



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:00 am BST

PDB ID : 3IMP
Title : New crystal form of the C-terminal domain of Helicobacter pylori MotB
(residues 125-256)
Authors : Roujeinikova, A.
Deposited on : 2009-08-11
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

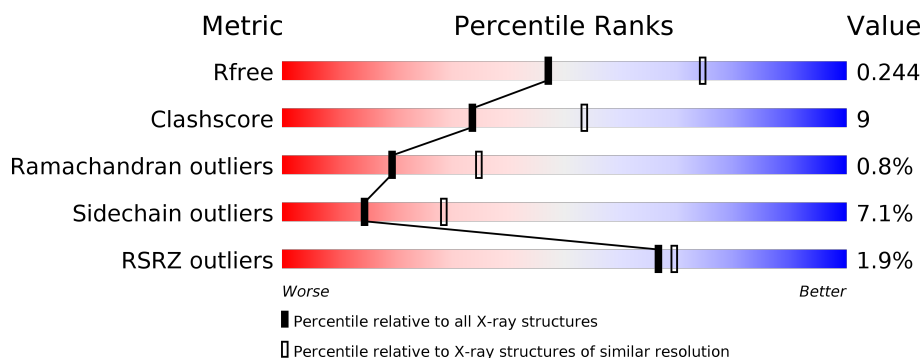
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	138	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 23%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 70% 23% • 5% </div> </div>
1	B	138	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 81%, yellow 15%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 15% • </div> </div>
1	C	138	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 74%, yellow 21%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 74% 21% • • </div> </div>
1	D	138	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 71%, yellow 21%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 71% 21% • • • </div> </div>
1	E	138	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 71%, yellow 22%, orange 3%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 71% 22% • • </div> </div>
1	F	138	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 79%, yellow 17%, orange 2%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 79% 17% • • </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	138	<div><div><div>%</div><div><div></div><div>75%</div><div>17%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div></div>
1	H	138	<div><div><div>%</div><div><div></div><div>75%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div></div>
1	I	138	<div><div><div>6%</div><div><div></div><div>71%</div><div>21%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div></div>
1	J	138	<div><div><div>2%</div><div><div></div><div>77%</div><div>17%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div></div>
1	K	138	<div><div><div>2%</div><div><div></div><div>76%</div><div>19%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div></div>
1	L	138	<div><div><div>3%</div><div><div></div><div>64%</div><div>29%</div><div></div><div></div></div><div><div></div><div></div><div></div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13220 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 Chemotaxis protein motB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	133	Total	C	N	O	S	0	0	0
			1071	676	188	203	4			
1	C	133	Total	C	N	O	S	0	0	0
			1071	676	188	203	4			
1	D	132	Total	C	N	O	S	0	0	0
			1064	671	187	202	4			
1	E	132	Total	C	N	O	S	0	0	0
			1064	671	187	202	4			
1	A	131	Total	C	N	O	S	0	0	0
			1056	667	185	200	4			
1	F	133	Total	C	N	O	S	0	0	0
			1071	676	188	203	4			
1	G	132	Total	C	N	O	S	0	1	0
			1064	671	187	202	4			
1	H	132	Total	C	N	O	S	0	0	0
			1064	671	187	202	4			
1	I	132	Total	C	N	O	S	0	0	0
			1064	671	187	202	4			
1	J	132	Total	C	N	O	S	0	0	0
			1064	671	187	202	4			
1	K	132	Total	C	N	O	S	0	1	0
			1064	671	187	202	4			
1	L	132	Total	C	N	O	S	0	0	0
			1064	671	187	202	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	119	GLY	-	EXPRESSION TAG	UNP P56427
B	120	ILE	-	EXPRESSION TAG	UNP P56427
B	121	ASP	-	EXPRESSION TAG	UNP P56427
B	122	PRO	-	EXPRESSION TAG	UNP P56427
B	123	PHE	-	EXPRESSION TAG	UNP P56427

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Chain	Residue	Modelled	Actual	Comment	Reference
B	124	THR	-	EXPRESSION TAG	UNP P56427
C	119	GLY	-	EXPRESSION TAG	UNP P56427
C	120	ILE	-	EXPRESSION TAG	UNP P56427
C	121	ASP	-	EXPRESSION TAG	UNP P56427
C	122	PRO	-	EXPRESSION TAG	UNP P56427
C	123	PHE	-	EXPRESSION TAG	UNP P56427
C	124	THR	-	EXPRESSION TAG	UNP P56427
D	119	GLY	-	EXPRESSION TAG	UNP P56427
D	120	ILE	-	EXPRESSION TAG	UNP P56427
D	121	ASP	-	EXPRESSION TAG	UNP P56427
D	122	PRO	-	EXPRESSION TAG	UNP P56427
D	123	PHE	-	EXPRESSION TAG	UNP P56427
D	124	THR	-	EXPRESSION TAG	UNP P56427
E	119	GLY	-	EXPRESSION TAG	UNP P56427
E	120	ILE	-	EXPRESSION TAG	UNP P56427
E	121	ASP	-	EXPRESSION TAG	UNP P56427
E	122	PRO	-	EXPRESSION TAG	UNP P56427
E	123	PHE	-	EXPRESSION TAG	UNP P56427
E	124	THR	-	EXPRESSION TAG	UNP P56427
A	119	GLY	-	EXPRESSION TAG	UNP P56427
A	120	ILE	-	EXPRESSION TAG	UNP P56427
A	121	ASP	-	EXPRESSION TAG	UNP P56427
A	122	PRO	-	EXPRESSION TAG	UNP P56427
A	123	PHE	-	EXPRESSION TAG	UNP P56427
A	124	THR	-	EXPRESSION TAG	UNP P56427
F	119	GLY	-	EXPRESSION TAG	UNP P56427
F	120	ILE	-	EXPRESSION TAG	UNP P56427
F	121	ASP	-	EXPRESSION TAG	UNP P56427
F	122	PRO	-	EXPRESSION TAG	UNP P56427
F	123	PHE	-	EXPRESSION TAG	UNP P56427
F	124	THR	-	EXPRESSION TAG	UNP P56427
G	119	GLY	-	EXPRESSION TAG	UNP P56427
G	120	ILE	-	EXPRESSION TAG	UNP P56427
G	121	ASP	-	EXPRESSION TAG	UNP P56427
G	122	PRO	-	EXPRESSION TAG	UNP P56427
G	123	PHE	-	EXPRESSION TAG	UNP P56427
G	124	THR	-	EXPRESSION TAG	UNP P56427
H	119	GLY	-	EXPRESSION TAG	UNP P56427
H	120	ILE	-	EXPRESSION TAG	UNP P56427
H	121	ASP	-	EXPRESSION TAG	UNP P56427
H	122	PRO	-	EXPRESSION TAG	UNP P56427
H	123	PHE	-	EXPRESSION TAG	UNP P56427

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Chain	Residue	Modelled	Actual	Comment	Reference
H	124	THR	-	EXPRESSION TAG	UNP P56427
I	119	GLY	-	EXPRESSION TAG	UNP P56427
I	120	ILE	-	EXPRESSION TAG	UNP P56427
I	121	ASP	-	EXPRESSION TAG	UNP P56427
I	122	PRO	-	EXPRESSION TAG	UNP P56427
I	123	PHE	-	EXPRESSION TAG	UNP P56427
I	124	THR	-	EXPRESSION TAG	UNP P56427
J	119	GLY	-	EXPRESSION TAG	UNP P56427
J	120	ILE	-	EXPRESSION TAG	UNP P56427
J	121	ASP	-	EXPRESSION TAG	UNP P56427
J	122	PRO	-	EXPRESSION TAG	UNP P56427
J	123	PHE	-	EXPRESSION TAG	UNP P56427
J	124	THR	-	EXPRESSION TAG	UNP P56427
K	119	GLY	-	EXPRESSION TAG	UNP P56427
K	120	ILE	-	EXPRESSION TAG	UNP P56427
K	121	ASP	-	EXPRESSION TAG	UNP P56427
K	122	PRO	-	EXPRESSION TAG	UNP P56427
K	123	PHE	-	EXPRESSION TAG	UNP P56427
K	124	THR	-	EXPRESSION TAG	UNP P56427
L	119	GLY	-	EXPRESSION TAG	UNP P56427
L	120	ILE	-	EXPRESSION TAG	UNP P56427
L	121	ASP	-	EXPRESSION TAG	UNP P56427
L	122	PRO	-	EXPRESSION TAG	UNP P56427
L	123	PHE	-	EXPRESSION TAG	UNP P56427
L	124	THR	-	EXPRESSION TAG	UNP P56427

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ni 1 1	0	0
2	K	1	Total Ni 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Cl 2 2	0	0
3	K	2	Total Cl 2 2	0	0

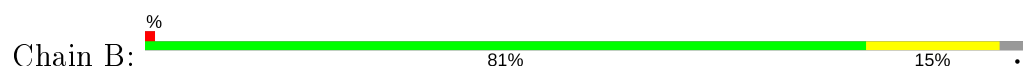
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	51	Total 51	O 51	0	0
4	C	35	Total 35	O 35	0	0
4	D	54	Total 54	O 54	0	0
4	E	40	Total 40	O 40	0	0
4	A	19	Total 19	O 19	0	0
4	F	25	Total 25	O 25	0	0
4	G	39	Total 39	O 39	0	0
4	H	42	Total 42	O 42	0	0
4	I	20	Total 20	O 20	0	0
4	J	22	Total 22	O 22	0	0
4	K	38	Total 38	O 38	0	0
4	L	48	Total 48	O 48	0	0

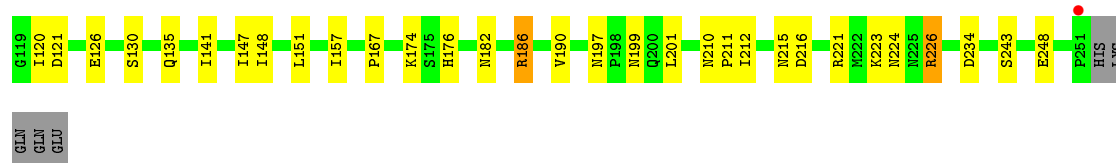
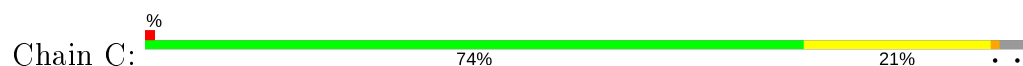
3 Residue-property plots [i](#)

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.

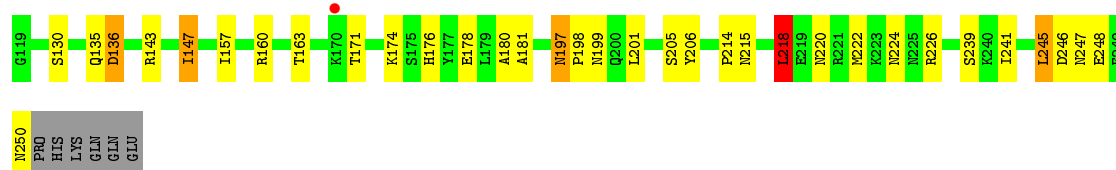
- Molecule 1: Chemotaxis protein motB



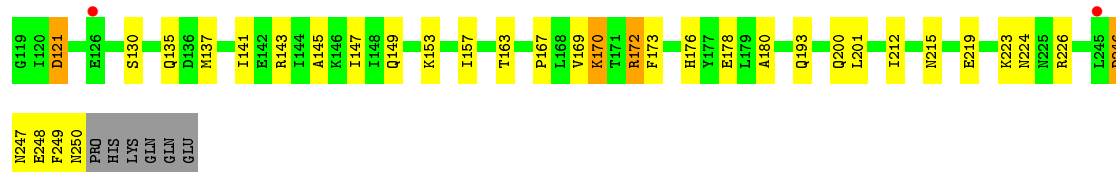
- Molecule 1: Chemotaxis protein motB



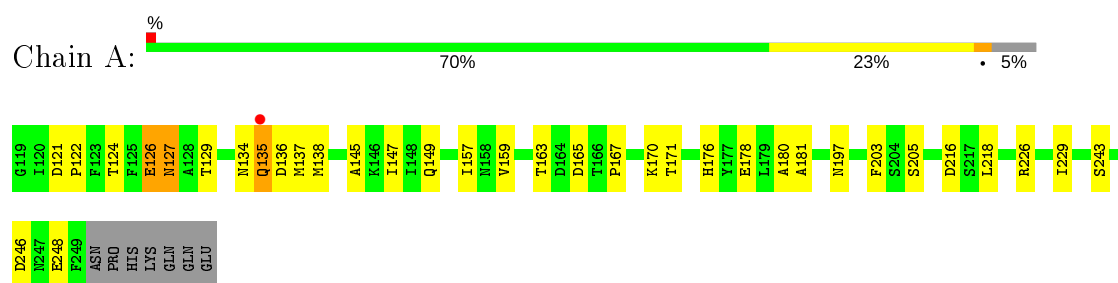
- Molecule 1: Chemotaxis protein motB



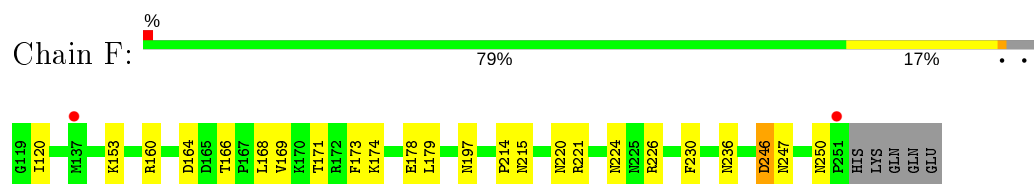
- Molecule 1: Chemotaxis protein motB



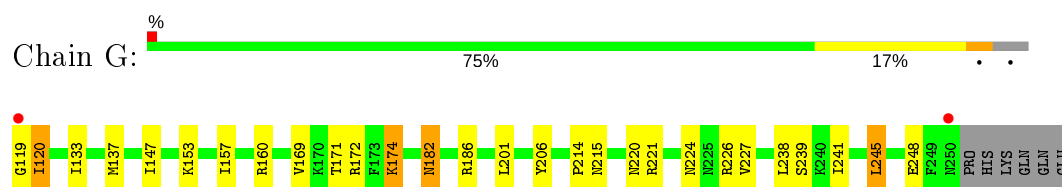
- Molecule 1: Chemotaxis protein motB



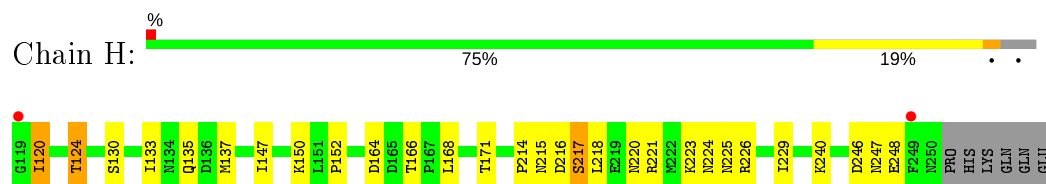
- Molecule 1: Chemotaxis protein motB



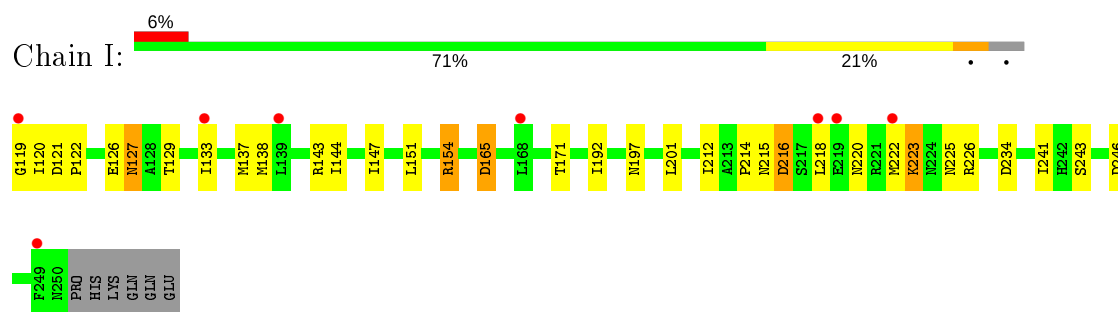
- Molecule 1: Chemotaxis protein motB



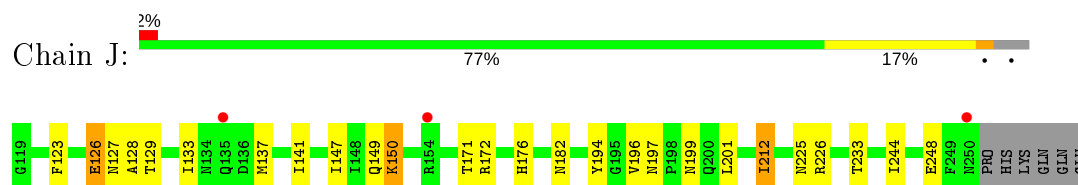
- Molecule 1: Chemotaxis protein motB



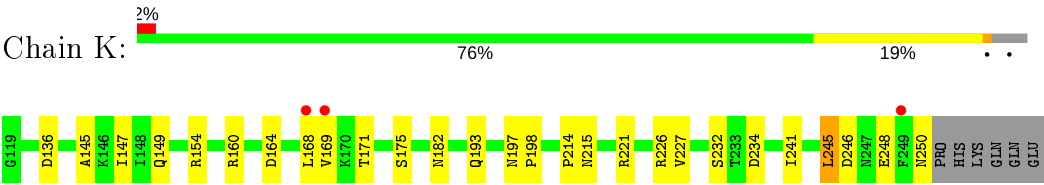
- Molecule 1: Chemotaxis protein motB



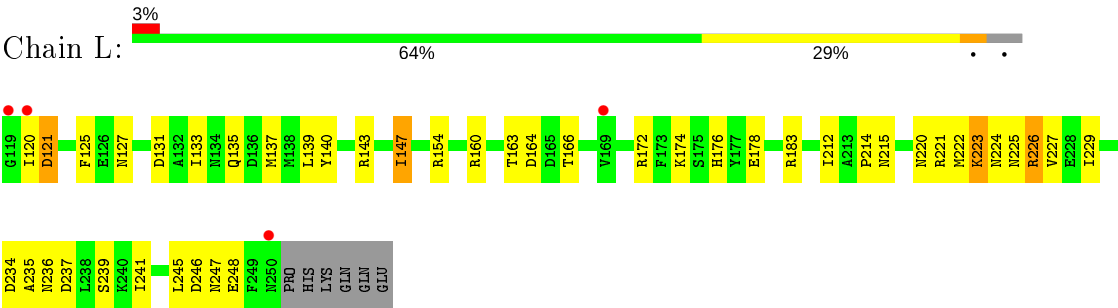
- Molecule 1: Chemotaxis protein motB



- Molecule 1: Chemotaxis protein motB



• Molecule 1: Chemotaxis protein motB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.56Å 100.34Å 108.49Å 90.00° 119.51° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-2.50) 99.0 (15.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.249 0.184 , 0.244	Depositor DCC
R_{free} test set	3498 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h-l,k,h 0.038 for l,k,-h-l 0.429 for h,-k,-h-l 0.026 for -h-l,-k,l 0.060 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13220	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.11% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, CL

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	0.79	2/1077 (0.2%)	0.73	0/1457
1	B	0.72	0/1093	0.72	1/1480 (0.1%)
1	C	0.67	0/1093	0.77	1/1480 (0.1%)
1	D	0.74	0/1085	0.78	1/1468 (0.1%)
1	E	0.70	0/1085	0.69	0/1468
1	F	0.61	0/1093	0.64	0/1480
1	G	0.68	0/1078	0.72	0/1457
1	H	0.66	0/1085	0.72	0/1468
1	I	0.82	3/1085 (0.3%)	0.73	2/1468 (0.1%)
1	J	0.56	0/1085	0.64	0/1468
1	K	0.70	0/1078	0.72	0/1457
1	L	0.68	0/1085	0.72	0/1468
All	All	0.70	5/13022 (0.0%)	0.72	5/17619 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	216	ASP	CG-OD2	9.70	1.47	1.25
1	I	216	ASP	CG-OD1	6.02	1.39	1.25
1	A	126	GLU	CD-OE1	5.70	1.31	1.25
1	I	143	ARG	CZ-NH1	5.68	1.40	1.33
1	A	126	GLU	CD-OE2	5.20	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	ASP	CB-CG-OD1	6.55	124.20	118.30
1	I	216	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	I	143	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	234	ASP	CB-CG-OD1	5.53	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	LEU	CA-CB-CG	-5.27	103.19	115.30

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	1056	0	1039	23	0
1	B	1071	0	1052	13	0
1	C	1071	0	1052	21	0
1	D	1064	0	1045	16	0
1	E	1064	0	1045	21	0
1	F	1071	0	1052	17	0
1	G	1064	0	1044	17	0
1	H	1064	0	1045	15	0
1	I	1064	0	1045	20	0
1	J	1064	0	1045	20	0
1	K	1064	0	1044	15	0
1	L	1064	0	1045	32	0
2	G	1	0	0	0	0
2	K	1	0	0	0	0
3	G	2	0	0	0	0
3	K	2	0	0	2	0
4	A	19	0	0	3	0
4	B	51	0	0	4	0
4	C	35	0	0	3	0
4	D	54	0	0	1	0
4	E	40	0	0	2	0
4	F	25	0	0	0	0
4	G	39	0	0	1	0
4	H	42	0	0	2	0
4	I	20	0	0	0	0
4	J	22	0	0	1	0
4	K	38	0	0	1	0
4	L	48	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13220	0	12553	216	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 9.

The worst 5 of 216 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:L:147:ILE:HD11	1:L:248:GLU:HG2	1.28	1.09
1:H:147:ILE:HD11	1:H:248:GLU:HG2	1.38	1.02
1:A:147:ILE:HD11	1:A:248:GLU:HG2	1.41	1.01
1:C:176:HIS:HE1	1:A:218:LEU:HD23	1.28	0.97
1:K:147:ILE:HD11	1:K:248:GLU:HG2	1.53	0.89

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	129/138 (94%)	117 (91%)	9 (7%)	3 (2%)	6	10
1	B	131/138 (95%)	125 (95%)	6 (5%)	0	100	100
1	C	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
1	D	130/138 (94%)	124 (95%)	5 (4%)	1 (1%)	19	35
1	E	130/138 (94%)	128 (98%)	1 (1%)	1 (1%)	19	35
1	F	131/138 (95%)	128 (98%)	2 (2%)	1 (1%)	19	35
1	G	130/138 (94%)	127 (98%)	2 (2%)	1 (1%)	19	35
1	H	130/138 (94%)	125 (96%)	1 (1%)	4 (3%)	4	5
1	I	130/138 (94%)	118 (91%)	11 (8%)	1 (1%)	19	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	130/138 (94%)	127 (98%)	3 (2%)	0	100	100
1	K	130/138 (94%)	129 (99%)	1 (1%)	0	100	100
1	L	130/138 (94%)	121 (93%)	9 (7%)	0	100	100
All	All	1562/1656 (94%)	1497 (96%)	53 (3%)	12 (1%)	19	35

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ASP
1	G	169	VAL
1	I	126	GLU
1	H	247	ASN
1	E	170	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	118/126 (94%)	111 (94%)	7 (6%)	19	37
1	B	120/126 (95%)	116 (97%)	4 (3%)	38	64
1	C	120/126 (95%)	112 (93%)	8 (7%)	16	31
1	D	119/126 (94%)	106 (89%)	13 (11%)	6	12
1	E	119/126 (94%)	109 (92%)	10 (8%)	11	21
1	F	120/126 (95%)	115 (96%)	5 (4%)	30	54
1	G	118/126 (94%)	109 (92%)	9 (8%)	13	25
1	H	119/126 (94%)	108 (91%)	11 (9%)	9	18
1	I	119/126 (94%)	110 (92%)	9 (8%)	13	25
1	J	119/126 (94%)	114 (96%)	5 (4%)	30	54
1	K	118/126 (94%)	109 (92%)	9 (8%)	13	25
1	L	119/126 (94%)	108 (91%)	11 (9%)	9	18
All	All	1428/1512 (94%)	1327 (93%)	101 (7%)	14	28

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	246	ASP
1	H	120	ILE
1	L	139	LEU
1	G	120	ILE
1	G	182	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	200	GLN
1	G	215	ASN
1	L	200	GLN
1	F	220	ASN
1	G	247	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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	131/138 (94%)	0.26	1 (0%) 86 87	39, 69, 106, 122	0
1	B	133/138 (96%)	-0.15	1 (0%) 86 87	18, 40, 68, 98	0
1	C	133/138 (96%)	-0.09	1 (0%) 86 87	22, 43, 72, 107	0
1	D	132/138 (95%)	-0.08	1 (0%) 86 87	20, 40, 68, 84	0
1	E	132/138 (95%)	-0.16	2 (1%) 73 75	24, 45, 71, 95	0
1	F	133/138 (96%)	0.06	2 (1%) 73 75	31, 59, 89, 123	0
1	G	132/138 (95%)	-0.04	2 (1%) 73 75	22, 45, 72, 92	0
1	H	132/138 (95%)	-0.03	2 (1%) 73 75	22, 44, 70, 107	0
1	I	132/138 (95%)	0.29	8 (6%) 21 22	36, 70, 111, 124	0
1	J	132/138 (95%)	0.04	3 (2%) 60 63	30, 60, 88, 110	0
1	K	132/138 (95%)	-0.07	3 (2%) 60 63	23, 44, 71, 96	0
1	L	132/138 (95%)	-0.08	4 (3%) 50 53	24, 44, 70, 102	0
All	All	1586/1656 (95%)	-0.00	30 (1%) 66 69	18, 49, 91, 124	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	120	ILE	5.5
1	G	119	GLY	4.5
1	I	222	MET	3.9
1	I	218	LEU	3.8
1	F	137	MET	3.7

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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	G	71	1/1	0.90	0.14	56,56,56,56	0
3	CL	K	95	1/1	0.92	0.13	53,53,53,53	0
3	CL	K	12	1/1	0.94	0.13	54,54,54,54	0
2	NI	K	2	1/1	0.95	0.19	37,37,37,37	0
3	CL	G	83	1/1	0.96	0.15	52,52,52,52	0
2	NI	G	1	1/1	0.97	0.20	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.