



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2017 – 07:27 AM EDT

PDB ID : 1T98
Title : Crystal Structure of MukF(1-287)
Authors : Fennell-Fezzie, R.; Berger, J.M.
Deposited on : unknown
Resolution : 2.90 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	:	rb-20030345
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-20030345

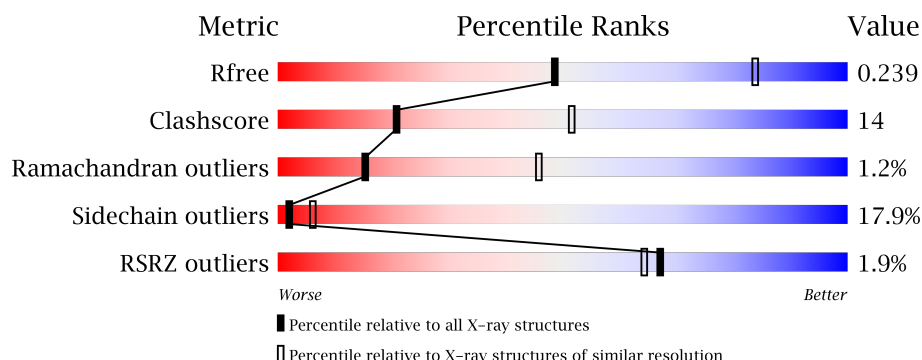
1 Overall quality at a glance

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	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 $\leq 5\%$. 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	287	<div> <div>0.1%</div> <div>57%</div> <div>30%</div> <div>5%</div> <div>7%</div> </div>
1	B	287	<div> <div>3%</div> <div>51%</div> <div>35%</div> <div>5%</div> <div>9%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4228 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	266	Total	C	N	O	S	Se	0	0	0
			2140	1342	378	414	1	5			
1	B	260	Total	C	N	O	S	Se	0	0	0
			2088	1308	368	407	1	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	81	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	127	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	178	MSE	MET	MODIFIED RESIDUE	UNP P60293
A	241	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	47	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	81	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	127	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	178	MSE	MET	MODIFIED RESIDUE	UNP P60293
B	241	MSE	MET	MODIFIED RESIDUE	UNP P60293

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.

Chain A:

57% 30% 5% 7%

Legend: MET, SER, GLU, PHE, SER, GLN, THR, V8, P9, H10, L11, V12, R16, K17, S23, R28, F31, L32, L33, A34, T37, R42, L43, D44, G45, E46, M47, S48, E49, V53, V59, Q65, E68, T69, V72, R73, A74, N75, N76, A77, D80, M81, Q84, L87, N88, P89.

Chain B:

Amino Acid	Category
W266	Green
Q268	Green
Q269	Green
S270	Green
L271	Orange
D272	Orange
L275	Yellow
D278	Yellow
R279	Yellow
H280	Yellow
V281	Green
HIS	Green
LYS	Green
PHE	Green
ILE	Green
ARG	Green
THR	Green
L193	Green
N194	Green
LYS	Green
ASP	Green
TRP	Green
ARG	Green
ALA	Green
I201	Yellow
C204	Yellow
E205	Yellow
L206	Green
L207	Green
L2107	Green
L208	Green
S209	Green
E210	Green
T211	Green
S212	Green
L215	Green
R216	Green
E217	Green
L218	Orange
Q219	Green
D220	Green
L221	Green
L222	Green
K228	Green
L229	Green
Q230	Green
L233	Green
T236	Green
Q237	Green
D238	Green
A239	Orange
THR	Grey
MSE	Grey
THR	Grey
H243	Yellow
L246	Yellow
H247	Orange
F248	Yellow
V249	Yellow
D250	Orange
R251	Yellow
L252	Orange
V253	Yellow
Q257	Green
S258	Green
K259	Green
R262	Green
L262	Green
GLN	Green
ALA	Green
GLU	Green
GLY	Green
ASN	Green
ALA	Green
I100	Green
Y101	Green
P105	Yellow
T111	Yellow
I114	Green
I115	Green
R116	Green
F120	Green
L123	Green
R124	Green
L125	Green
L129	Orange
S130	Orange
D141	Green
E144	Green
E145	Green
G146	Green
L147	Green
D148	Orange
E149	Orange
H152	Green
H153	Green
R154	Green
H155	Green
Y156	Orange
Y157	Yellow
A158	Yellow
P159	Yellow
L160	Green
K161	Yellow
Y162	Yellow
E166	Yellow
I167	Yellow
F168	Green
D169	Yellow
S170	Green
I171	Yellow
D172	Orange
L173	Green
T174	Green
Q175	Green
R176	Green
L177	Green
M178	Grey
GLU	Grey
SER	Grey
T91	Green
F90	Green
R89	Green
M81	Yellow
A77	Yellow
I70	Yellow
F63	Yellow
R57	Yellow
D54	Yellow
L52	Yellow
V53	Yellow
E51	Green
G50	Green
S48	Yellow
E49	Yellow
M47	Yellow
L43	Yellow
R42	Yellow
E41	Yellow
G40	Yellow
N39	Orange
L38	Yellow
T37	Yellow
A36	Yellow
V35	Yellow
A34	Green
L33	Orange
L32	Orange
F31	Yellow
R28	Orange
P25	Yellow
D19	Yellow
N18	Yellow
W14	Yellow
A13	Green
V12	Orange
L11	Orange
E10	Green
P9	Yellow
V8	Orange
T7	Orange
Q6	Orange
S5	Orange
PHE	Orange
GLU	Orange
SER	Orange
MET	Orange

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	58.70 Å 58.70 Å 307.41 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 51.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-2.90) 95.5 (51.24-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.233 , 0.273 0.201 , 0.239	Depositor DCC
R_{free} test set	625 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.118 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4228	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	A	0.45	0/2169	0.80	11/2926 (0.4%)
1	B	0.44	0/2114	0.79	11/2850 (0.4%)
All	All	0.44	0/4283	0.80	22/5776 (0.4%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	172	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	172	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	245	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	19	ASP	CB-CG-OD2	5.77	123.50	118.30

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	2140	0	2103	54	0
1	B	2088	0	2048	69	0
All	All	4228	0	4151	116	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 14.

The worst 5 of 116 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:B:120:PHE:HZ	1:B:218:LEU:HD21	1.17	1.09
1:A:138:ARG:HH11	1:A:138:ARG:HG3	1.13	1.08
1:A:90:PHE:O	1:A:100:ILE:HG13	1.68	0.92
1:B:124:ARG:HD2	1:B:174:THR:HG23	1.51	0.91
1:A:37:THR:HG21	1:B:11:LEU:HD11	1.54	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	262/287 (91%)	245 (94%)	14 (5%)	3 (1%)	17	48
1	B	252/287 (88%)	234 (93%)	15 (6%)	3 (1%)	15	46
All	All	514/574 (90%)	479 (93%)	29 (6%)	6 (1%)	15	46

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLY
1	A	244	ASP
1	B	146	GLY
1	B	43	LEU
1	A	43	LEU

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	231/244 (95%)	185 (80%)	46 (20%)	1	4
1	B	227/244 (93%)	191 (84%)	36 (16%)	3	8
All	All	458/488 (94%)	376 (82%)	82 (18%)	2	6

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	LYS
1	A	268	GLN
1	B	250	ASP
1	A	197	TRP
1	A	234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	184	GLN
1	B	219	GLN
1	A	155	ASN
1	B	230	GLN

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 [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	261/287 (90%)	0.06	2 (0%) 86 85	15, 32, 53, 65	0
1	B	256/287 (89%)	0.16	8 (3%) 49 43	13, 32, 54, 65	0
All	All	517/574 (90%)	0.11	10 (1%) 67 64	13, 32, 54, 65	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	GLN	3.7
1	B	5	SER	3.0
1	A	195	LYS	2.7
1	B	236	ILE	2.7
1	B	247	HIS	2.5

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.