



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:24 am GMT

PDB ID : 3RPU
Title : Crystal structure of the MukE-MukF complex
Authors : Guarne, A.; Gloyd, M.; Ghirlando, R.
Deposited on : 2011-04-27
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

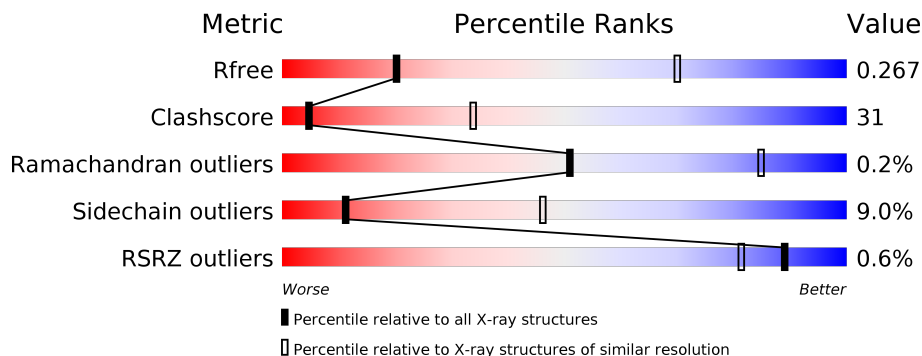
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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 $\leq 5\%$. 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	460	<div> <div style="width: 35%; background-color: green;"></div> <div style="width: 30%; background-color: yellow;"></div> <div style="width: 33%; background-color: grey;"></div> </div> <div> <div style="width: 35%; background-color: green;"></div> <div style="width: 30%; background-color: yellow;"></div> <div style="width: 33%; background-color: grey;"></div> </div>
1	B	460	<div> <div style="width: 29%; background-color: green;"></div> <div style="width: 33%; background-color: yellow;"></div> <div style="width: 34%; background-color: grey;"></div> </div> <div> <div style="width: 29%; background-color: green;"></div> <div style="width: 33%; background-color: yellow;"></div> <div style="width: 34%; background-color: grey;"></div> </div>
1	X	460	<div> <div style="width: 40%; background-color: green;"></div> <div style="width: 25%; background-color: yellow;"></div> <div style="width: 33%; background-color: grey;"></div> </div> <div> <div style="width: 40%; background-color: green;"></div> <div style="width: 25%; background-color: yellow;"></div> <div style="width: 33%; background-color: grey;"></div> </div>
2	D	245	<div> <div style="width: 37%; background-color: green;"></div> <div style="width: 39%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 17%; background-color: grey;"></div> </div> <div> <div style="width: 37%; background-color: green;"></div> <div style="width: 39%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 17%; background-color: grey;"></div> </div>
2	E	245	<div> <div style="width: 44%; background-color: green;"></div> <div style="width: 31%; background-color: yellow;"></div> <div style="width: 22%; background-color: grey;"></div> </div> <div> <div style="width: 44%; background-color: green;"></div> <div style="width: 31%; background-color: yellow;"></div> <div style="width: 22%; background-color: grey;"></div> </div>
2	G	245	<div> <div style="width: 42%; background-color: green;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 17%; background-color: grey;"></div> </div> <div> <div style="width: 42%; background-color: green;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 17%; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	H	245	<div><div></div><div>39%36%22%</div></div>
2	Y	245	<div><div></div><div>41%36%7%16%</div></div>
2	Z	245	<div><div></div><div>%45%27%5%23%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17083 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 Chromosome partition protein mukF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2503	1573	447	475	8			
1	B	302	Total	C	N	O	S	0	0	0
			2443	1536	438	462	7			
1	X	310	Total	C	N	O	S	0	0	0
			2504	1573	448	476	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P60293
A	-18	GLY	-	EXPRESSION TAG	UNP P60293
A	-17	SER	-	EXPRESSION TAG	UNP P60293
A	-16	SER	-	EXPRESSION TAG	UNP P60293
A	-15	HIS	-	EXPRESSION TAG	UNP P60293
A	-14	HIS	-	EXPRESSION TAG	UNP P60293
A	-13	HIS	-	EXPRESSION TAG	UNP P60293
A	-12	HIS	-	EXPRESSION TAG	UNP P60293
A	-11	HIS	-	EXPRESSION TAG	UNP P60293
A	-10	HIS	-	EXPRESSION TAG	UNP P60293
A	-9	SER	-	EXPRESSION TAG	UNP P60293
A	-8	SER	-	EXPRESSION TAG	UNP P60293
A	-7	GLY	-	EXPRESSION TAG	UNP P60293
A	-6	LEU	-	EXPRESSION TAG	UNP P60293
A	-5	VAL	-	EXPRESSION TAG	UNP P60293
A	-4	PRO	-	EXPRESSION TAG	UNP P60293
A	-3	ARG	-	EXPRESSION TAG	UNP P60293
A	-2	GLY	-	EXPRESSION TAG	UNP P60293
A	-1	SER	-	EXPRESSION TAG	UNP P60293
A	0	HIS	-	EXPRESSION TAG	UNP P60293
B	-19	MET	-	EXPRESSION TAG	UNP P60293
B	-18	GLY	-	EXPRESSION TAG	UNP P60293
B	-17	SER	-	EXPRESSION TAG	UNP P60293

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP P60293
B	-15	HIS	-	EXPRESSION TAG	UNP P60293
B	-14	HIS	-	EXPRESSION TAG	UNP P60293
B	-13	HIS	-	EXPRESSION TAG	UNP P60293
B	-12	HIS	-	EXPRESSION TAG	UNP P60293
B	-11	HIS	-	EXPRESSION TAG	UNP P60293
B	-10	HIS	-	EXPRESSION TAG	UNP P60293
B	-9	SER	-	EXPRESSION TAG	UNP P60293
B	-8	SER	-	EXPRESSION TAG	UNP P60293
B	-7	GLY	-	EXPRESSION TAG	UNP P60293
B	-6	LEU	-	EXPRESSION TAG	UNP P60293
B	-5	VAL	-	EXPRESSION TAG	UNP P60293
B	-4	PRO	-	EXPRESSION TAG	UNP P60293
B	-3	ARG	-	EXPRESSION TAG	UNP P60293
B	-2	GLY	-	EXPRESSION TAG	UNP P60293
B	-1	SER	-	EXPRESSION TAG	UNP P60293
B	0	HIS	-	EXPRESSION TAG	UNP P60293
X	-19	MET	-	EXPRESSION TAG	UNP P60293
X	-18	GLY	-	EXPRESSION TAG	UNP P60293
X	-17	SER	-	EXPRESSION TAG	UNP P60293
X	-16	SER	-	EXPRESSION TAG	UNP P60293
X	-15	HIS	-	EXPRESSION TAG	UNP P60293
X	-14	HIS	-	EXPRESSION TAG	UNP P60293
X	-13	HIS	-	EXPRESSION TAG	UNP P60293
X	-12	HIS	-	EXPRESSION TAG	UNP P60293
X	-11	HIS	-	EXPRESSION TAG	UNP P60293
X	-10	HIS	-	EXPRESSION TAG	UNP P60293
X	-9	SER	-	EXPRESSION TAG	UNP P60293
X	-8	SER	-	EXPRESSION TAG	UNP P60293
X	-7	GLY	-	EXPRESSION TAG	UNP P60293
X	-6	LEU	-	EXPRESSION TAG	UNP P60293
X	-5	VAL	-	EXPRESSION TAG	UNP P60293
X	-4	PRO	-	EXPRESSION TAG	UNP P60293
X	-3	ARG	-	EXPRESSION TAG	UNP P60293
X	-2	GLY	-	EXPRESSION TAG	UNP P60293
X	-1	SER	-	EXPRESSION TAG	UNP P60293
X	0	HIS	-	EXPRESSION TAG	UNP P60293

- Molecule 2 is a protein called Chromosome partition protein mukE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	204	Total	C	N	O	S	0	0	0
			1656	1049	295	304	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	191	Total	C	N	O	S	0	0	0
			1561	994	277	283	7			
2	D	203	Total	C	N	O	S	0	0	0
			1649	1045	294	302	8			
2	E	191	Total	C	N	O	S	0	0	0
			1562	995	276	284	7			
2	Y	205	Total	C	N	O	S	0	0	0
			1661	1052	296	305	8			
2	Z	188	Total	C	N	O	S	0	0	0
			1542	983	272	280	7			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	MET	-	EXPRESSION TAG	UNP P22524
G	-9	GLY	-	EXPRESSION TAG	UNP P22524
G	-8	SER	-	EXPRESSION TAG	UNP P22524
G	-7	SER	-	EXPRESSION TAG	UNP P22524
G	-6	HIS	-	EXPRESSION TAG	UNP P22524
G	-5	HIS	-	EXPRESSION TAG	UNP P22524
G	-4	HIS	-	EXPRESSION TAG	UNP P22524
G	-3	HIS	-	EXPRESSION TAG	UNP P22524
G	-2	HIS	-	EXPRESSION TAG	UNP P22524
G	-1	HIS	-	EXPRESSION TAG	UNP P22524
G	0	SER	-	EXPRESSION TAG	UNP P22524
G	1	SER	-	EXPRESSION TAG	UNP P22524
G	2	GLY	-	EXPRESSION TAG	UNP P22524
G	3	LEU	-	EXPRESSION TAG	UNP P22524
G	4	VAL	-	EXPRESSION TAG	UNP P22524
G	5	PRO	-	EXPRESSION TAG	UNP P22524
G	6	ARG	-	EXPRESSION TAG	UNP P22524
G	7	GLY	-	EXPRESSION TAG	UNP P22524
G	8	SER	-	EXPRESSION TAG	UNP P22524
G	9	HIS	-	EXPRESSION TAG	UNP P22524
H	-10	MET	-	EXPRESSION TAG	UNP P22524
H	-9	GLY	-	EXPRESSION TAG	UNP P22524
H	-8	SER	-	EXPRESSION TAG	UNP P22524
H	-7	SER	-	EXPRESSION TAG	UNP P22524
H	-6	HIS	-	EXPRESSION TAG	UNP P22524
H	-5	HIS	-	EXPRESSION TAG	UNP P22524
H	-4	HIS	-	EXPRESSION TAG	UNP P22524
H	-3	HIS	-	EXPRESSION TAG	UNP P22524
H	-2	HIS	-	EXPRESSION TAG	UNP P22524

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	HIS	-	EXPRESSION TAG	UNP P22524
H	0	SER	-	EXPRESSION TAG	UNP P22524
H	1	SER	-	EXPRESSION TAG	UNP P22524
H	2	GLY	-	EXPRESSION TAG	UNP P22524
H	3	LEU	-	EXPRESSION TAG	UNP P22524
H	4	VAL	-	EXPRESSION TAG	UNP P22524
H	5	PRO	-	EXPRESSION TAG	UNP P22524
H	6	ARG	-	EXPRESSION TAG	UNP P22524
H	7	GLY	-	EXPRESSION TAG	UNP P22524
H	8	SER	-	EXPRESSION TAG	UNP P22524
H	9	HIS	-	EXPRESSION TAG	UNP P22524
D	-10	MET	-	EXPRESSION TAG	UNP P22524
D	-9	GLY	-	EXPRESSION TAG	UNP P22524
D	-8	SER	-	EXPRESSION TAG	UNP P22524
D	-7	SER	-	EXPRESSION TAG	UNP P22524
D	-6	HIS	-	EXPRESSION TAG	UNP P22524
D	-5	HIS	-	EXPRESSION TAG	UNP P22524
D	-4	HIS	-	EXPRESSION TAG	UNP P22524
D	-3	HIS	-	EXPRESSION TAG	UNP P22524
D	-2	HIS	-	EXPRESSION TAG	UNP P22524
D	-1	HIS	-	EXPRESSION TAG	UNP P22524
D	0	SER	-	EXPRESSION TAG	UNP P22524
D	1	SER	-	EXPRESSION TAG	UNP P22524
D	2	GLY	-	EXPRESSION TAG	UNP P22524
D	3	LEU	-	EXPRESSION TAG	UNP P22524
D	4	VAL	-	EXPRESSION TAG	UNP P22524
D	5	PRO	-	EXPRESSION TAG	UNP P22524
D	6	ARG	-	EXPRESSION TAG	UNP P22524
D	7	GLY	-	EXPRESSION TAG	UNP P22524
D	8	SER	-	EXPRESSION TAG	UNP P22524
D	9	HIS	-	EXPRESSION TAG	UNP P22524
E	-10	MET	-	EXPRESSION TAG	UNP P22524
E	-9	GLY	-	EXPRESSION TAG	UNP P22524
E	-8	SER	-	EXPRESSION TAG	UNP P22524
E	-7	SER	-	EXPRESSION TAG	UNP P22524
E	-6	HIS	-	EXPRESSION TAG	UNP P22524
E	-5	HIS	-	EXPRESSION TAG	UNP P22524
E	-4	HIS	-	EXPRESSION TAG	UNP P22524
E	-3	HIS	-	EXPRESSION TAG	UNP P22524
E	-2	HIS	-	EXPRESSION TAG	UNP P22524
E	-1	HIS	-	EXPRESSION TAG	UNP P22524
E	0	SER	-	EXPRESSION TAG	UNP P22524

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	SER	-	EXPRESSION TAG	UNP P22524
E	2	GLY	-	EXPRESSION TAG	UNP P22524
E	3	LEU	-	EXPRESSION TAG	UNP P22524
E	4	VAL	-	EXPRESSION TAG	UNP P22524
E	5	PRO	-	EXPRESSION TAG	UNP P22524
E	6	ARG	-	EXPRESSION TAG	UNP P22524
E	7	GLY	-	EXPRESSION TAG	UNP P22524
E	8	SER	-	EXPRESSION TAG	UNP P22524
E	9	HIS	-	EXPRESSION TAG	UNP P22524
Y	-10	MET	-	EXPRESSION TAG	UNP P22524
Y	-9	GLY	-	EXPRESSION TAG	UNP P22524
Y	-8	SER	-	EXPRESSION TAG	UNP P22524
Y	-7	SER	-	EXPRESSION TAG	UNP P22524
Y	-6	HIS	-	EXPRESSION TAG	UNP P22524
Y	-5	HIS	-	EXPRESSION TAG	UNP P22524
Y	-4	HIS	-	EXPRESSION TAG	UNP P22524
Y	-3	HIS	-	EXPRESSION TAG	UNP P22524
Y	-2	HIS	-	EXPRESSION TAG	UNP P22524
Y	-1	HIS	-	EXPRESSION TAG	UNP P22524
Y	0	SER	-	EXPRESSION TAG	UNP P22524
Y	1	SER	-	EXPRESSION TAG	UNP P22524
Y	2	GLY	-	EXPRESSION TAG	UNP P22524
Y	3	LEU	-	EXPRESSION TAG	UNP P22524
Y	4	VAL	-	EXPRESSION TAG	UNP P22524
Y	5	PRO	-	EXPRESSION TAG	UNP P22524
Y	6	ARG	-	EXPRESSION TAG	UNP P22524
Y	7	GLY	-	EXPRESSION TAG	UNP P22524
Y	8	SER	-	EXPRESSION TAG	UNP P22524
Y	9	HIS	-	EXPRESSION TAG	UNP P22524
Z	-10	MET	-	EXPRESSION TAG	UNP P22524
Z	-9	GLY	-	EXPRESSION TAG	UNP P22524
Z	-8	SER	-	EXPRESSION TAG	UNP P22524
Z	-7	SER	-	EXPRESSION TAG	UNP P22524
Z	-6	HIS	-	EXPRESSION TAG	UNP P22524
Z	-5	HIS	-	EXPRESSION TAG	UNP P22524
Z	-4	HIS	-	EXPRESSION TAG	UNP P22524
Z	-3	HIS	-	EXPRESSION TAG	UNP P22524
Z	-2	HIS	-	EXPRESSION TAG	UNP P22524
Z	-1	HIS	-	EXPRESSION TAG	UNP P22524
Z	0	SER	-	EXPRESSION TAG	UNP P22524
Z	1	SER	-	EXPRESSION TAG	UNP P22524
Z	2	GLY	-	EXPRESSION TAG	UNP P22524

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	3	LEU	-	EXPRESSION TAG	UNP P22524
Z	4	VAL	-	EXPRESSION TAG	UNP P22524
Z	5	PRO	-	EXPRESSION TAG	UNP P22524
Z	6	ARG	-	EXPRESSION TAG	UNP P22524
Z	7	GLY	-	EXPRESSION TAG	UNP P22524
Z	8	SER	-	EXPRESSION TAG	UNP P22524
Z	9	HIS	-	EXPRESSION TAG	UNP P22524

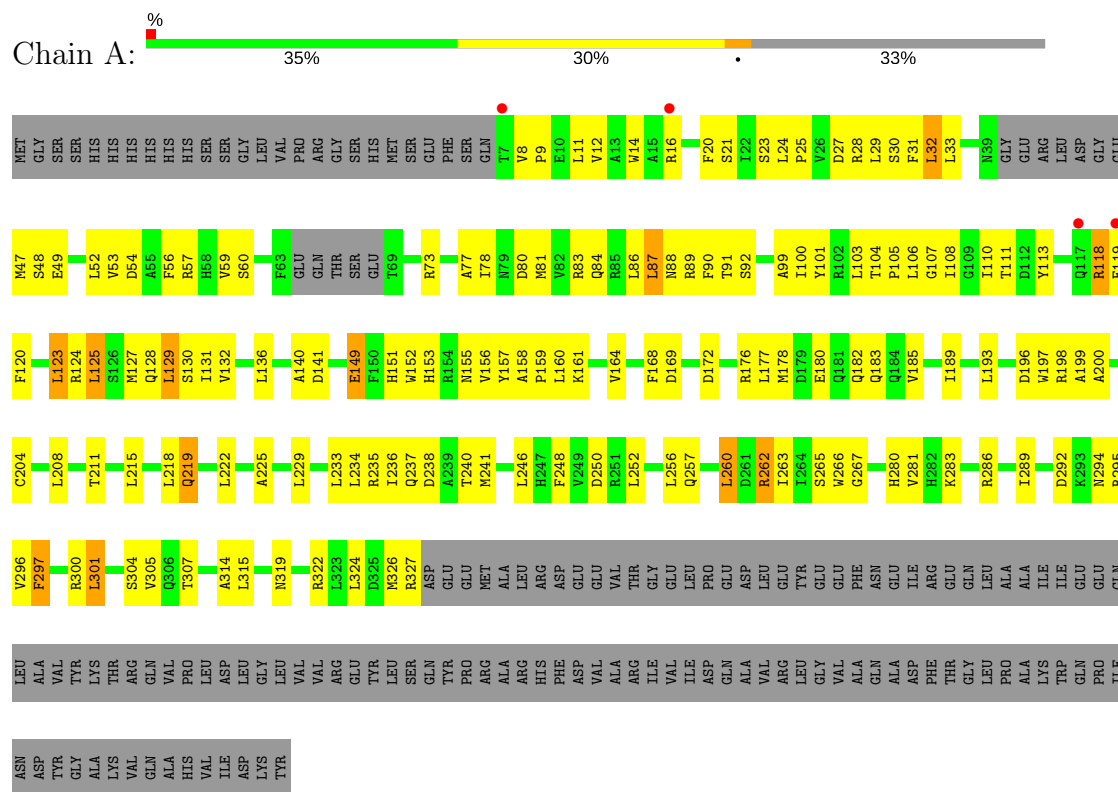
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O 1 1	0	0
3	Y	1	Total O 1 1	0	0

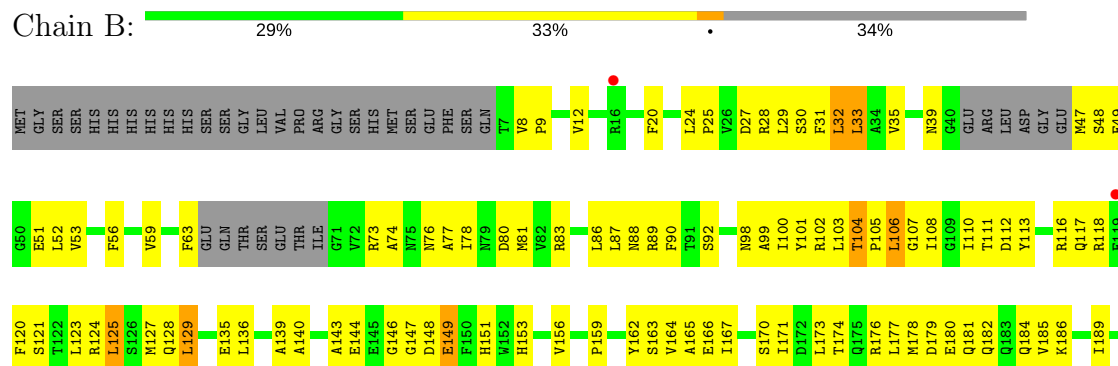
3 Residue-property plots

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: Chromosome partition protein mukF

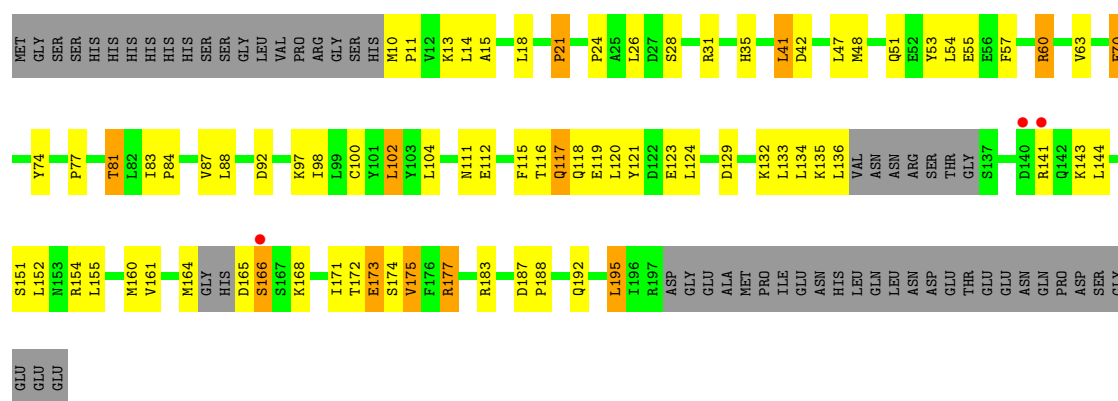
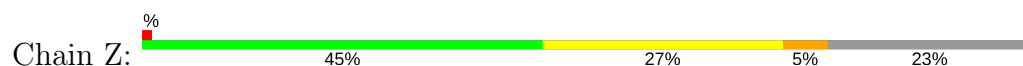


• Molecule 1: Chromosome partition protein mukF





- Molecule 2: Chromosome partition protein mukE



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	149.89Å 149.89Å 738.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.60 19.98 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.98-3.60) 98.4 (19.98-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.217 , 0.274 0.204 , 0.267	Depositor DCC
R_{free} test set	2888 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	105.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17083	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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

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	0.65	0/2545	0.85	1/3442 (0.0%)
1	B	0.58	0/2483	0.74	0/3355
1	X	0.60	0/2546	0.82	1/3443 (0.0%)
2	D	0.70	0/1679	0.92	2/2260 (0.1%)
2	E	0.65	0/1589	0.81	1/2138 (0.0%)
2	G	0.68	0/1687	0.86	0/2273
2	H	0.62	0/1590	0.80	0/2140
2	Y	0.80	1/1692 (0.1%)	0.97	5/2280 (0.2%)
2	Z	0.71	0/1569	0.89	1/2110 (0.0%)
All	All	0.66	1/17380 (0.0%)	0.85	11/23441 (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
2	Y	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	108	ARG	CG-CD	6.25	1.67	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	41	LEU	CA-CB-CG	-6.22	101.00	115.30
2	D	81	THR	CB-CA-C	-6.13	95.05	111.60
2	Y	203	ARG	NE-CZ-NH1	-5.69	117.45	120.30
2	Y	108	ARG	CB-CG-CD	5.67	126.36	111.60
1	X	300	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	194	GLY	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	2503	0	2463	195	0
1	B	2443	0	2405	229	0
1	X	2504	0	2453	122	0
2	D	1649	0	1652	144	0
2	E	1562	0	1571	89	0
2	G	1656	0	1660	104	0
2	H	1561	0	1567	82	0
2	Y	1661	0	1662	120	0
2	Z	1542	0	1554	75	0
3	G	1	0	0	0	0
3	Y	1	0	0	0	0
All	All	17083	0	16987	1047	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 31.

The worst 5 of 1047 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:A:281:VAL:HG22	2:G:109:LEU:HD22	1.28	1.15
1:X:118:ARG:HB3	1:X:177:LEU:HD21	1.12	1.11
1:B:300:ARG:HH22	2:D:193:GLY:HA2	1.06	1.10
2:D:180:THR:O	2:D:183:VAL:HG23	1.51	1.09
1:X:219:GLN:HE21	1:X:267:GLY:HA3	0.98	1.09

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	303/460 (66%)	284 (94%)	19 (6%)	0	100	100
1	B	294/460 (64%)	277 (94%)	17 (6%)	0	100	100
1	X	304/460 (66%)	286 (94%)	18 (6%)	0	100	100
2	D	199/245 (81%)	190 (96%)	8 (4%)	1 (0%)	32	73
2	E	185/245 (76%)	167 (90%)	17 (9%)	1 (0%)	32	73
2	G	202/245 (82%)	189 (94%)	11 (5%)	2 (1%)	18	62
2	H	187/245 (76%)	181 (97%)	6 (3%)	0	100	100
2	Y	203/245 (83%)	191 (94%)	12 (6%)	0	100	100
2	Z	182/245 (74%)	171 (94%)	11 (6%)	0	100	100
All	All	2059/2850 (72%)	1936 (94%)	119 (6%)	4 (0%)	51	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	126	THR
2	E	131	ALA
2	G	126	THR
2	G	137	VAL

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	268/397 (68%)	254 (95%)	14 (5%)	27	65
1	B	260/397 (66%)	241 (93%)	19 (7%)	16	54
1	X	266/397 (67%)	248 (93%)	18 (7%)	18	57
2	D	177/215 (82%)	157 (89%)	20 (11%)	7	35
2	E	168/215 (78%)	158 (94%)	10 (6%)	22	62
2	G	178/215 (83%)	157 (88%)	21 (12%)	6	33
2	H	167/215 (78%)	155 (93%)	12 (7%)	17	55
2	Y	178/215 (83%)	145 (82%)	33 (18%)	2	12
2	Z	166/215 (77%)	149 (90%)	17 (10%)	8	40
All	All	1828/2481 (74%)	1664 (91%)	164 (9%)	11	46

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	90	GLU
2	E	117	GLN
2	Z	70	GLU
2	D	112	GLU
2	D	191	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	ASN
1	B	219	GLN
2	Y	117	GLN
1	B	39	ASN
2	Z	35	HIS

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 [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(Å ²)	Q<0.9
1	A	309/460 (67%)	-0.53	4 (1%) 77 64	75, 131, 215, 275	0
1	B	302/460 (65%)	-0.52	2 (0%) 87 78	81, 149, 217, 294	0
1	X	310/460 (67%)	-0.52	2 (0%) 89 81	61, 141, 209, 280	0
2	D	203/245 (82%)	-0.62	1 (0%) 90 84	73, 113, 175, 222	0
2	E	191/245 (77%)	-0.60	1 (0%) 90 84	72, 110, 184, 244	0
2	G	204/245 (83%)	-0.67	0 100 100	75, 110, 178, 217	0
2	H	191/245 (77%)	-0.62	0 100 100	79, 111, 171, 222	0
2	Y	205/245 (83%)	-0.73	0 100 100	57, 94, 168, 205	0
2	Z	188/245 (76%)	-0.60	3 (1%) 72 59	64, 108, 169, 264	0
All	All	2103/2850 (73%)	-0.59	13 (0%) 89 81	57, 123, 200, 294	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ARG	4.1
1	A	117	GLN	3.0
1	A	7	THR	2.8
1	A	119	GLU	2.5
2	Z	141	ARG	2.4

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.