1:P:131:LYS:NZ	2.09	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:ARG:NH2	1:I:62:CYS:O[2_555]	2.17	0.03

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	244/273 (89%)	217 (89%)	24 (10%)	3 (1%)	13	27
1	B	239/273 (88%)	216 (90%)	21 (9%)	2 (1%)	19	39
1	C	241/273 (88%)	215 (89%)	25 (10%)	1 (0%)	34	57
1	D	242/273 (89%)	221 (91%)	20 (8%)	1 (0%)	34	57
1	E	240/273 (88%)	213 (89%)	22 (9%)	5 (2%)	7	13
1	F	241/273 (88%)	212 (88%)	24 (10%)	5 (2%)	7	13
1	G	240/273 (88%)	214 (89%)	23 (10%)	3 (1%)	12	24
1	H	244/273 (89%)	224 (92%)	16 (7%)	4 (2%)	9	19
1	I	240/273 (88%)	217 (90%)	22 (9%)	1 (0%)	34	57
1	J	241/273 (88%)	209 (87%)	27 (11%)	5 (2%)	7	13
1	K	242/273 (89%)	211 (87%)	26 (11%)	5 (2%)	7	13
1	L	240/273 (88%)	217 (90%)	21 (9%)	2 (1%)	19	39
1	M	241/273 (88%)	218 (90%)	21 (9%)	2 (1%)	19	39
1	N	240/273 (88%)	213 (89%)	26 (11%)	1 (0%)	34	57
1	O	243/273 (89%)	211 (87%)	28 (12%)	4 (2%)	9	19
1	P	244/273 (89%)	217 (89%)	26 (11%)	1 (0%)	34	57
All	All	3862/4368 (88%)	3445 (89%)	372 (10%)	45 (1%)	13	27

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	59	PRO
1	E	215	ARG
1	F	103	ASP
1	F	131	LYS
1	G	214	GLU

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	184/205 (90%)	181 (98%)	3 (2%)	62	82
1	B	179/205 (87%)	176 (98%)	3 (2%)	60	81
1	C	181/205 (88%)	180 (99%)	1 (1%)	86	95
1	D	182/205 (89%)	177 (97%)	5 (3%)	44	71
1	E	180/205 (88%)	179 (99%)	1 (1%)	86	95
1	F	181/205 (88%)	173 (96%)	8 (4%)	28	53
1	G	180/205 (88%)	175 (97%)	5 (3%)	43	69
1	H	184/205 (90%)	182 (99%)	2 (1%)	73	88
1	I	180/205 (88%)	172 (96%)	8 (4%)	28	53
1	J	181/205 (88%)	180 (99%)	1 (1%)	86	95
1	K	182/205 (89%)	176 (97%)	6 (3%)	38	64
1	L	180/205 (88%)	174 (97%)	6 (3%)	38	64
1	M	181/205 (88%)	179 (99%)	2 (1%)	73	88
1	N	181/205 (88%)	177 (98%)	4 (2%)	52	76
1	O	183/205 (89%)	176 (96%)	7 (4%)	33	59
1	P	183/205 (89%)	176 (96%)	7 (4%)	33	59
All	All	2902/3280 (88%)	2833 (98%)	69 (2%)	49	74

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	50	GLU
1	O	85	ASP
1	P	53	SER
1	G	141	ASN
1	G	107	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	41	ASN
1	P	213	ASN
1	F	101	GLN
1	F	216	GLN
1	N	101	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	248/273 (90%)	-0.51	2 (0%) 86 84	19, 29, 53, 77	0
1	B	243/273 (89%)	-0.47	0 100 100	27, 37, 55, 66	0
1	C	245/273 (89%)	-0.58	0 100 100	17, 28, 45, 62	0
1	D	246/273 (90%)	-0.42	1 (0%) 92 91	26, 41, 58, 88	0
1	E	244/273 (89%)	-0.14	3 (1%) 79 76	28, 46, 68, 75	0
1	F	245/273 (89%)	-0.50	0 100 100	22, 35, 54, 64	0
1	G	244/273 (89%)	-0.55	0 100 100	22, 33, 49, 75	0
1	H	248/273 (90%)	-0.59	2 (0%) 86 84	21, 30, 54, 85	0
1	I	244/273 (89%)	-0.51	3 (1%) 79 76	18, 32, 57, 76	0
1	J	245/273 (89%)	-0.29	1 (0%) 92 91	26, 45, 63, 76	0
1	K	246/273 (90%)	-0.48	1 (0%) 92 91	23, 36, 59, 82	0
1	L	244/273 (89%)	-0.32	2 (0%) 86 84	27, 45, 61, 72	0
1	M	245/273 (89%)	-0.35	1 (0%) 92 91	31, 43, 58, 67	0
1	N	244/273 (89%)	-0.33	2 (0%) 86 84	26, 37, 64, 76	0
1	O	247/273 (90%)	0.07	8 (3%) 47 40	34, 51, 71, 80	0
1	P	248/273 (90%)	-0.24	6 (2%) 59 53	27, 40, 66, 80	0
All	All	3926/4368 (89%)	-0.39	32 (0%) 86 84	17, 38, 62, 88	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	209	MET	4.1
1	A	99	GLY	3.7
1	O	81	GLY	3.5
1	I	215	ARG	3.4
1	N	102	LEU	3.2

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.