

Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 01:43 pm BST

PDB ID 5EIP

Title apo-structure of YTH domain of SpMmi1 Authors Wu, B.X.; Xu, J.H.; Su, S.C.; Ma, J.B.

2015-10-30 Deposited on

1.49 Å(reported) Resolution

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 https://www.wwpdb.org/validation/2017/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:

4.02b-467MolProbity Xtriage (Phenix) 1.13

EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

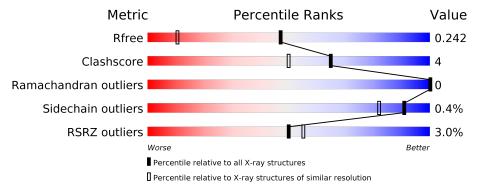
Validation Pipeline (wwPDB-VP) 2.11

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 1.49 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	134	93%	7%
1	В	134	90%	10%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2335 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 YTH domain-containing protein mmi1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	134	Total 1065			O 205	S 8	0	0	0
1	В	134	Total 1065			O 205	S 8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	SER	_	expression tag	UNP O74958
A	345	GLU	-	expression tag	UNP O74958
A	346	PHE	_	expression tag	UNP O74958
A	347	GLU	_	expression tag	UNP O74958
A	348	LEU	_	expression tag	UNP O74958
В	344	SER	-	expression tag	UNP O74958
В	345	GLU	-	expression tag	UNP O74958
В	346	PHE	-	expression tag	UNP O74958
В	347	GLU	_	expression tag	UNP O74958
В	348	LEU	_	expression tag	UNP O74958

• Molecule 2 is water.

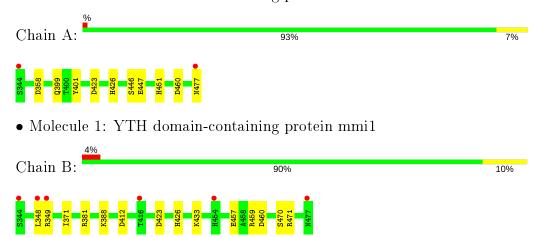
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	106	Total O 106 106	0	0
2	В	99	Total O 99 99	0	0



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: YTH domain-containing protein mmi1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	33.84Å 60.26Å 119.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.81 - 1.49	Depositor
Resolution (A)	33.25 - 1.49	EDS
% Data completeness	98.5 (59.81-1.49)	Depositor
(in resolution range)	98.5 (33.25-1.49)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.88 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
P. P.	0.194 , 0.230	Depositor
R, R_{free}	0.203 , 0.242	DCC
R_{free} test set	2006 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 41.6	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2335	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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	Boı	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	1.04	1/1087 (0.1%)	1.03	1/1464 (0.1%)	
1	В	1.13	1/1087 (0.1%)	1.15	7/1464 (0.5%)	
All	All	1.09	2/2174~(0.1%)	1.09	8/2928 (0.3%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
1	A	401	TYR	CE1-CZ	-6.81	1.29	1.38
1	В	470	SER	CB-OG	-6.38	1.33	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	В	471	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	В	412	ASP	CB-CG-OD1	8.05	125.54	118.30
1	В	471	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	460	ASP	CB-CG-OD1	5.56	123.30	118.30
1	В	459	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	В	412	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	В	381	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	В	460	ASP	CB-CG-OD1	5.02	122.82	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	Α	1065	0	1033	8	0
1	В	1065	0	1033	9	0
2	A	106	0	0	3	0
2	В	99	0	0	7	0
All	All	2335	0	2066	17	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 4.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}\;({ m \AA})$	${ m overlap}({ m \AA})$
1:A:446:SER:HB2	2:A:501:HOH:O	1.00	1.18
1:B:348:LEU:HD21	2:B:536:HOH:O	1.75	0.85
1:B:371:ILE:HB	2:B:502:HOH:O	1.82	0.78
1:A:446:SER:CB	2:A:501:HOH:O	1.75	0.77
1:B:423:ASP:H	1:B:426:HIS:HD2	1.31	0.74
1:A:447:GLU:OE2	1:A:451:HIS:HD2	1.79	0.66
1:A:423:ASP:H	1:A:426:HIS:HD2	1.44	0.64
1:A:477:ASN:C	2:A:552:HOH:O	2.37	0.62
1:A:399:GLN:HA	1:A:399:GLN:NE2	2.26	0.50
1:B:433:LYS:HE3	2:B:562:HOH:O	2.16	0.46
1:A:423:ASP:N	1:A:426:HIS:HD2	2.13	0.44
1:B:371:ILE:HD11	2:B:527:HOH:O	2.17	0.43
1:B:388:LYS:HG3	2:B:510:HOH:O	2.18	0.42
1:A:399:GLN:HA	1:A:399:GLN:HE21	1.82	0.42
1:B:349:ARG:CD	2:B:565:HOH:O	2.69	0.41
1:B:457:GLU:HG2	2:B:513:HOH:O	2.21	0.41
1:B:423:ASP:N	1:B:426:HIS:HD2	2.10	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	Perce	\mathbf{ntiles}
1	A	132/134~(98%)	129 (98%)	3 (2%)	0	100	100
1	В	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
All	All	$264/268 \; (98\%)$	260 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	Percei	$_{ m tiles}$
1	A	116/116 (100%)	115 (99%)	1 (1%)	78	61
1	В	116/116 (100%)	116 (100%)	0	100	100
All	All	232/232 (100%)	231 (100%)	1 (0%)	91	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	GLN
1	A	426	HIS
1	A	451	HIS
1	A	454	HIS
1	В	426	HIS
1	В	451	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.



5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	134/134 (100%)	-0.09	2 (1%) 73 78	11, 17, 34, 39	0
1	В	134/134 (100%)	0.02	6 (4%) 33 36	9, 16, 31, 48	0
All	All	268/268 (100%)	-0.03	8 (2%) 50 55	9, 17, 34, 48	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	348	LEU	4.2
1	В	344	SER	4.0
1	В	349	ARG	3.7
1	A	477	ASN	3.3
1	В	416	THR	3.2
1	A	344	SER	2.8
1	В	454	HIS	2.4
1	В	477	ASN	2.1

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.

