wwPDB X-ray Structure Validation Summary Report (i)

Jun 8, 2017 – 08:06 AM EDT

PDB ID	:	5LOX
Title	:	Helical Assembly of the Anbu Complex from Pseudomonas aeruginosa
Authors	:	Fuchs, A.C.D.; Albrecht, R.; Martin, J.; Hartmann, M.D.
Deposited on	:	2016-08-10
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

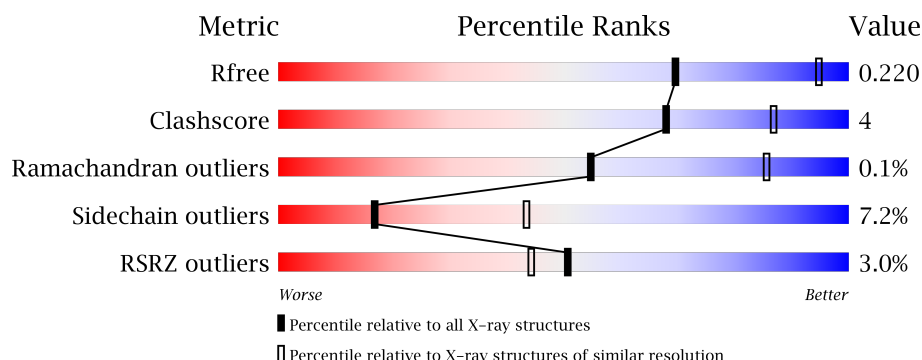|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

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 2.90 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	Percentile Ranks	Value
Rfree		0.220
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		7.2%
RSRZ outliers		3.0%

Worse .... *Better*

█ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 >=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 <=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	1	242	4% / 87% / 11% •
1	2	242	5% / 86% / 13% •
1	3	242	4% / 86% / 12% •
1	4	242	3% / 87% / 11% •
1	5	242	5% / 88% / 10% •

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Mol	Chain	Length	Quality of chain
1	6	242	5% ... 88% ... 10%
1	7	242	4% ... 86% ... 12%
1	8	242	2% ... 89% ... 10%
1	A	242	3% ... 86% ... 12%
1	B	242	2% ... 88% ... 10%
1	C	242	3% ... 88% ... 10%
1	D	242	3% ... 87% ... 12%
1	E	242	3% ... 86% ... 13%
1	F	242	3% ... 85% ... 12%
1	G	242	2% ... 86% ... 13%
1	H	242	3% ... 86% ... 13%
1	I	242	88% ... 11%
1	J	242	3% ... 88% ... 10%
1	K	242	2% ... 87% ... 11%
1	L	242	2% ... 87% ... 12%
1	M	242	3% ... 87% ... 12%
1	N	242	87% ... 12%
1	O	242	3% ... 86% ... 12%
1	P	242	2% ... 85% ... 13%
1	Q	242	3% ... 85% ... 14%
1	R	242	2% ... 86% ... 13%
1	S	242	3% ... 83% ... 15%
1	T	242	3% ... 87% ... 12%
1	U	242	2% ... 87% ... 10%
1	V	242	2% ... 87% ... 11%

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Mol	Chain	Length	Quality of chain
1	W	242	3% 87% 11%
1	X	242	2% 86% 12%
1	Y	242	4% 86% 13%
1	Z	242	5% 87% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 62186 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 Peptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	B	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	C	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	D	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	E	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	F	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	G	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	H	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	I	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	J	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	K	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	L	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	M	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	N	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	O	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0
1	P	241	Total 1829	C 1155	N 315	O 351	S 3	Se 5	0	0	0

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	Q	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	R	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	S	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	T	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	U	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	V	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	W	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	X	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	Y	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	Z	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	1	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	2	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	3	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	4	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	5	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	6	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	7	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				
1	8	241	Total	C	N	O	S	Se		0	0	0
			1829	1155	315	351	3	5				

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
A	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
A	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
B	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
B	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
C	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
C	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
C	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
D	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
D	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
D	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
E	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
E	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
E	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
F	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
F	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
F	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
G	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
G	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
G	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
H	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
H	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
H	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
I	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
I	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
I	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
J	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
J	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
J	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
K	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
K	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
K	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
L	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
L	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
L	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
M	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
M	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
M	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
N	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
N	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
N	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
O	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
O	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
O	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
P	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
P	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Q	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Q	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Q	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
R	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
R	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
R	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
S	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
S	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
S	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
T	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
T	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
T	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
U	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
U	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
U	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
V	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
V	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
V	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
W	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
W	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
W	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
X	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
X	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
X	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Y	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Y	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Y	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Z	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Z	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
Z	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
1	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
1	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
1	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
2	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
2	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
2	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
3	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
3	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
3	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

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Chain	Residue	Modelled	Actual	Comment	Reference
4	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
4	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
4	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
5	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
6	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
6	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
6	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
7	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
7	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
7	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
8	94	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
8	112	MSE	LEU	engineered mutation	UNP A0A0D6I0H1
8	229	MSE	LEU	engineered mutation	UNP A0A0D6I0H1

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 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: Peptidase

Chain A:

- Molecule 1: Peptidase

Chain B:

- Molecule 1: Peptidase

Chain C:

- Molecule 1: Peptidase

Chain D:

- Molecule 1: Peptidase

Chain E:

T1 M6 I24 T38 E41 R42 A49 N60 I66 L74 Y80 R91 M94 A95 R96 D97 N100 L101 A102 G103 N104 T105 S108 C109 Q130 D139 K149 Y150 C171 A172 E210 W222 G225 L226 M229 L230 E231 R232 L233

P234 S235 N241 ILE

• **Molecule 1: Peptidase**

Chain F:

3%

85% 12% •

T1 M6 I24 T38 E41 R42 A49 N60 I66 D69 L74 N75 Y80 R91 M94 G99 N100 L101 A102 G103 N104 T105 S108 C109 M112 I117 Q130 G131 N132 F133 D139 K149 A172 E210 R220 Q221 W222

L226 M229 L230 E231 R232 L233 P234 S235 N241 ILE

• **Molecule 1: Peptidase**

Chain G:

2%

86% 13% •

T1 M6 I24 T38 E41 R42 A49 N60 I66 L74 N75 Y80 R91 M94 A95 R96 N100 L101 A102 G103 N104 T105 S108 C109 M112 Q130 G131 D139 K149 Y150 A172 E210 W222 G225 L226 M229 R232

L233 P234 S235 N241 ILE

• **Molecule 1: Peptidase**

Chain H:

3%

86% 13% •

T1 M6 I24 T38 E41 R42 A49 N60 I66 L74 N75 Y80 R91 M94 A95 R96 D97 S98 G99 N100 L101 A102 G103 N104 T105 S108 C109 Y128 P129 Q130 D139 K149 Y150 C171 A172 E210 L226 M229 L230 E231 R232

L233 P234 S235 N241 ILE

• **Molecule 1: Peptidase**

Chain I:

88% 11% •

T1 M6 I24 T38 E41 R42 A49 N60 I66 L74 N75 Y80 R91 M94 L101 A102 G103 N104 T105 S108 C109 Q130 D139 A172 E210 L226 H227 D228 M229 R232 L233 P234 S235 A239 Y240 N241 ILE

• **Molecule 1: Peptidase**

Chain J:

3%

88% 10% •

T1 M6 A22 G23 I24 T38 E41 R42 A49 N60 I66 D69 L74 N75 M94 A95 R96 G99 N100 L101 A102 G103 N104 T105 S108 C109 Q130 D139 A172 E210 G225 M229 R232 L233 P234 S235 A239 Y240 N241 ILE

• Molecule 1: Peptidase

Chain K:

• Molecule 1: Peptidase

Chain L:

• Molecule 1: Peptidase

Chain M:

• Molecule 1: Peptidase

Chain N:

• Molecule 1: Peptidase

Chain O:

• Molecule 1: Peptidase

Chain P:

• Molecule 1: Peptidase

Chain Q:

• Molecule 1: Peptidase

Chain R:

• Molecule 1: Peptidase

Chain S:

• Molecule 1: Peptidase

Chain T:

• Molecule 1: Peptidase

Chain U:

2%

87%   10%

ILE

• Molecule 1: Peptidase

Chain V:

2%

87%   11%

ILE

• Molecule 1: Peptidase

Chain W:

3%

87%   11%

ILE

• Molecule 1: Peptidase

Chain X:

2%

86%   12%

ILE

• Molecule 1: Peptidase

Chain Y:

4%

86%   13%

ILE

• Molecule 1: Peptidase

Chain Z:

• Molecule 1: Peptidase

Chain 1:

• Molecule 1: Peptidase

Chain 2:

• Molecule 1: Peptidase

Chain 3:

• Molecule 1: Peptidase

Chain 4:

• Molecule 1: Peptidase

Chain 5:

• Molecule 1: Peptidase

Chain 6:

• Molecule 1: Peptidase

Chain 7:

• Molecule 1: Peptidase
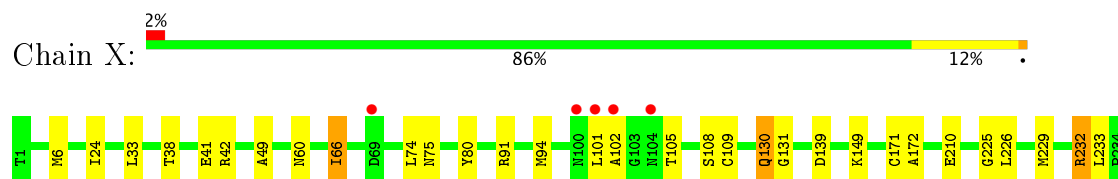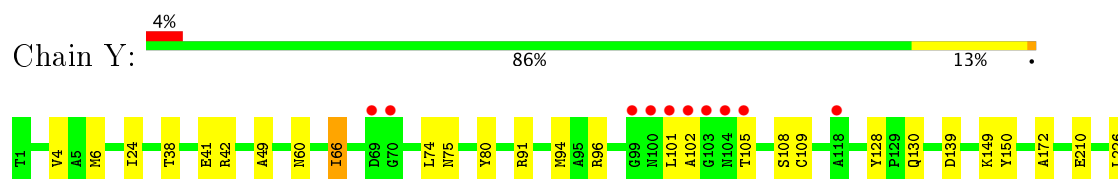
Chain 8:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	150.07Å 230.08Å 171.72Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	39.60 – 2.90 39.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.60-2.90) 99.7 (39.57-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.56 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.198 , 0.218 0.203 , 0.220	Depositor DCC
R_{free} test set	12245 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.0	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	62186	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	1	0.57	0/1862	0.80	3/2530 (0.1%)
1	2	0.56	0/1862	0.74	0/2530
1	3	0.58	0/1862	0.78	2/2530 (0.1%)
1	4	0.57	0/1862	0.77	1/2530 (0.0%)
1	5	0.53	0/1862	0.75	1/2530 (0.0%)
1	6	0.54	0/1862	0.72	0/2530
1	7	0.61	0/1862	0.78	2/2530 (0.1%)
1	8	0.59	0/1862	0.76	1/2530 (0.0%)
1	A	0.61	0/1862	0.77	1/2530 (0.0%)
1	B	0.59	0/1862	0.78	1/2530 (0.0%)
1	C	0.58	0/1862	0.76	2/2530 (0.1%)
1	D	0.60	0/1862	0.74	1/2530 (0.0%)
1	E	0.60	0/1862	0.83	3/2530 (0.1%)
1	F	0.68	1/1862 (0.1%)	0.80	4/2530 (0.2%)
1	G	0.62	0/1862	0.79	2/2530 (0.1%)
1	H	0.59	0/1862	0.74	0/2530
1	I	0.59	0/1862	0.77	2/2530 (0.1%)
1	J	0.62	0/1862	0.79	4/2530 (0.2%)
1	K	0.63	0/1862	0.78	2/2530 (0.1%)
1	L	0.62	0/1862	0.75	0/2530
1	M	0.66	0/1862	0.75	0/2530
1	N	0.63	0/1862	0.78	3/2530 (0.1%)
1	O	0.62	0/1862	0.81	2/2530 (0.1%)
1	P	0.59	0/1862	0.77	2/2530 (0.1%)
1	Q	0.64	0/1862	0.75	0/2530
1	R	0.59	0/1862	0.73	0/2530
1	S	0.63	0/1862	0.79	2/2530 (0.1%)
1	T	0.60	0/1862	0.78	3/2530 (0.1%)
1	U	0.60	0/1862	0.83	6/2530 (0.2%)
1	V	0.61	0/1862	0.79	1/2530 (0.0%)
1	W	0.63	0/1862	0.79	2/2530 (0.1%)
1	X	0.62	0/1862	0.79	2/2530 (0.1%)
1	Y	0.56	0/1862	0.72	1/2530 (0.0%)
1	Z	0.56	0/1862	0.73	0/2530

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.60	1/63308 (0.0%)	0.77	56/86020 (0.1%)

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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	221	GLN	CD-OE1	-6.75	1.09	1.24

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	229	MSE	CA-CB-CG	-12.61	91.86	113.30
1	O	232	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	7	232	ARG	NE-CZ-NH2	-12.03	114.29	120.30
1	E	229	MSE	N-CA-CB	-11.69	89.57	110.60
1	3	232	ARG	NE-CZ-NH2	-11.32	114.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	133	PHE	Mainchain

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	1	1829	0	1800	30	0
1	2	1829	0	1800	31	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	1829	0	1800	27	0
1	4	1829	0	1800	26	1
1	5	1829	0	1800	15	0
1	6	1829	0	1800	14	0
1	7	1829	0	1800	18	1
1	8	1829	0	1800	16	1
1	A	1829	0	1800	20	0
1	B	1829	0	1800	17	0
1	C	1829	0	1800	18	0
1	D	1829	0	1800	19	0
1	E	1829	0	1800	36	0
1	F	1829	0	1800	45	1
1	G	1829	0	1800	33	0
1	H	1829	0	1800	41	0
1	I	1829	0	1800	18	1
1	J	1829	0	1800	21	0
1	K	1829	0	1800	23	0
1	L	1829	0	1800	23	0
1	M	1829	0	1800	21	2
1	N	1829	0	1800	19	0
1	O	1829	0	1800	32	1
1	P	1829	0	1800	32	0
1	Q	1829	0	1800	36	0
1	R	1829	0	1800	33	0
1	S	1829	0	1800	29	0
1	T	1829	0	1800	18	0
1	U	1829	0	1800	17	2
1	V	1829	0	1800	17	0
1	W	1829	0	1800	28	0
1	X	1829	0	1800	27	0
1	Y	1829	0	1800	31	0
1	Z	1829	0	1800	32	0
All	All	62186	0	61200	547	6

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 4.

The worst 5 of 547 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:117:ILE:HG21	1:S:69:ASP:CB	1.26	1.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:ILE:CG2	1:S:69:ASP:CB	1.97	1.40
1:J:69:ASP:CB	1:W:69:ASP:O	1.73	1.34
1:A:229:MSE:HE1	1:B:229:MSE:HE1	1.19	1.18
1:D:69:ASP:CB	1:Q:117:ILE:HG21	1.74	1.16

The worst 5 of 6 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:M:197:ARG:NH2	1:U:232:ARG:O[1_655]	1.65	0.55
1:M:162:ASP:OD1	1:U:231:GLU:OE1[1_655]	1.71	0.49
1:2:228:ASP:OD2	1:8:220:ARG:NH1[2_744]	1.91	0.29
1:2:231:GLU:OE1	1:7:234:PRO:CB[2_744]	2.03	0.17
1:F:220:ARG:NH1	1:4:232:ARG:O[1_556]	2.08	0.12

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	1	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	2	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	3	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	4	239/242 (99%)	228 (95%)	11 (5%)	0	100	100
1	5	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	6	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	7	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	8	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	A	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	B	239/242 (99%)	229 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	D	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	E	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	F	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	G	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	H	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	I	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	38	72
1	J	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	38	72
1	K	239/242 (99%)	230 (96%)	8 (3%)	1 (0%)	38	72
1	L	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	38	72
1	M	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	N	239/242 (99%)	228 (95%)	10 (4%)	1 (0%)	38	72
1	O	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	P	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	Q	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	R	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	S	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	T	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	U	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	V	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	W	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	X	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
1	Y	239/242 (99%)	229 (96%)	9 (4%)	1 (0%)	38	72
1	Z	239/242 (99%)	229 (96%)	10 (4%)	0	100	100
All	All	8126/8228 (99%)	7785 (96%)	335 (4%)	6 (0%)	55	85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	239	ALA
1	N	239	ALA
1	I	239	ALA
1	K	239	ALA
1	L	239	ALA

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	1	197/197 (100%)	182 (92%)	15 (8%)	15	41
1	2	197/197 (100%)	184 (93%)	13 (7%)	19	49
1	3	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	4	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	5	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	6	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	7	197/197 (100%)	182 (92%)	15 (8%)	15	41
1	8	197/197 (100%)	185 (94%)	12 (6%)	22	53
1	A	197/197 (100%)	182 (92%)	15 (8%)	15	41
1	B	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	C	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	D	197/197 (100%)	184 (93%)	13 (7%)	19	49
1	E	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	F	197/197 (100%)	181 (92%)	16 (8%)	14	38
1	G	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	H	197/197 (100%)	180 (91%)	17 (9%)	12	35
1	I	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	J	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	K	197/197 (100%)	182 (92%)	15 (8%)	15	41
1	L	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	M	197/197 (100%)	184 (93%)	13 (7%)	19	49
1	N	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	O	197/197 (100%)	182 (92%)	15 (8%)	15	41
1	P	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	Q	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	R	197/197 (100%)	183 (93%)	14 (7%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	T	197/197 (100%)	184 (93%)	13 (7%)	19	49
1	U	197/197 (100%)	182 (92%)	15 (8%)	15	41
1	V	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	W	197/197 (100%)	184 (93%)	13 (7%)	19	49
1	X	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	Y	197/197 (100%)	183 (93%)	14 (7%)	17	44
1	Z	197/197 (100%)	182 (92%)	15 (8%)	15	41
All	All	6698/6698 (100%)	6217 (93%)	481 (7%)	17	43

5 of 481 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	38	THR
1	S	232	ARG
1	6	60	ASN
1	P	130	GLN
1	R	24	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	130	GLN
1	V	130	GLN
1	6	60	ASN
1	Q	75	ASN
1	S	75	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 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, 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(Å²)	Q<0.9
1	1	236/242 (97%)	0.04	10 (4%)	37	32	56, 86, 131, 215	0
1	2	236/242 (97%)	-0.05	11 (4%)	32	28	59, 87, 135, 203	0
1	3	236/242 (97%)	-0.10	9 (3%)	41	35	57, 80, 140, 221	0
1	4	236/242 (97%)	-0.05	8 (3%)	46	39	56, 83, 129, 220	0
1	5	236/242 (97%)	0.16	12 (5%)	29	24	60, 97, 147, 204	0
1	6	236/242 (97%)	0.14	11 (4%)	32	28	64, 94, 138, 205	0
1	7	236/242 (97%)	0.02	10 (4%)	37	32	56, 79, 118, 227	0
1	8	236/242 (97%)	-0.14	5 (2%)	64	60	57, 79, 135, 186	0
1	A	236/242 (97%)	-0.13	7 (2%)	51	44	54, 72, 120, 163	0
1	B	236/242 (97%)	-0.20	6 (2%)	58	53	55, 76, 117, 208	0
1	C	236/242 (97%)	-0.08	7 (2%)	51	44	54, 77, 119, 208	0
1	D	236/242 (97%)	-0.16	7 (2%)	51	44	53, 70, 128, 190	0
1	E	236/242 (97%)	-0.13	7 (2%)	51	44	53, 77, 122, 216	0
1	F	236/242 (97%)	-0.14	7 (2%)	51	44	50, 66, 121, 234	0
1	G	236/242 (97%)	-0.14	4 (1%)	70	68	56, 74, 127, 186	0
1	H	236/242 (97%)	-0.13	7 (2%)	51	44	52, 74, 126, 210	0
1	I	236/242 (97%)	-0.33	1 (0%)	92	92	52, 72, 107, 134	0
1	J	236/242 (97%)	-0.19	7 (2%)	51	44	50, 70, 137, 226	0
1	K	236/242 (97%)	-0.23	5 (2%)	64	60	46, 64, 106, 174	0
1	L	236/242 (97%)	-0.20	4 (1%)	70	68	48, 67, 109, 153	0
1	M	236/242 (97%)	-0.18	8 (3%)	46	39	47, 65, 113, 200	0
1	N	236/242 (97%)	-0.28	1 (0%)	92	92	43, 69, 107, 136	0
1	O	236/242 (97%)	-0.15	7 (2%)	51	44	50, 70, 117, 195	0
1	P	236/242 (97%)	-0.13	5 (2%)	64	60	50, 75, 124, 192	0

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Mol	Chain	Analysed	\<RSRZ\>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	Q	236/242 (97%)	-0.13	7 (2%)	51	44	49, 66, 114, 216	0
1	R	236/242 (97%)	-0.20	6 (2%)	58	53	49, 78, 120, 199	0
1	S	236/242 (97%)	-0.03	7 (2%)	51	44	51, 69, 132, 179	0
1	T	236/242 (97%)	-0.14	7 (2%)	51	44	52, 79, 126, 202	0
1	U	236/242 (97%)	-0.06	5 (2%)	64	60	54, 79, 124, 160	0
1	V	236/242 (97%)	-0.22	6 (2%)	58	53	54, 69, 124, 206	0
1	W	236/242 (97%)	-0.15	8 (3%)	46	39	47, 70, 137, 215	0
1	X	236/242 (97%)	-0.19	5 (2%)	64	60	47, 69, 112, 148	0
1	Y	236/242 (97%)	-0.02	10 (4%)	37	32	57, 89, 142, 213	0
1	Z	236/242 (97%)	0.06	13 (5%)	26	21	56, 87, 136, 199	0
All	All	8024/8228 (97%)	-0.11	240 (2%)	51	44	43, 75, 128, 234	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	69	ASP	15.5
1	H	100	ASN	11.3
1	O	100	ASN	11.2
1	H	101	LEU	10.1
1	Q	100	ASN	10.0

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3   Carbohydrates ⓘ

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.