Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:30 AM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

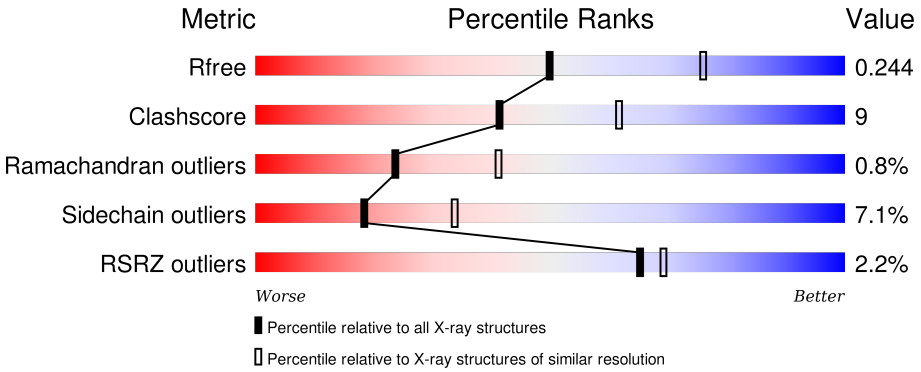
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	138	% 70% 23% • 5%
1	B	138	% 81% 15% •
1	C	138	% 74% 21% • •
1	D	138	% 71% 21% • • •
1	E	138	% 71% 22% • •

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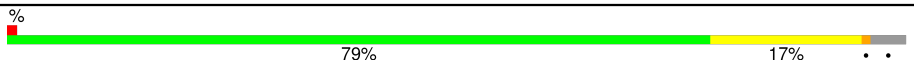
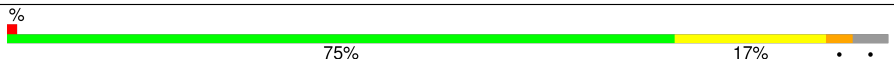
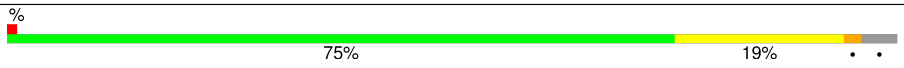
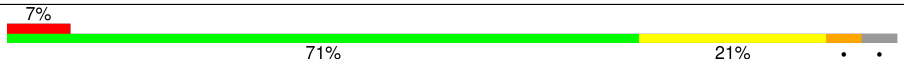
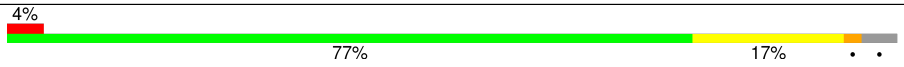
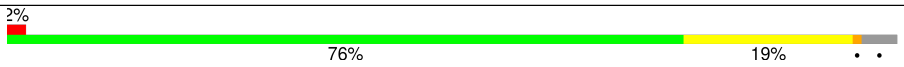
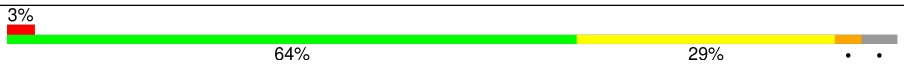
Mol	Chain	Length	Quality of chain
1	F	138	
1	G	138	
1	H	138	
1	I	138	
1	J	138	
1	K	138	
1	L	138	

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.

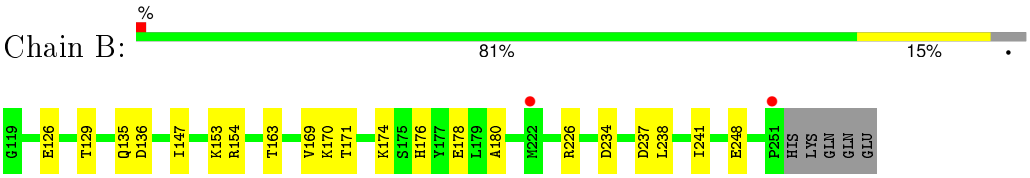
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	51	Total O 51 51	0	0
4	C	35	Total O 35 35	0	0
4	D	54	Total O 54 54	0	0
4	E	40	Total O 40 40	0	0
4	A	19	Total O 19 19	0	0
4	F	25	Total O 25 25	0	0
4	G	39	Total O 39 39	0	0
4	H	42	Total O 42 42	0	0
4	I	20	Total O 20 20	0	0
4	J	22	Total O 22 22	0	0
4	K	38	Total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

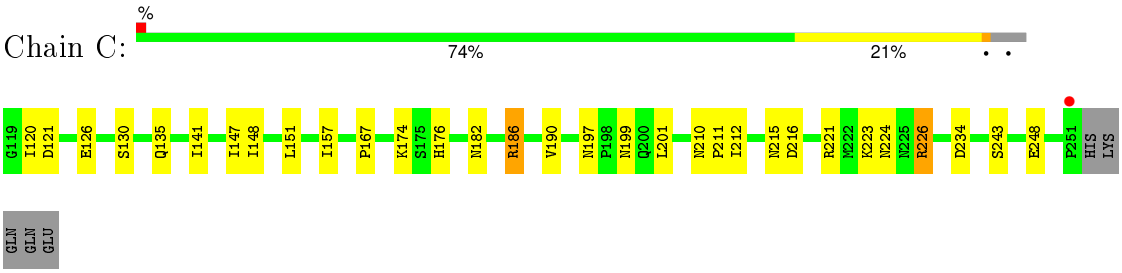
- Molecule 1: Chemotaxis protein motB

Chain B:



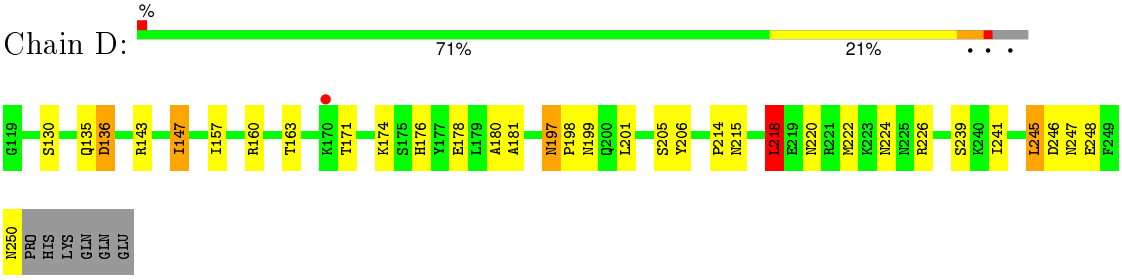
- Molecule 1: Chemotaxis protein motB

Chain C:



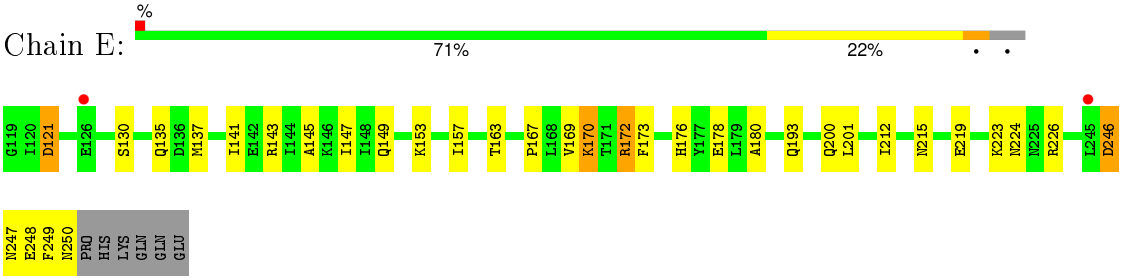
- Molecule 1: Chemotaxis protein motB

Chain D:



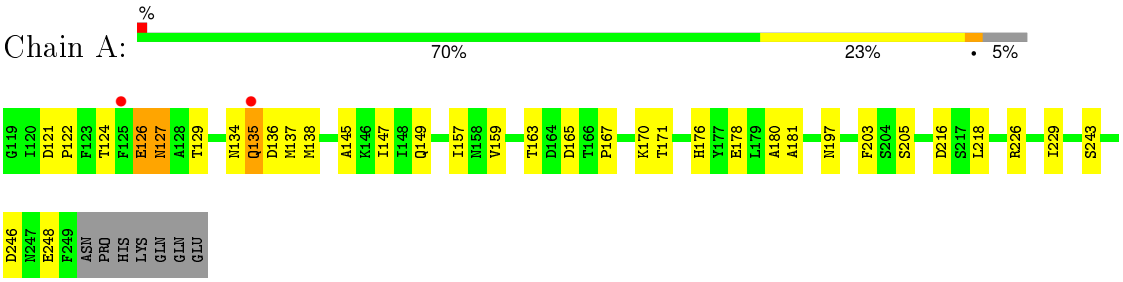
- Molecule 1: Chemotaxis protein motB

Chain E:



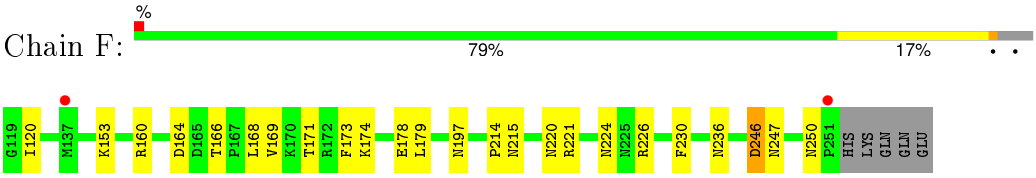
- Molecule 1: Chemotaxis protein motB

Chain A:



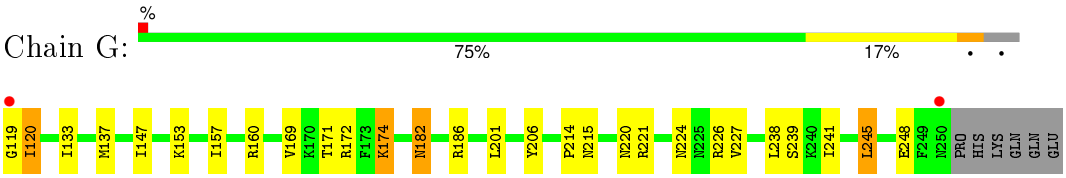
• Molecule 1: Chemotaxis protein motB

Chain F:



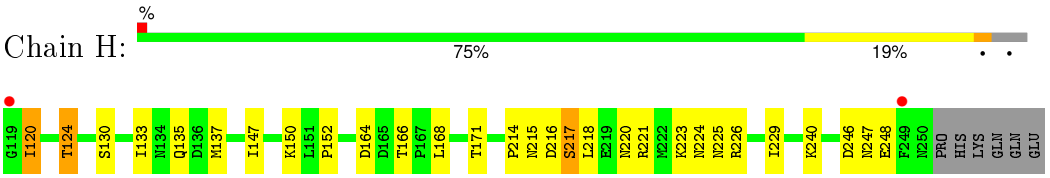
• Molecule 1: Chemotaxis protein motB

Chain G:



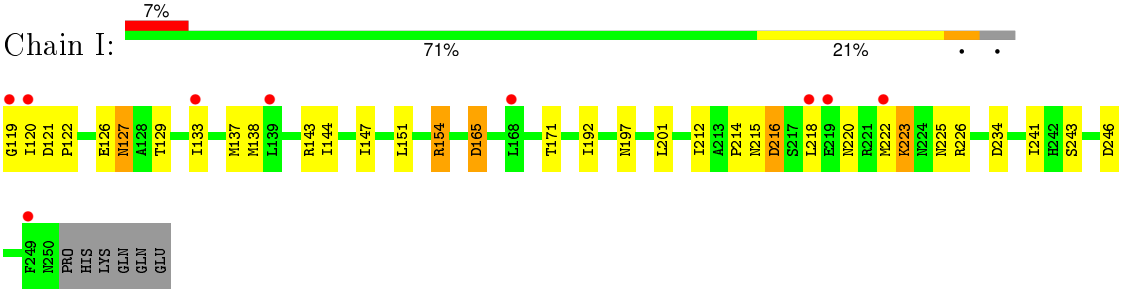
• Molecule 1: Chemotaxis protein motB

Chain H:



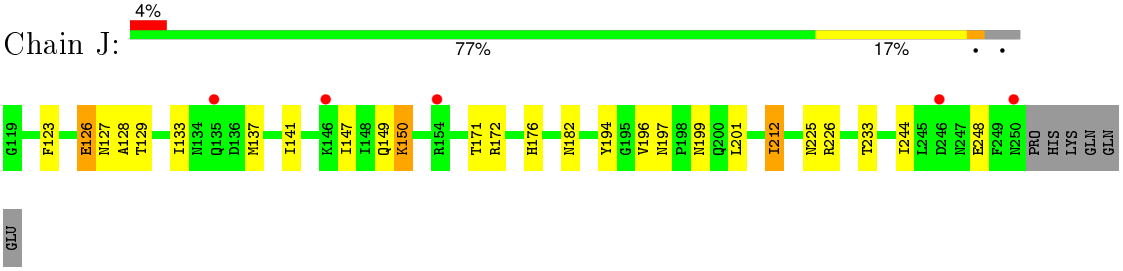
• Molecule 1: Chemotaxis protein motB

Chain I:



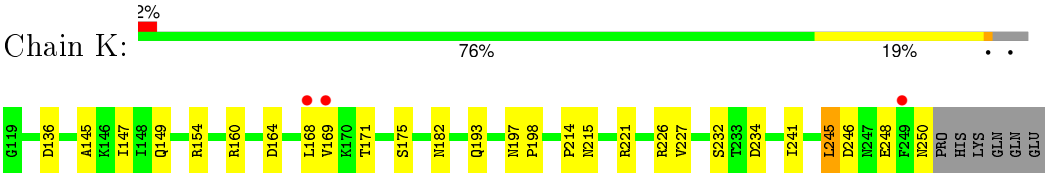
• Molecule 1: Chemotaxis protein motB

Chain J:



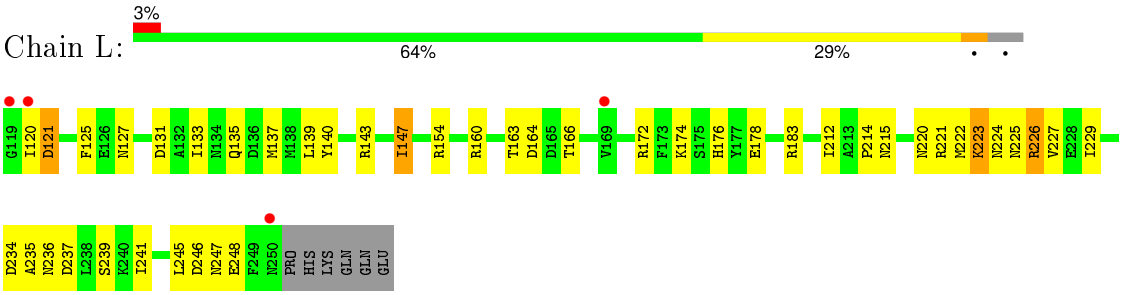
• Molecule 1: Chemotaxis protein motB

Chain K:



• Molecule 1: Chemotaxis protein motB

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.33%)	DCC
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
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
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 69177 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	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.

All (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
1:J:176:HIS:ND1	4:J:5:HOH:O	2.06	0.88
1:H:215:ASN:HD22	1:H:221:ARG:HG2	1.39	0.87
1:B:176:HIS:ND1	4:B:3:HOH:O	2.07	0.87
1:H:137:MET:HG3	4:H:10:HOH:O	1.77	0.83
1:H:168:LEU:HA	4:H:274:HOH:O	1.78	0.82
1:D:147:ILE:HD11	1:D:248:GLU:HG2	1.61	0.80
1:G:120:ILE:HD13	1:G:120:ILE:N	1.98	0.78
1:L:222:MET:HG3	4:L:257:HOH:O	1.84	0.77
1:J:147:ILE:HD11	1:J:248:GLU:HG2	1.68	0.76
1:J:133:ILE:HG12	1:J:137:MET:HE1	1.68	0.76
1:D:176:HIS:ND1	4:D:4:HOH:O	2.18	0.75
1:D:241:ILE:HG22	1:D:245:LEU:HD22	1.70	0.74
1:J:133:ILE:HG23	1:J:137:MET:HE2	1.70	0.74
1:L:223:LYS:HE2	4:L:344:HOH:O	1.87	0.73
1:C:176:HIS:CE1	1:A:218:LEU:HD23	2.20	0.73
1:G:147:ILE:HD11	1:G:248:GLU:HG2	1.69	0.73
1:C:216:ASP:OD2	4:C:117:HOH:O	2.06	0.73
1:L:147:ILE:HD11	1:L:248:GLU:CG	2.16	0.72
1:I:127:ASN:HD22	1:I:129:THR:H	1.38	0.71
1:E:172:ARG:NH1	1:E:178:GLU:OE1	2.25	0.69
4:C:110:HOH:O	3:K:12:CL:CL	2.48	0.68
1:E:169:VAL:O	1:E:170:LYS:CB	2.42	0.67
1:L:176:HIS:ND1	4:L:2:HOH:O	2.27	0.67
1:F:120:ILE:H	1:F:120:ILE:HD12	1.59	0.67
1:F:166:THR:HG23	1:F:221:ARG:HD2	1.77	0.66
1:J:197:ASN:HD21	1:J:199:ASN:HB3	1.59	0.66
1:A:127:ASN:HD22	1:A:129:THR:H	1.43	0.66
1:K:241:ILE:HG22	1:K:245:LEU:HD22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASN:HD22	1:C:199:ASN:H	1.43	0.66
4:C:110:HOH:O	3:K:95:CL:CL	2.51	0.66
1:C:215:ASN:ND2	1:C:224:ASN:HD22	1.94	0.65
1:A:178:GLU:HG3	1:F:197:ASN:HD21	1.62	0.65
1:L:183:ARG:HH12	1:L:225:ASN:HD22	1.42	0.65
1:G:174:LYS:HB2	1:G:174:LYS:HZ3	1.62	0.64
1:K:193:GLN:HB2	4:K:68:HOH:O	1.98	0.64
1:I:120:ILE:HD13	1:L:235:ALA:HB1	1.80	0.64
1:B:126:GLU:HG3	4:B:305:HOH:O	1.98	0.63
1:B:135:GLN:NE2	4:B:265:HOH:O	2.28	0.62
1:K:215:ASN:HD22	1:K:221:ARG:HG2	1.63	0.62
1:C:167:PRO:HA	1:A:218:LEU:HD21	1.80	0.62
1:C:182:ASN:O	1:C:186:ARG:HD2	1.99	0.62
1:F:214:PRO:O	1:F:220:ASN:HB3	2.00	0.62
1:B:147:ILE:HD11	1:B:248:GLU:HG2	1.82	0.61
1:J:133:ILE:HG23	1:J:137:MET:CE	2.31	0.61
1:E:167:PRO:HA	1:I:218:LEU:HD21	1.83	0.61
1:A:129:THR:HB	1:A:171:THR:HG21	1.83	0.61
1:G:214:PRO:HB3	1:I:171:THR:HA	1.82	0.60
1:L:174:LYS:HD3	4:L:268:HOH:O	2.00	0.60
1:J:197:ASN:ND2	1:J:199:ASN:HB3	2.17	0.60
1:H:164:ASP:H	1:H:225:ASN:ND2	2.00	0.60
1:L:215:ASN:HD22	1:L:221:ARG:HG2	1.66	0.60
1:G:120:ILE:N	1:G:120:ILE:CD1	2.65	0.59
1:C:147:ILE:HD11	1:C:248:GLU:HG2	1.85	0.58
1:L:154:ARG:NH2	1:L:234:ASP:OD2	2.36	0.58
1:F:236:ASN:OD1	1:G:119:GLY:HA3	2.04	0.58
1:J:149:GLN:NE2	1:J:194:TYR:O	2.36	0.58
1:E:153:LYS:HG2	4:E:56:HOH:O	2.04	0.57
1:J:172:ARG:HH22	1:J:182:ASN:ND2	2.02	0.57
1:L:121:ASP:N	1:L:121:ASP:OD2	2.37	0.57
1:L:147:ILE:CD1	1:L:248:GLU:HG2	2.20	0.57
1:F:160:ARG:HD2	1:F:230:PHE:CD1	2.39	0.57
1:D:215:ASN:ND2	1:D:224:ASN:HD22	2.02	0.57
1:B:248:GLU:OE2	1:B:248:GLU:HA	2.04	0.56
1:J:147:ILE:HD11	1:J:248:GLU:CG	2.35	0.56
1:D:197:ASN:ND2	1:D:199:ASN:H	2.04	0.56
1:D:157:ILE:HB	1:D:201:LEU:HD23	1.87	0.56
1:L:133:ILE:HG23	1:L:137:MET:HB3	1.87	0.56
1:I:214:PRO:HB2	1:I:216:ASP:OD2	2.05	0.56
1:E:215:ASN:ND2	1:E:224:ASN:HD22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:THR:HB	1:J:171:THR:HG21	1.87	0.55
1:K:164:ASP:HB2	1:K:215:ASN:HD21	1.71	0.55
1:D:215:ASN:HD21	1:D:224:ASN:HD22	1.55	0.55
1:A:178:GLU:CG	1:F:197:ASN:HD21	2.18	0.55
1:E:212:ILE:HD12	1:E:223:LYS:O	2.06	0.55
1:J:126:GLU:H	1:J:126:GLU:CD	2.08	0.55
1:J:150:LYS:HD2	1:J:244:ILE:HG12	1.90	0.54
1:H:147:ILE:HD11	1:H:248:GLU:CG	2.25	0.54
1:E:172:ARG:O	1:E:172:ARG:NE	2.40	0.54
1:L:120:ILE:HG23	1:L:140:TYR:OH	2.07	0.54
1:F:168:LEU:HB3	1:F:171:THR:CG2	2.37	0.54
1:A:124:THR:HG21	4:A:6:HOH:O	2.08	0.54
1:K:145:ALA:O	1:K:149:GLN:HG2	2.08	0.53
1:A:176:HIS:HD2	4:A:263:HOH:O	1.90	0.53
1:C:215:ASN:HD22	1:C:221:ARG:HG2	1.73	0.53
1:D:136:ASP:OD1	1:D:136:ASP:N	2.38	0.53
1:C:212:ILE:HD12	1:C:223:LYS:O	2.08	0.53
1:E:137:MET:O	1:E:141:ILE:HG13	2.08	0.53
1:E:147:ILE:HD11	1:E:248:GLU:HG2	1.90	0.53
1:G:171:THR:HG23	4:G:265:HOH:O	2.09	0.53
1:C:197:ASN:ND2	1:C:199:ASN:H	2.06	0.52
1:L:174:LYS:N	1:L:178:GLU:OE2	2.30	0.52
1:F:246:ASP:O	1:F:250:ASN:HB2	2.09	0.52
1:L:120:ILE:HD11	1:L:245:LEU:HD22	1.91	0.52
1:E:173:PHE:HD2	1:E:178:GLU:HG2	1.74	0.52
1:F:215:ASN:ND2	1:F:224:ASN:HD22	2.07	0.52
1:K:147:ILE:CD1	1:K:248:GLU:HG2	2.34	0.52
1:C:210:ASN:N	1:C:211:PRO:HD3	2.25	0.52
1:L:214:PRO:O	1:L:220:ASN:HB3	2.09	0.52
1:D:174:LYS:HE3	1:D:178:GLU:OE2	2.10	0.52
1:I:144:ILE:HA	1:I:147:ILE:HD12	1.90	0.52
1:H:164:ASP:H	1:H:225:ASN:HD21	1.57	0.52
1:E:147:ILE:CD1	1:E:249:PHE:CE2	2.93	0.51
1:L:131:ASP:OD1	1:L:172:ARG:NH2	2.36	0.51
1:I:154:ARG:NH2	1:I:234:ASP:OD2	2.41	0.51
1:J:128:ALA:HA	1:J:225:ASN:ND2	2.25	0.51
1:H:133:ILE:HG23	1:H:137:MET:HB3	1.92	0.51
1:F:215:ASN:HD22	1:F:221:ARG:HG2	1.75	0.51
1:L:125:PHE:CZ	1:L:183:ARG:HG2	2.46	0.51
1:L:215:ASN:ND2	1:L:224:ASN:HD22	2.09	0.51
1:A:145:ALA:O	1:A:149:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:222:MET:HA	1:I:225:ASN:HD22	1.75	0.50
1:F:173:PHE:CE1	1:F:179:LEU:HD13	2.47	0.50
1:C:223:LYS:O	1:C:226:ARG:HD2	2.12	0.49
1:G:160:ARG:HD3	1:G:206:TYR:CE2	2.47	0.49
1:E:147:ILE:CD1	1:E:249:PHE:HE2	2.26	0.49
1:A:159:VAL:O	1:A:203:PHE:HA	2.12	0.49
1:J:137:MET:HE2	1:J:141:ILE:HD11	1.94	0.48
1:J:196:VAL:CG1	1:J:201:LEU:HD11	2.42	0.48
1:D:218:LEU:O	1:D:222:MET:HG2	2.14	0.48
1:E:157:ILE:HB	1:E:201:LEU:HD23	1.95	0.48
1:G:215:ASN:HD22	1:G:221:ARG:HG2	1.78	0.48
1:A:197:ASN:HD21	1:F:178:GLU:HG2	1.78	0.48
1:H:124:THR:O	1:H:137:MET:HE2	2.14	0.48
1:G:160:ARG:O	1:G:227:VAL:HA	2.13	0.48
1:B:178:GLU:HG2	1:C:197:ASN:ND2	2.29	0.48
1:D:160:ARG:HD3	1:D:206:TYR:CE2	2.48	0.48
1:G:241:ILE:HG22	1:G:245:LEU:HD22	1.95	0.48
1:F:120:ILE:N	1:F:120:ILE:HD12	2.28	0.48
1:L:164:ASP:H	1:L:225:ASN:ND2	2.12	0.47
1:E:176:HIS:HE1	1:I:218:LEU:HD23	1.77	0.47
1:H:216:ASP:O	1:H:217:SER:HB3	2.14	0.47
1:C:147:ILE:HD11	1:C:248:GLU:CG	2.44	0.47
1:I:119:GLY:HA3	1:L:236:ASN:OD1	2.15	0.47
1:A:163:THR:HG23	1:A:180:ALA:HB2	1.97	0.46
1:I:165:ASP:HB2	1:I:215:ASN:ND2	2.31	0.46
1:F:215:ASN:HD21	1:F:224:ASN:HD22	1.62	0.46
1:L:143:ARG:NH2	1:L:248:GLU:O	2.49	0.46
1:G:133:ILE:HG23	1:G:137:MET:HB3	1.98	0.46
1:D:214:PRO:O	1:D:220:ASN:HB3	2.16	0.46
1:G:214:PRO:O	1:G:220:ASN:HB3	2.16	0.45
1:F:164:ASP:C	1:F:164:ASP:OD1	2.54	0.45
1:D:197:ASN:HD22	1:D:198:PRO:N	2.14	0.45
1:A:124:THR:CG2	4:A:6:HOH:O	2.64	0.45
1:I:192:ILE:HG13	1:I:201:LEU:CD1	2.46	0.45
1:E:200:GLN:NE2	4:E:6:HOH:O	2.50	0.45
1:A:181:ALA:HB2	1:A:205:SER:HB2	1.99	0.45
1:C:141:ILE:HG21	1:C:190:VAL:CG1	2.46	0.45
1:C:215:ASN:HD21	1:C:224:ASN:HD22	1.65	0.45
1:C:147:ILE:HD11	1:C:248:GLU:CB	2.47	0.45
1:I:151:LEU:HD22	1:I:241:ILE:HG12	1.99	0.45
1:J:127:ASN:C	1:J:127:ASN:OD1	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:ARG:HH12	1:L:225:ASN:ND2	2.13	0.44
1:K:154:ARG:NH2	1:K:234:ASP:OD2	2.42	0.44
1:F:120:ILE:H	1:F:120:ILE:CD1	2.30	0.44
1:J:123:PHE:HB3	1:J:137:MET:SD	2.58	0.44
1:B:248:GLU:CA	1:B:248:GLU:OE2	2.66	0.44
1:J:172:ARG:HH22	1:J:182:ASN:HD21	1.64	0.44
1:E:147:ILE:HD11	1:E:249:PHE:CE2	2.52	0.44
1:G:215:ASN:ND2	1:G:224:ASN:HD22	2.16	0.44
1:H:214:PRO:O	1:H:220:ASN:HB3	2.18	0.44
1:G:182:ASN:O	1:G:186:ARG:HG3	2.17	0.44
1:A:127:ASN:ND2	1:A:129:THR:H	2.13	0.43
1:I:133:ILE:HG23	1:I:137:MET:HB3	2.00	0.43
1:B:129:THR:HB	1:B:171:THR:HG21	2.00	0.43
1:J:212:ILE:H	1:J:212:ILE:HG12	1.70	0.43
1:A:170:LYS:O	1:K:214:PRO:HA	2.19	0.43
1:D:163:THR:HG23	1:D:180:ALA:HB2	1.99	0.43
1:C:148:ILE:HA	1:C:151:LEU:HD12	2.00	0.43
1:G:120:ILE:H	1:G:120:ILE:HD13	1.76	0.43
1:L:164:ASP:OD1	1:L:166:THR:HB	2.19	0.43
1:A:135:GLN:O	1:A:138:MET:HB2	2.18	0.43
1:K:164:ASP:HB2	1:K:215:ASN:ND2	2.33	0.43
1:A:157:ILE:HG23	1:A:229:ILE:HG23	2.00	0.43
1:K:164:ASP:OD1	1:K:164:ASP:C	2.58	0.43
1:L:163:THR:HA	1:L:225:ASN:HD22	1.84	0.42
1:C:157:ILE:HB	1:C:201:LEU:HD23	2.01	0.42
1:H:248:GLU:HG3	1:H:248:GLU:O	2.18	0.42
1:E:145:ALA:O	1:E:149:GLN:HG3	2.19	0.42
1:H:133:ILE:HA	1:H:137:MET:HE3	2.01	0.42
1:K:197:ASN:HA	1:K:198:PRO:HD3	1.91	0.42
1:A:170:LYS:O	1:K:215:ASN:N	2.50	0.42
1:I:133:ILE:HG22	1:I:138:MET:HG2	2.00	0.42
1:H:152:PRO:HG3	1:H:240:LYS:HD2	2.01	0.42
1:K:168:LEU:HB3	1:K:171:THR:HG21	2.02	0.42
1:I:121:ASP:HA	1:I:122:PRO:HD3	1.85	0.42
1:E:167:PRO:HA	1:I:218:LEU:CD2	2.50	0.42
1:E:246:ASP:O	1:E:250:ASN:HB2	2.20	0.42
1:B:237:ASP:O	1:B:241:ILE:HG13	2.20	0.42
1:L:160:ARG:O	1:L:227:VAL:HA	2.20	0.41
1:G:157:ILE:HB	1:G:201:LEU:HD23	2.02	0.41
1:B:169:VAL:HG12	1:B:170:LYS:N	2.35	0.41
1:H:215:ASN:ND2	1:H:224:ASN:HD22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:ARG:O	1:K:227:VAL:HA	2.20	0.41
1:E:163:THR:HG23	1:E:180:ALA:HB2	2.01	0.41
1:A:134:ASN:HD21	1:A:137:MET:HE3	1.86	0.41
1:B:154:ARG:HB2	4:B:18:HOH:O	2.19	0.41
1:I:220:ASN:O	1:I:223:LYS:HB2	2.20	0.41
1:D:197:ASN:HD22	1:D:197:ASN:C	2.24	0.41
1:I:165:ASP:HB2	1:I:215:ASN:HD21	1.86	0.41
1:B:163:THR:HG23	1:B:180:ALA:HB2	2.03	0.41
1:A:121:ASP:HA	1:A:122:PRO:HD3	1.91	0.41
1:L:125:PHE:CE1	1:L:183:ARG:HG2	2.56	0.41
1:I:121:ASP:OD2	1:I:121:ASP:N	2.53	0.40
1:B:174:LYS:HE3	1:B:178:GLU:OE2	2.21	0.40
1:E:121:ASP:OD1	1:E:121:ASP:N	2.53	0.40
1:D:181:ALA:HA	1:D:205:SER:HB2	2.03	0.40
1:L:164:ASP:H	1:L:225:ASN:HD21	1.69	0.40
1:L:237:ASP:O	1:L:241:ILE:HG13	2.22	0.40
1:L:215:ASN:HD21	1:L:224:ASN:HD22	1.70	0.40
1:L:212:ILE:HG13	1:L:226:ARG:CZ	2.52	0.40
1:C:120:ILE:N	1:C:120:ILE:HD12	2.37	0.40

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%)	8 12
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%)	24 41
1	E	130/138 (94%)	128 (98%)	1 (1%)	1 (1%)	24 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	131/138 (95%)	128 (98%)	2 (2%)	1 (1%)	24 41
1	G	130/138 (94%)	127 (98%)	2 (2%)	1 (1%)	24 41
1	H	130/138 (94%)	125 (96%)	1 (1%)	4 (3%)	5 7
1	I	130/138 (94%)	118 (91%)	11 (8%)	1 (1%)	24 41
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%)	24 41

All (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
1	A	126	GLU
1	F	169	VAL
1	D	247	ASN
1	A	167	PRO
1	H	217	SER
1	H	218	LEU
1	H	120	ILE

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	118/126 (94%)	111 (94%)	7 (6%)	24 44
1	B	120/126 (95%)	116 (97%)	4 (3%)	45 73
1	C	120/126 (95%)	112 (93%)	8 (7%)	20 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	119/126 (94%)	106 (89%)	13 (11%)	8 15
1	E	119/126 (94%)	109 (92%)	10 (8%)	14 25
1	F	120/126 (95%)	115 (96%)	5 (4%)	36 62
1	G	118/126 (94%)	109 (92%)	9 (8%)	16 30
1	H	119/126 (94%)	108 (91%)	11 (9%)	11 21
1	I	119/126 (94%)	110 (92%)	9 (8%)	16 30
1	J	119/126 (94%)	114 (96%)	5 (4%)	36 62
1	K	118/126 (94%)	109 (92%)	9 (8%)	16 30
1	L	119/126 (94%)	108 (91%)	11 (9%)	11 21
All	All	1428/1512 (94%)	1327 (93%)	101 (7%)	18 34

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	136	ASP
1	B	153	LYS
1	B	226	ARG
1	B	238	LEU
1	C	121	ASP
1	C	126	GLU
1	C	130	SER
1	C	135	GLN
1	C	174	LYS
1	C	186	ARG
1	C	226	ARG
1	C	243	SER
1	D	130	SER
1	D	135	GLN
1	D	136	ASP
1	D	143	ARG
1	D	147	ILE
1	D	171	THR
1	D	197	ASN
1	D	218	LEU
1	D	226	ARG
1	D	239	SER
1	D	245	LEU
1	D	246	ASP
1	D	250	ASN

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Mol	Chain	Res	Type
1	E	121	ASP
1	E	130	SER
1	E	135	GLN
1	E	143	ARG
1	E	172	ARG
1	E	193	GLN
1	E	219	GLU
1	E	226	ARG
1	E	246	ASP
1	E	247	ASN
1	A	127	ASN
1	A	135	GLN
1	A	136	ASP
1	A	165	ASP
1	A	226	ARG
1	A	243	SER
1	A	246	ASP
1	F	153	LYS
1	F	174	LYS
1	F	226	ARG
1	F	246	ASP
1	F	247	ASN
1	G	120	ILE
1	G	153	LYS
1	G	172	ARG
1	G	174	LYS
1	G	182	ASN
1	G	226	ARG
1	G	238	LEU
1	G	239	SER
1	G	245	LEU
1	H	120	ILE
1	H	124	THR
1	H	130	SER
1	H	135	GLN
1	H	150	LYS
1	H	166	THR
1	H	171	THR
1	H	223	LYS
1	H	226	ARG
1	H	229	ILE
1	H	246	ASP

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Mol	Chain	Res	Type
1	I	127	ASN
1	I	154	ARG
1	I	165	ASP
1	I	197	ASN
1	I	212	ILE
1	I	223	LYS
1	I	226	ARG
1	I	243	SER
1	I	246	ASP
1	J	126	GLU
1	J	150	LYS
1	J	212	ILE
1	J	226	ARG
1	J	233	THR
1	K	136	ASP
1	K	169	VAL
1	K	175	SER
1	K	182	ASN
1	K	226	ARG
1	K	232	SER
1	K	245	LEU
1	K	246	ASP
1	K	250	ASN
1	L	121	ASP
1	L	127	ASN
1	L	135	GLN
1	L	139	LEU
1	L	147	ILE
1	L	223	LYS
1	L	226	ARG
1	L	229	ILE
1	L	239	SER
1	L	246	ASP
1	L	247	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	156	HIS
1	C	197	ASN
1	C	215	ASN
1	C	220	ASN

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Mol	Chain	Res	Type
1	C	242	HIS
1	D	197	ASN
1	D	215	ASN
1	E	135	GLN
1	E	215	ASN
1	A	127	ASN
1	A	134	ASN
1	A	176	HIS
1	A	210	ASN
1	A	247	ASN
1	F	200	GLN
1	F	215	ASN
1	F	220	ASN
1	G	215	ASN
1	G	247	ASN
1	H	215	ASN
1	H	225	ASN
1	I	127	ASN
1	I	134	ASN
1	I	176	HIS
1	J	182	ASN
1	J	210	ASN
1	J	215	ASN
1	J	220	ASN
1	K	215	ASN
1	L	200	GLN
1	L	215	ASN
1	L	225	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

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	131/138 (94%)	0.32	2 (1%)	76	79	39, 69, 106, 122	0
1	B	133/138 (96%)	-0.10	2 (1%)	76	79	18, 40, 68, 98	0
1	C	133/138 (96%)	-0.04	1 (0%)	87	89	22, 43, 72, 107	0
1	D	132/138 (95%)	-0.03	1 (0%)	87	89	20, 40, 68, 84	0
1	E	132/138 (95%)	-0.11	2 (1%)	76	79	24, 45, 71, 95	0
1	F	133/138 (96%)	0.12	2 (1%)	76	79	31, 59, 89, 123	0
1	G	132/138 (95%)	0.01	2 (1%)	76	79	22, 45, 72, 92	0
1	H	132/138 (95%)	0.02	2 (1%)	76	79	22, 44, 70, 107	0
1	I	132/138 (95%)	0.35	9 (6%)	20	23	36, 70, 111, 124	0
1	J	132/138 (95%)	0.10	5 (3%)	44	49	30, 60, 88, 110	0
1	K	132/138 (95%)	-0.02	3 (2%)	64	67	23, 44, 71, 96	0
1	L	132/138 (95%)	-0.03	4 (3%)	54	59	24, 44, 70, 102	0
All	All	1586/1656 (95%)	0.05	35 (2%)	65	69	18, 49, 91, 124	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	120	ILE	5.7
1	G	119	GLY	4.7
1	I	222	MET	4.1
1	I	218	LEU	4.0
1	F	137	MET	3.9
1	K	249	PHE	3.8
1	E	126	GLU	3.7
1	G	250	ASN	3.7
1	K	168	LEU	3.7
1	K	169	VAL	3.7
1	H	119	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	119	GLY	3.6
1	I	249	PHE	3.5
1	I	133	ILE	3.2
1	F	251	PRO	3.2
1	E	245	LEU	3.1
1	I	219	GLU	3.1
1	B	251	PRO	3.0
1	H	249	PHE	2.9
1	D	170	LYS	2.8
1	I	119	GLY	2.8
1	C	251	PRO	2.7
1	J	135	GLN	2.5
1	I	168	LEU	2.4
1	L	250	ASN	2.4
1	J	250	ASN	2.4
1	L	169	VAL	2.3
1	A	135	GLN	2.2
1	I	139	LEU	2.2
1	J	154	ARG	2.2
1	B	222	MET	2.1
1	I	120	ILE	2.1
1	J	146	LYS	2.1
1	J	246	ASP	2.0
1	A	125	PHE	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	NI	G	1	1/1	0.97	0.20	-	39,39,39,39	0
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
2	NI	K	2	1/1	0.95	0.19	-	37,37,37,37	0
3	CL	K	12	1/1	0.94	0.13	-	54,54,54,54	0
3	CL	G	83	1/1	0.96	0.15	-	52,52,52,52	0

6.5 Other polymers

There are no such residues in this entry.