



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2016 – 05:26 PM EDT

PDB ID : 5ENY  
Title : Ketosynthase from module 6 connected to acyl carrier protein from module 5 (unobservable) of the bacillaene synthase from *Bacillus subtilis* 168  
Authors : Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.  
Deposited on : 2015-11-09  
Resolution : 4.00 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](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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

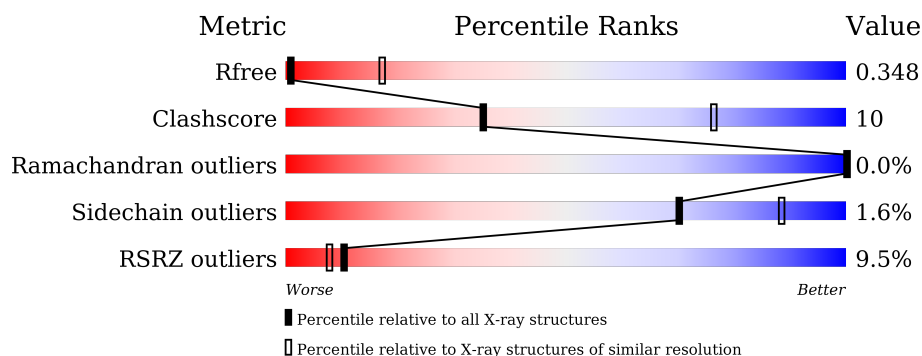
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.






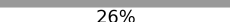

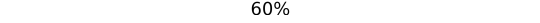

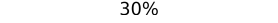
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	764	<div> <div>7%</div> <div>62%</div> <div>11%</div> <div>26%</div> </div>
1	B	764	<div> <div>8%</div> <div>59%</div> <div>10%</div> <div>30%</div> </div>
1	C	764	<div> <div>6%</div> <div>62%</div> <div>11%</div> <div>26%</div> </div>
1	D	764	<div> <div>5%</div> <div>60%</div> <div>9%</div> <div>30%</div> </div>
1	E	764	<div> <div>7%</div> <div>62%</div> <div>11%</div> <div>26%</div> </div>
1	F	764	<div> <div>7%</div> <div>59%</div> <div>10%</div> <div>30%</div> </div>

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Mol	Chain	Length	Quality of chain			
			5%	62%	11%	26%
1	G	764				
1	H	764				

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34416 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 Polyketide synthase PksL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	B	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			
1	C	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	D	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			
1	E	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	F	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			
1	G	563	Total	C	N	O	S	0	0	0
			4419	2811	738	844	26			
1	H	533	Total	C	N	O	S	0	0	0
			4185	2663	703	797	22			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-172	MET	-	initiating methionine	UNP Q05470
A	-171	GLY	-	expression tag	UNP Q05470
A	-170	SER	-	expression tag	UNP Q05470
A	-169	SER	-	expression tag	UNP Q05470
A	-168	HIS	-	expression tag	UNP Q05470
A	-167	HIS	-	expression tag	UNP Q05470
A	-166	HIS	-	expression tag	UNP Q05470
A	-165	HIS	-	expression tag	UNP Q05470
A	-164	HIS	-	expression tag	UNP Q05470
A	-163	HIS	-	expression tag	UNP Q05470
A	-162	SER	-	expression tag	UNP Q05470
A	-161	SER	-	expression tag	UNP Q05470
A	-160	GLY	-	expression tag	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-159	LEU	-	expression tag	UNP Q05470
A	-158	VAL	-	expression tag	UNP Q05470
A	-157	PRO	-	expression tag	UNP Q05470
A	-156	ARG	-	expression tag	UNP Q05470
A	-155	GLY	-	expression tag	UNP Q05470
A	-154	SER	-	expression tag	UNP Q05470
A	-153	SER	-	expression tag	UNP Q05470
B	-172	MET	-	initiating methionine	UNP Q05470
B	-171	GLY	-	expression tag	UNP Q05470
B	-170	SER	-	expression tag	UNP Q05470
B	-169	SER	-	expression tag	UNP Q05470
B	-168	HIS	-	expression tag	UNP Q05470
B	-167	HIS	-	expression tag	UNP Q05470
B	-166	HIS	-	expression tag	UNP Q05470
B	-165	HIS	-	expression tag	UNP Q05470
B	-164	HIS	-	expression tag	UNP Q05470
B	-163	HIS	-	expression tag	UNP Q05470
B	-162	SER	-	expression tag	UNP Q05470
B	-161	SER	-	expression tag	UNP Q05470
B	-160	GLY	-	expression tag	UNP Q05470
B	-159	LEU	-	expression tag	UNP Q05470
B	-158	VAL	-	expression tag	UNP Q05470
B	-157	PRO	-	expression tag	UNP Q05470
B	-156	ARG	-	expression tag	UNP Q05470
B	-155	GLY	-	expression tag	UNP Q05470
B	-154	SER	-	expression tag	UNP Q05470
B	-153	SER	-	expression tag	UNP Q05470
C	-172	MET	-	initiating methionine	UNP Q05470
C	-171	GLY	-	expression tag	UNP Q05470
C	-170	SER	-	expression tag	UNP Q05470
C	-169	SER	-	expression tag	UNP Q05470
C	-168	HIS	-	expression tag	UNP Q05470
C	-167	HIS	-	expression tag	UNP Q05470
C	-166	HIS	-	expression tag	UNP Q05470
C	-165	HIS	-	expression tag	UNP Q05470
C	-164	HIS	-	expression tag	UNP Q05470
C	-163	HIS	-	expression tag	UNP Q05470
C	-162	SER	-	expression tag	UNP Q05470
C	-161	SER	-	expression tag	UNP Q05470
C	-160	GLY	-	expression tag	UNP Q05470
C	-159	LEU	-	expression tag	UNP Q05470
C	-158	VAL	-	expression tag	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-157	PRO	-	expression tag	UNP Q05470
C	-156	ARG	-	expression tag	UNP Q05470
C	-155	GLY	-	expression tag	UNP Q05470
C	-154	SER	-	expression tag	UNP Q05470
C	-153	SER	-	expression tag	UNP Q05470
D	-172	MET	-	initiating methionine	UNP Q05470
D	-171	GLY	-	expression tag	UNP Q05470
D	-170	SER	-	expression tag	UNP Q05470
D	-169	SER	-	expression tag	UNP Q05470
D	-168	HIS	-	expression tag	UNP Q05470
D	-167	HIS	-	expression tag	UNP Q05470
D	-166	HIS	-	expression tag	UNP Q05470
D	-165	HIS	-	expression tag	UNP Q05470
D	-164	HIS	-	expression tag	UNP Q05470
D	-163	HIS	-	expression tag	UNP Q05470
D	-162	SER	-	expression tag	UNP Q05470
D	-161	SER	-	expression tag	UNP Q05470
D	-160	GLY	-	expression tag	UNP Q05470
D	-159	LEU	-	expression tag	UNP Q05470
D	-158	VAL	-	expression tag	UNP Q05470
D	-157	PRO	-	expression tag	UNP Q05470
D	-156	ARG	-	expression tag	UNP Q05470
D	-155	GLY	-	expression tag	UNP Q05470
D	-154	SER	-	expression tag	UNP Q05470
D	-153	SER	-	expression tag	UNP Q05470
E	-172	MET	-	initiating methionine	UNP Q05470
E	-171	GLY	-	expression tag	UNP Q05470
E	-170	SER	-	expression tag	UNP Q05470
E	-169	SER	-	expression tag	UNP Q05470
E	-168	HIS	-	expression tag	UNP Q05470
E	-167	HIS	-	expression tag	UNP Q05470
E	-166	HIS	-	expression tag	UNP Q05470
E	-165	HIS	-	expression tag	UNP Q05470
E	-164	HIS	-	expression tag	UNP Q05470
E	-163	HIS	-	expression tag	UNP Q05470
E	-162	SER	-	expression tag	UNP Q05470
E	-161	SER	-	expression tag	UNP Q05470
E	-160	GLY	-	expression tag	UNP Q05470
E	-159	LEU	-	expression tag	UNP Q05470
E	-158	VAL	-	expression tag	UNP Q05470
E	-157	PRO	-	expression tag	UNP Q05470
E	-156	ARG	-	expression tag	UNP Q05470

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-155	GLY	-	expression tag	UNP Q05470
E	-154	SER	-	expression tag	UNP Q05470
E	-153	SER	-	expression tag	UNP Q05470
F	-172	MET	-	initiating methionine	UNP Q05470
F	-171	GLY	-	expression tag	UNP Q05470
F	-170	SER	-	expression tag	UNP Q05470
F	-169	SER	-	expression tag	UNP Q05470
F	-168	HIS	-	expression tag	UNP Q05470
F	-167	HIS	-	expression tag	UNP Q05470
F	-166	HIS	-	expression tag	UNP Q05470
F	-165	HIS	-	expression tag	UNP Q05470
F	-164	HIS	-	expression tag	UNP Q05470
F	-163	HIS	-	expression tag	UNP Q05470
F	-162	SER	-	expression tag	UNP Q05470
F	-161	SER	-	expression tag	UNP Q05470
F	-160	GLY	-	expression tag	UNP Q05470
F	-159	LEU	-	expression tag	UNP Q05470
F	-158	VAL	-	expression tag	UNP Q05470
F	-157	PRO	-	expression tag	UNP Q05470
F	-156	ARG	-	expression tag	UNP Q05470
F	-155	GLY	-	expression tag	UNP Q05470
F	-154	SER	-	expression tag	UNP Q05470
F	-153	SER	-	expression tag	UNP Q05470
G	-172	MET	-	initiating methionine	UNP Q05470
G	-171	GLY	-	expression tag	UNP Q05470
G	-170	SER	-	expression tag	UNP Q05470
G	-169	SER	-	expression tag	UNP Q05470
G	-168	HIS	-	expression tag	UNP Q05470
G	-167	HIS	-	expression tag	UNP Q05470
G	-166	HIS	-	expression tag	UNP Q05470
G	-165	HIS	-	expression tag	UNP Q05470
G	-164	HIS	-	expression tag	UNP Q05470
G	-163	HIS	-	expression tag	UNP Q05470
G	-162	SER	-	expression tag	UNP Q05470
G	-161	SER	-	expression tag	UNP Q05470
G	-160	GLY	-	expression tag	UNP Q05470
G	-159	LEU	-	expression tag	UNP Q05470
G	-158	VAL	-	expression tag	UNP Q05470
G	-157	PRO	-	expression tag	UNP Q05470
G	-156	ARG	-	expression tag	UNP Q05470
G	-155	GLY	-	expression tag	UNP Q05470
G	-154	SER	-	expression tag	UNP Q05470

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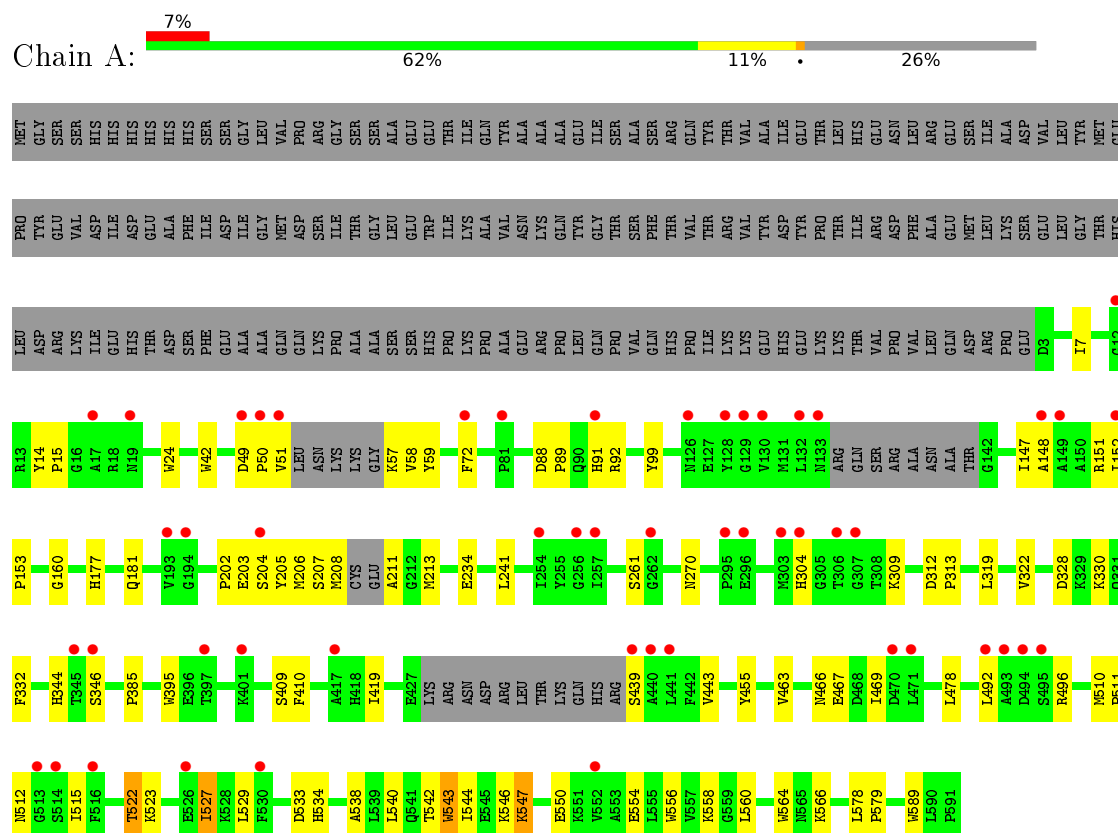
Chain	Residue	Modelled	Actual	Comment	Reference
G	-153	SER	-	expression tag	UNP Q05470
H	-172	MET	-	initiating methionine	UNP Q05470
H	-171	GLY	-	expression tag	UNP Q05470
H	-170	SER	-	expression tag	UNP Q05470
H	-169	SER	-	expression tag	UNP Q05470
H	-168	HIS	-	expression tag	UNP Q05470
H	-167	HIS	-	expression tag	UNP Q05470
H	-166	HIS	-	expression tag	UNP Q05470
H	-165	HIS	-	expression tag	UNP Q05470
H	-164	HIS	-	expression tag	UNP Q05470
H	-163	HIS	-	expression tag	UNP Q05470
H	-162	SER	-	expression tag	UNP Q05470
H	-161	SER	-	expression tag	UNP Q05470
H	-160	GLY	-	expression tag	UNP Q05470
H	-159	LEU	-	expression tag	UNP Q05470
H	-158	VAL	-	expression tag	UNP Q05470
H	-157	PRO	-	expression tag	UNP Q05470
H	-156	ARG	-	expression tag	UNP Q05470
H	-155	GLY	-	expression tag	UNP Q05470
H	-154	SER	-	expression tag	UNP Q05470
H	-153	SER	-	expression tag	UNP Q05470



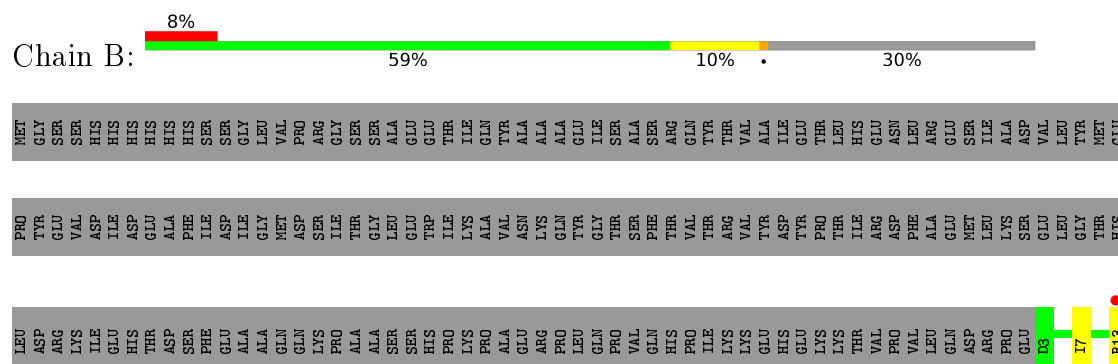
### 3 Residue-property plots

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: Polyketide synthase PksL



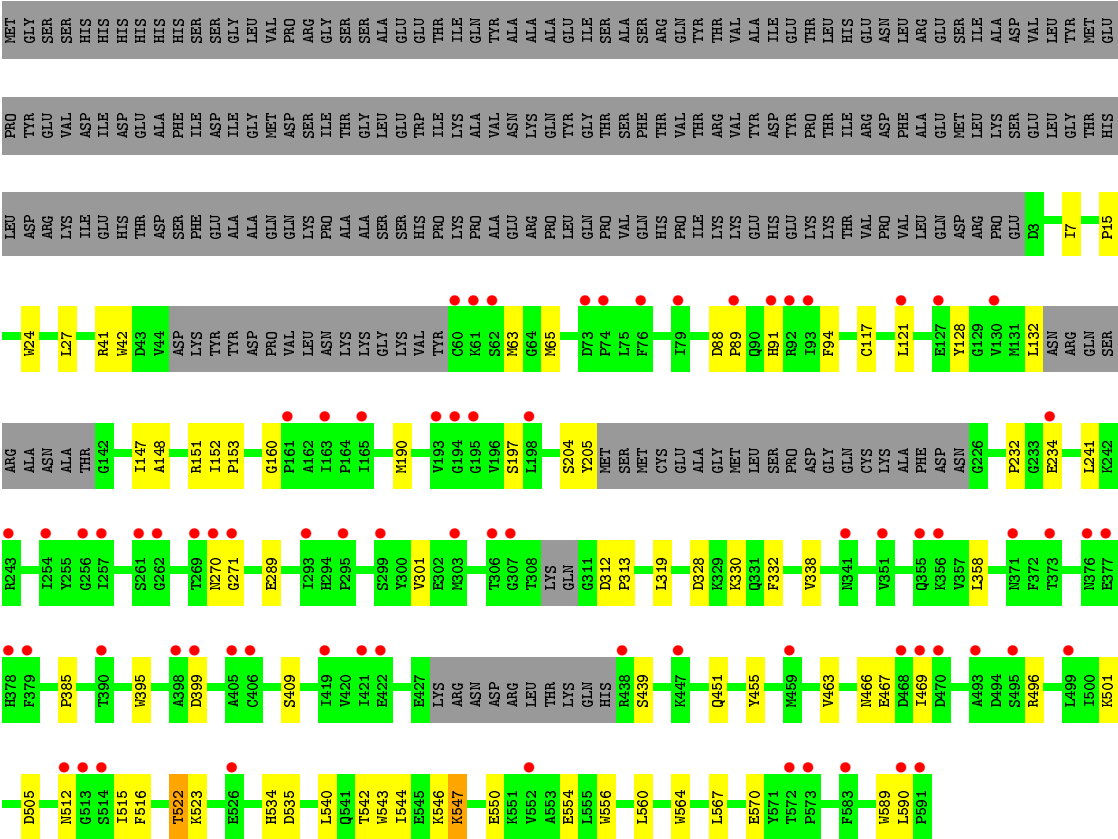
#### • Molecule 1: Polyketide synthase PksL











## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.11Å 112.73Å 211.44Å 104.96° 90.07° 106.32°	Depositor
Resolution (Å)	39.77 – 4.00 39.77 – 4.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (39.77-4.00) 84.5 (39.77-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.333 , 0.354 0.327 , 0.348	Depositor DCC
$R_{free}$ test set	2126 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	138.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 102.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.347 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	34416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.09 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.2714e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.42	7/4518 (0.2%)	0.45	0/6110
1	B	0.43	7/4277 (0.2%)	0.58	7/5784 (0.1%)
1	C	0.42	7/4518 (0.2%)	0.53	2/6110 (0.0%)
1	D	0.41	6/4277 (0.1%)	0.56	7/5784 (0.1%)
1	E	0.42	7/4518 (0.2%)	0.45	0/6110
1	F	0.43	7/4277 (0.2%)	0.54	6/5784 (0.1%)
1	G	0.42	7/4518 (0.2%)	0.45	0/6110
1	H	0.41	6/4277 (0.1%)	0.45	0/5784
All	All	0.42	54/35180 (0.2%)	0.50	22/47576 (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	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	H	0	1
All	All	0	5

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	TRP	CD2-CE2	6.34	1.49	1.41
1	F	564	TRP	CD2-CE2	6.24	1.48	1.41
1	G	42	TRP	CD2-CE2	6.24	1.48	1.41
1	E	42	TRP	CD2-CE2	6.23	1.48	1.41
1	E	589	TRP	CD2-CE2	6.21	1.48	1.41

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	546	LYS	CB-CA-C	-19.44	71.52	110.40
1	D	546	LYS	CB-CA-C	-19.21	71.98	110.40
1	B	546	LYS	N-CA-CB	-18.38	77.51	110.60
1	B	545	GLU	CB-CA-C	15.26	140.91	110.40
1	F	546	LYS	N-CA-C	13.36	147.08	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	570	GLU	Peptide
1	C	546	LYS	Peptide
1	D	570	GLU	Peptide
1	F	570	GLU	Peptide
1	H	570	GLU	Peptide

## 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	4419	0	4322	86	2
1	B	4185	0	4102	76	11
1	C	4419	0	4323	84	8
1	D	4185	0	4102	70	2
1	E	4419	0	4323	59	6
1	F	4185	0	4102	193	0
1	G	4419	0	4323	144	0
1	H	4185	0	4102	83	3
All	All	34416	0	33699	670	16

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 10.

The worst 5 of 670 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:535:ASP:CB	1:G:539:LEU:HB2	1.33	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:535:ASP:HB2	1:G:539:LEU:CB	1.28	1.52
1:F:545:GLU:CA	1:F:546:LYS:HG3	1.36	1.51
1:A:270:ASN:HD21	1:F:378:HIS:CA	1.23	1.51
1:F:539:LEU:CD1	1:G:533:ASP:CG	1.80	1.50

The worst 5 of 16 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:B:547:LYS:O	1:E:29:HIS:NE2[1_665]	1.53	0.67
1:B:547:LYS:O	1:E:29:HIS:CD2[1_665]	1.78	0.42
1:B:539:LEU:CB	1:C:535:ASP:CB[1_655]	1.88	0.32
1:B:539:LEU:CD2	1:C:533:ASP:OD2[1_655]	1.93	0.27
1:E:546:LYS:NZ	1:H:535:ASP:OD2[1_656]	1.96	0.24

## 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	553/764 (72%)	541 (98%)	12 (2%)	0	100	100
1	B	521/764 (68%)	503 (96%)	17 (3%)	1 (0%)	52	86
1	C	553/764 (72%)	539 (98%)	14 (2%)	0	100	100
1	D	521/764 (68%)	508 (98%)	12 (2%)	1 (0%)	52	86
1	E	553/764 (72%)	541 (98%)	12 (2%)	0	100	100
1	F	521/764 (68%)	508 (98%)	13 (2%)	0	100	100
1	G	553/764 (72%)	540 (98%)	13 (2%)	0	100	100
1	H	521/764 (68%)	507 (97%)	14 (3%)	0	100	100
All	All	4296/6112 (70%)	4187 (98%)	107 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	570	GLU
1	B	569	GLY

### 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	468/644 (73%)	461 (98%)	7 (2%)	72	89
1	B	442/644 (69%)	432 (98%)	10 (2%)	58	83
1	C	468/644 (73%)	462 (99%)	6 (1%)	76	90
1	D	442/644 (69%)	433 (98%)	9 (2%)	63	86
1	E	468/644 (73%)	461 (98%)	7 (2%)	72	89
1	F	442/644 (69%)	436 (99%)	6 (1%)	74	89
1	G	468/644 (73%)	463 (99%)	5 (1%)	80	91
1	H	442/644 (69%)	433 (98%)	9 (2%)	63	86
All	All	3640/5152 (71%)	3581 (98%)	59 (2%)	70	88

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	439	SER
1	E	309	LYS
1	H	439	SER
1	D	455	TYR
1	D	525	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	541	GLN
1	E	344	HIS
1	G	344	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	91	HIS
1	G	91	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 carbohydrates 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, 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	563/764 (73%)	0.40	51 (9%) 11 8	24, 154, 186, 226	0
1	B	533/764 (69%)	0.46	61 (11%) 7 6	24, 156, 195, 222	0
1	C	563/764 (73%)	0.33	46 (8%) 14 10	24, 153, 185, 226	0
1	D	533/764 (69%)	0.27	39 (7%) 18 13	24, 156, 191, 216	0
1	E	563/764 (73%)	0.32	51 (9%) 11 8	100, 153, 187, 213	0
1	F	533/764 (69%)	0.42	55 (10%) 9 7	24, 156, 189, 216	0
1	G	563/764 (73%)	0.30	39 (6%) 20 13	101, 153, 186, 206	0
1	H	533/764 (69%)	0.53	74 (13%) 4 4	24, 157, 193, 225	0
All	All	4384/6112 (71%)	0.38	416 (9%) 10 8	24, 155, 189, 226	0

The worst 5 of 416 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	60	CYS	9.6
1	A	493	ALA	8.0
1	G	529	LEU	7.6
1	A	513	GLY	7.4
1	F	261	SER	7.3

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.