



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 04:25 pm BST

PDB ID : 8S6O  
Title : Structure of MLLE3 in complex with PAMPL2  
Authors : Devan, S.; Shanmugasundaram, S.; Muentjes, K.; Smits, S.H.; Altegoer, F.;  
Feldbruegge, M.  
Deposited on : 2024-02-28  
Resolution : 2.40 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

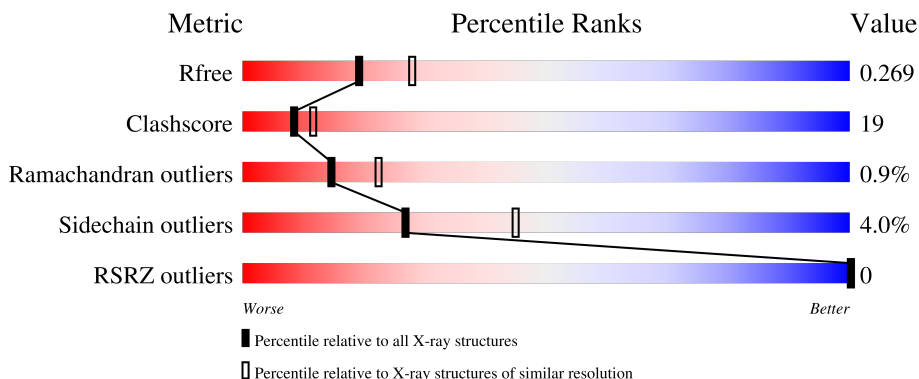
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.








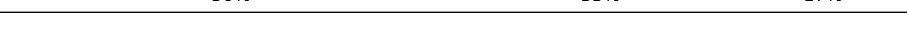
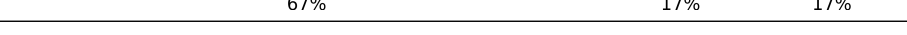
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	133	
1	C	133	
1	D	133	
1	F	133	
1	I	133	

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Mol	Chain	Length	Quality of chain
1	K	133	 62% 22% 14%
1	M	133	 56% 26% 14%
1	O	133	 66% 15% 14%
2	B	6	 83% 17%
2	E	6	 50% 50%
2	G	6	 67% 33%
2	H	6	 50% 33% 17%
2	J	6	 50% 33% 17%
2	L	6	 67% 33%
2	N	6	 67% 17% 17%
2	P	6	 67% 17% 17%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15073 atoms, of which 7616 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 RNA-binding protein RRM4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	D	115	1781	551	908	156	165	1	0	0	0
1	A	115	1781	551	908	156	165	1	0	0	0
1	C	115	1781	551	908	156	165	1	0	0	0
1	F	115	1781	551	908	156	165	1	0	0	0
1	I	115	1781	551	908	156	165	1	0	0	0
1	K	115	1781	551	908	156	165	1	0	0	0
1	M	115	1781	551	908	156	165	1	0	0	0
1	O	115	1781	551	908	156	165	1	0	0	0

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	HIS	-	expression tag	UNP A0A0D1DWZ5
D	118	VAL	-	expression tag	UNP A0A0D1DWZ5
D	119	LYS	-	expression tag	UNP A0A0D1DWZ5
D	120	GLY	-	expression tag	UNP A0A0D1DWZ5
D	121	ALA	-	expression tag	UNP A0A0D1DWZ5
D	122	PRO	-	expression tag	UNP A0A0D1DWZ5
D	123	LYS	-	expression tag	UNP A0A0D1DWZ5
D	124	LEU	-	expression tag	UNP A0A0D1DWZ5
D	125	THR	-	expression tag	UNP A0A0D1DWZ5
D	126	ILE	-	expression tag	UNP A0A0D1DWZ5
D	127	HIS	-	expression tag	UNP A0A0D1DWZ5
D	128	LEU	-	expression tag	UNP A0A0D1DWZ5
D	129	LEU	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	130	ASP	-	expression tag	UNP A0A0D1DWZ5
D	131	SER	-	expression tag	UNP A0A0D1DWZ5
D	132	GLU	-	expression tag	UNP A0A0D1DWZ5
D	133	ASP	-	expression tag	UNP A0A0D1DWZ5
D	134	LEU	-	expression tag	UNP A0A0D1DWZ5
D	135	ARG	-	expression tag	UNP A0A0D1DWZ5
A	3	HIS	-	expression tag	UNP A0A0D1DWZ5
A	118	VAL	-	expression tag	UNP A0A0D1DWZ5
A	119	LYS	-	expression tag	UNP A0A0D1DWZ5
A	120	GLY	-	expression tag	UNP A0A0D1DWZ5
A	121	ALA	-	expression tag	UNP A0A0D1DWZ5
A	122	PRO	-	expression tag	UNP A0A0D1DWZ5
A	123	LYS	-	expression tag	UNP A0A0D1DWZ5
A	124	LEU	-	expression tag	UNP A0A0D1DWZ5
A	125	THR	-	expression tag	UNP A0A0D1DWZ5
A	126	ILE	-	expression tag	UNP A0A0D1DWZ5
A	127	HIS	-	expression tag	UNP A0A0D1DWZ5
A	128	LEU	-	expression tag	UNP A0A0D1DWZ5
A	129	LEU	-	expression tag	UNP A0A0D1DWZ5
A	130	ASP	-	expression tag	UNP A0A0D1DWZ5
A	131	SER	-	expression tag	UNP A0A0D1DWZ5
A	132	GLU	-	expression tag	UNP A0A0D1DWZ5
A	133	ASP	-	expression tag	UNP A0A0D1DWZ5
A	134	LEU	-	expression tag	UNP A0A0D1DWZ5
A	135	ARG	-	expression tag	UNP A0A0D1DWZ5
C	3	HIS	-	expression tag	UNP A0A0D1DWZ5
C	118	VAL	-	expression tag	UNP A0A0D1DWZ5
C	119	LYS	-	expression tag	UNP A0A0D1DWZ5
C	120	GLY	-	expression tag	UNP A0A0D1DWZ5
C	121	ALA	-	expression tag	UNP A0A0D1DWZ5
C	122	PRO	-	expression tag	UNP A0A0D1DWZ5
C	123	LYS	-	expression tag	UNP A0A0D1DWZ5
C	124	LEU	-	expression tag	UNP A0A0D1DWZ5
C	125	THR	-	expression tag	UNP A0A0D1DWZ5
C	126	ILE	-	expression tag	UNP A0A0D1DWZ5
C	127	HIS	-	expression tag	UNP A0A0D1DWZ5
C	128	LEU	-	expression tag	UNP A0A0D1DWZ5
C	129	LEU	-	expression tag	UNP A0A0D1DWZ5
C	130	ASP	-	expression tag	UNP A0A0D1DWZ5
C	131	SER	-	expression tag	UNP A0A0D1DWZ5
C	132	GLU	-	expression tag	UNP A0A0D1DWZ5
C	133	ASP	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	134	LEU	-	expression tag	UNP A0A0D1DWZ5
C	135	ARG	-	expression tag	UNP A0A0D1DWZ5
F	3	HIS	-	expression tag	UNP A0A0D1DWZ5
F	118	VAL	-	expression tag	UNP A0A0D1DWZ5
F	119	LYS	-	expression tag	UNP A0A0D1DWZ5
F	120	GLY	-	expression tag	UNP A0A0D1DWZ5
F	121	ALA	-	expression tag	UNP A0A0D1DWZ5
F	122	PRO	-	expression tag	UNP A0A0D1DWZ5
F	123	LYS	-	expression tag	UNP A0A0D1DWZ5
F	124	LEU	-	expression tag	UNP A0A0D1DWZ5
F	125	THR	-	expression tag	UNP A0A0D1DWZ5
F	126	ILE	-	expression tag	UNP A0A0D1DWZ5
F	127	HIS	-	expression tag	UNP A0A0D1DWZ5
F	128	LEU	-	expression tag	UNP A0A0D1DWZ5
F	129	LEU	-	expression tag	UNP A0A0D1DWZ5
F	130	ASP	-	expression tag	UNP A0A0D1DWZ5
F	131	SER	-	expression tag	UNP A0A0D1DWZ5
F	132	GLU	-	expression tag	UNP A0A0D1DWZ5
F	133	ASP	-	expression tag	UNP A0A0D1DWZ5
F	134	LEU	-	expression tag	UNP A0A0D1DWZ5
F	135	ARG	-	expression tag	UNP A0A0D1DWZ5
I	3	HIS	-	expression tag	UNP A0A0D1DWZ5
I	118	VAL	-	expression tag	UNP A0A0D1DWZ5
I	119	LYS	-	expression tag	UNP A0A0D1DWZ5
I	120	GLY	-	expression tag	UNP A0A0D1DWZ5
I	121	ALA	-	expression tag	UNP A0A0D1DWZ5
I	122	PRO	-	expression tag	UNP A0A0D1DWZ5
I	123	LYS	-	expression tag	UNP A0A0D1DWZ5
I	124	LEU	-	expression tag	UNP A0A0D1DWZ5
I	125	THR	-	expression tag	UNP A0A0D1DWZ5
I	126	ILE	-	expression tag	UNP A0A0D1DWZ5
I	127	HIS	-	expression tag	UNP A0A0D1DWZ5
I	128	LEU	-	expression tag	UNP A0A0D1DWZ5
I	129	LEU	-	expression tag	UNP A0A0D1DWZ5
I	130	ASP	-	expression tag	UNP A0A0D1DWZ5
I	131	SER	-	expression tag	UNP A0A0D1DWZ5
I	132	GLU	-	expression tag	UNP A0A0D1DWZ5
I	133	ASP	-	expression tag	UNP A0A0D1DWZ5
I	134	LEU	-	expression tag	UNP A0A0D1DWZ5
I	135	ARG	-	expression tag	UNP A0A0D1DWZ5
K	3	HIS	-	expression tag	UNP A0A0D1DWZ5
K	118	VAL	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	119	LYS	-	expression tag	UNP A0A0D1DWZ5
K	120	GLY	-	expression tag	UNP A0A0D1DWZ5
K	121	ALA	-	expression tag	UNP A0A0D1DWZ5
K	122	PRO	-	expression tag	UNP A0A0D1DWZ5
K	123	LYS	-	expression tag	UNP A0A0D1DWZ5
K	124	LEU	-	expression tag	UNP A0A0D1DWZ5
K	125	THR	-	expression tag	UNP A0A0D1DWZ5
K	126	ILE	-	expression tag	UNP A0A0D1DWZ5
K	127	HIS	-	expression tag	UNP A0A0D1DWZ5
K	128	LEU	-	expression tag	UNP A0A0D1DWZ5
K	129	LEU	-	expression tag	UNP A0A0D1DWZ5
K	130	ASP	-	expression tag	UNP A0A0D1DWZ5
K	131	SER	-	expression tag	UNP A0A0D1DWZ5
K	132	GLU	-	expression tag	UNP A0A0D1DWZ5
K	133	ASP	-	expression tag	UNP A0A0D1DWZ5
K	134	LEU	-	expression tag	UNP A0A0D1DWZ5
K	135	ARG	-	expression tag	UNP A0A0D1DWZ5
M	3	HIS	-	expression tag	UNP A0A0D1DWZ5
M	118	VAL	-	expression tag	UNP A0A0D1DWZ5
M	119	LYS	-	expression tag	UNP A0A0D1DWZ5
M	120	GLY	-	expression tag	UNP A0A0D1DWZ5
M	121	ALA	-	expression tag	UNP A0A0D1DWZ5
M	122	PRO	-	expression tag	UNP A0A0D1DWZ5
M	123	LYS	-	expression tag	UNP A0A0D1DWZ5
M	124	LEU	-	expression tag	UNP A0A0D1DWZ5
M	125	THR	-	expression tag	UNP A0A0D1DWZ5
M	126	ILE	-	expression tag	UNP A0A0D1DWZ5
M	127	HIS	-	expression tag	UNP A0A0D1DWZ5
M	128	LEU	-	expression tag	UNP A0A0D1DWZ5
M	129	LEU	-	expression tag	UNP A0A0D1DWZ5
M	130	ASP	-	expression tag	UNP A0A0D1DWZ5
M	131	SER	-	expression tag	UNP A0A0D1DWZ5
M	132	GLU	-	expression tag	UNP A0A0D1DWZ5
M	133	ASP	-	expression tag	UNP A0A0D1DWZ5
M	134	LEU	-	expression tag	UNP A0A0D1DWZ5
M	135	ARG	-	expression tag	UNP A0A0D1DWZ5
O	3	HIS	-	expression tag	UNP A0A0D1DWZ5
O	118	VAL	-	expression tag	UNP A0A0D1DWZ5
O	119	LYS	-	expression tag	UNP A0A0D1DWZ5
O	120	GLY	-	expression tag	UNP A0A0D1DWZ5
O	121	ALA	-	expression tag	UNP A0A0D1DWZ5
O	122	PRO	-	expression tag	UNP A0A0D1DWZ5

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Chain	Residue	Modelled	Actual	Comment	Reference
O	123	LYS	-	expression tag	UNP A0A0D1DWZ5
O	124	LEU	-	expression tag	UNP A0A0D1DWZ5
O	125	THR	-	expression tag	UNP A0A0D1DWZ5
O	126	ILE	-	expression tag	UNP A0A0D1DWZ5
O	127	HIS	-	expression tag	UNP A0A0D1DWZ5
O	128	LEU	-	expression tag	UNP A0A0D1DWZ5
O	129	LEU	-	expression tag	UNP A0A0D1DWZ5
O	130	ASP	-	expression tag	UNP A0A0D1DWZ5
O	131	SER	-	expression tag	UNP A0A0D1DWZ5
O	132	GLU	-	expression tag	UNP A0A0D1DWZ5
O	133	ASP	-	expression tag	UNP A0A0D1DWZ5
O	134	LEU	-	expression tag	UNP A0A0D1DWZ5
O	135	ARG	-	expression tag	UNP A0A0D1DWZ5

- Molecule 2 is a protein called PAMPL2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	H	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	B	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	E	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	G	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	J	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	L	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	N	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			
2	P	6	Total	C	H	N	O	0	0	0
			99	38	44	6	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	5	Total	O	0	0
			5	5		
3	A	4	Total	O	0	0
			4	4		
3	C	4	Total	O	0	0
			4	4		

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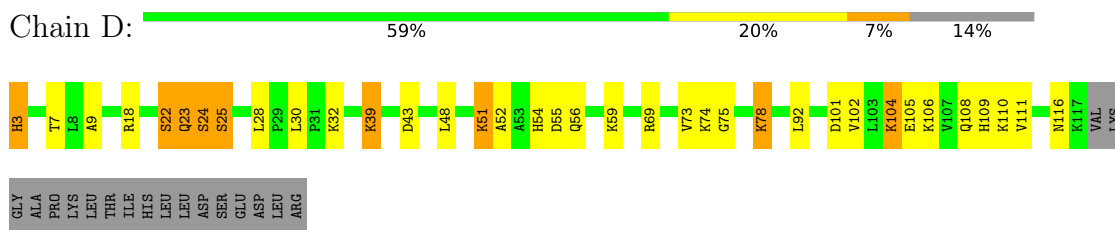
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	F	4	Total O 4 4	0	0
3	G	1	Total O 1 1	0	0
3	I	6	Total O 6 6	0	0
3	J	1	Total O 1 1	0	0
3	K	5	Total O 5 5	0	0
3	M	2	Total O 2 2	0	0
3	P	1	Total O 1 1	0	0

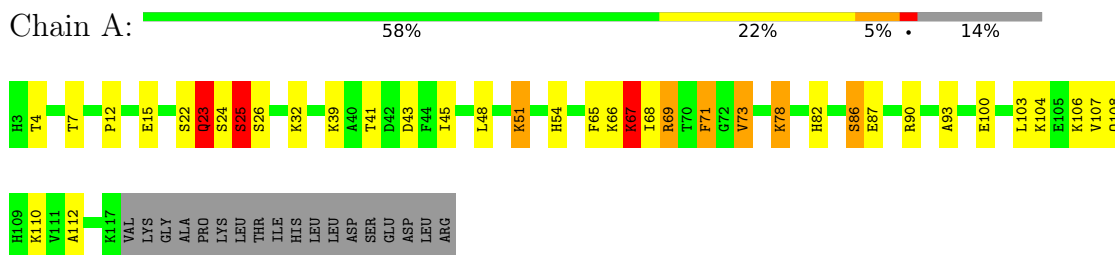
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

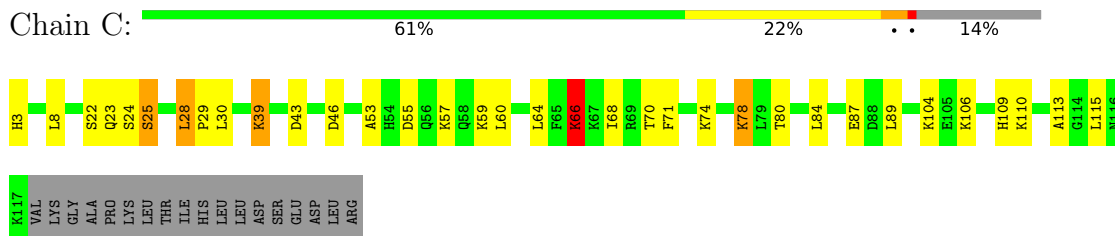
- Molecule 1: RNA-binding protein RRM4



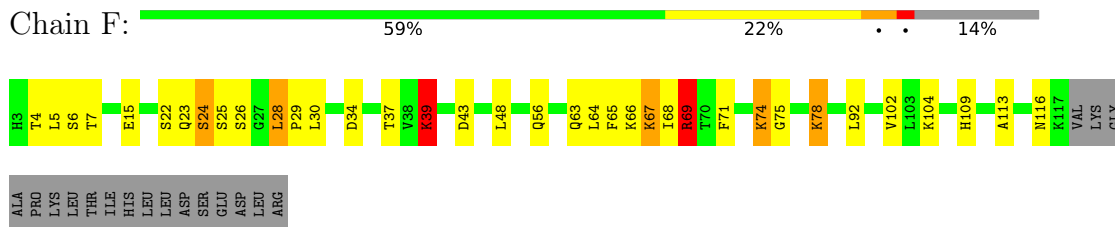
- Molecule 1: RNA-binding protein RRM4



- Molecule 1: RNA-binding protein RRM4

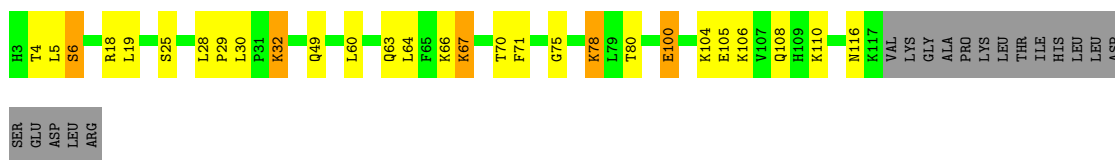


- Molecule 1: RNA-binding protein RRM4



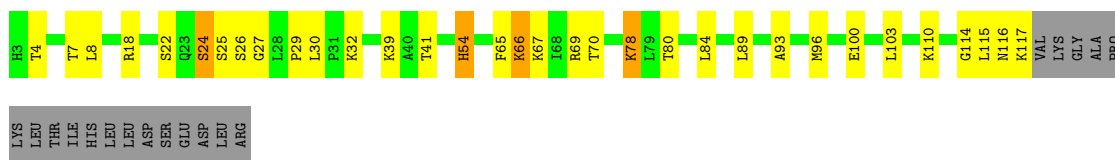
- Molecule 1: RNA-binding protein RRM4

Chain I:  65% 17% 14%



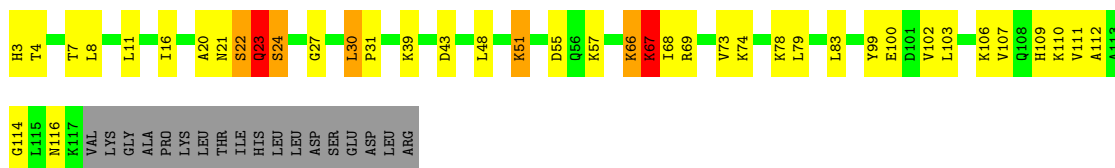
- Molecule 1: RNA-binding protein RRM4

Chain K:  62% 22% 14%



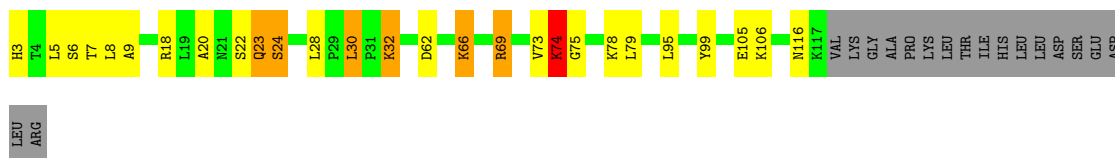
- Molecule 1: RNA-binding protein RRM4

Chain M:  56% 26% 14%



- Molecule 1: RNA-binding protein RRM4

Chain O:  66% 15% 5% 14%




- Molecule 2: PAMPL2

Chain H:  50% 33% 17%



- Molecule 2: PAMPL2

Chain B:  83% 17%



- Molecule 2: PAMPL2



- Molecule 2: PAMPL2



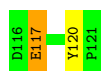
- Molecule 2: PAMPL2



- Molecule 2: PAMPL2



- Molecule 2: PAMPL2



- Molecule 2: PAMPL2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.88Å 74.63Å 168.51Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	56.17 – 2.40 56.17 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (56.17-2.40) 81.2 (56.17-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.21 (at 1.64Å)	Xtrriage
Refinement program	PHENIX 1.17	Depositor
R, $R_{free}$	0.240 , 0.276 0.230 , 0.269	Depositor DCC
$R_{free}$ test set	32173 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtrriage
Anisotropy	0.388	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.318 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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	1.26	9/886 (1.0%)	1.13	8/1195 (0.7%)
1	C	1.03	8/886 (0.9%)	1.09	10/1195 (0.8%)
1	D	1.11	7/886 (0.8%)	1.01	4/1195 (0.3%)
1	F	0.96	5/886 (0.6%)	1.26	8/1195 (0.7%)
1	I	0.96	3/886 (0.3%)	0.99	4/1195 (0.3%)
1	K	1.01	8/886 (0.9%)	1.11	8/1195 (0.7%)
1	M	0.97	6/886 (0.7%)	1.34	15/1195 (1.3%)
1	O	1.12	5/886 (0.6%)	1.44	14/1195 (1.2%)
2	B	1.11	0/57	1.45	1/77 (1.3%)
2	E	1.69	2/57 (3.5%)	1.24	0/77
2	G	1.29	0/57	1.14	0/77
2	H	2.11	3/57 (5.3%)	1.23	0/77
2	J	0.87	0/57	1.43	1/77 (1.3%)
2	L	1.12	0/57	1.44	0/77
2	N	2.11	2/57 (3.5%)	1.87	4/77 (5.2%)
2	P	0.90	0/57	0.91	0/77
All	All	1.09	58/7544 (0.8%)	1.19	77/10176 (0.8%)

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	LYS	CD-CE	18.68	1.98	1.51
1	O	74	LYS	CD-CE	14.35	1.87	1.51
1	A	51	LYS	CE-NZ	13.99	1.84	1.49
1	I	32	LYS	CD-CE	13.61	1.85	1.51
1	O	74	LYS	CE-NZ	12.12	1.79	1.49

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	5	LEU	CB-CG-CD2	18.38	142.25	111.00
1	F	69	ARG	NE-CZ-NH1	17.60	129.10	120.30
1	F	69	ARG	NE-CZ-NH2	-17.14	111.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	5	LEU	CB-CG-CD1	-15.88	84.00	111.00
1	O	30	LEU	CA-CB-CG	14.69	149.08	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	873	908	908	44	2
1	C	873	908	908	37	0
1	D	873	908	908	31	2
1	F	873	908	908	45	1
1	I	873	908	908	23	0
1	K	873	908	908	25	0
1	M	873	908	908	38	0
1	O	873	908	908	34	0
2	B	55	44	45	3	0
2	E	55	44	45	1	0
2	G	55	44	45	2	0
2	H	55	44	45	3	0
2	J	55	44	45	4	0
2	L	55	44	45	4	0
2	N	55	44	45	2	1
2	P	55	44	45	1	0
3	A	4	0	0	1	0
3	C	4	0	0	0	0
3	D	5	0	0	0	0
3	F	4	0	0	2	0
3	G	1	0	0	0	0
3	I	6	0	0	2	0
3	J	1	0	0	0	0
3	K	5	0	0	0	0
3	M	2	0	0	0	0
3	P	1	0	0	1	0
All	All	7457	7616	7624	281	3

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 19.

The worst 5 of 281 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:C:39:LYS:CD	1:C:39:LYS:CG	1.76	1.60
1:C:78:LYS:CE	1:C:78:LYS:CD	1.74	1.58
1:C:66:LYS:CE	1:C:66:LYS:CD	1.79	1.57
1:K:78:LYS:CD	1:K:78:LYS:CG	1.81	1.56
1:D:78:LYS:CD	1:D:78:LYS:CE	1.80	1.56

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ASP:OD2	1:A:32:LYS:NZ[4_455]	1.82	0.38
1:F:23:GLN:OE1	2:N:117:GLU:OE1[4_456]	1.88	0.32
1:D:101:ASP:OD2	1:A:32:LYS:HZ2[4_455]	1.58	0.02

## 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	113/133 (85%)	110 (97%)	2 (2%)	1 (1%)	14	22
1	C	113/133 (85%)	109 (96%)	3 (3%)	1 (1%)	14	22
1	D	113/133 (85%)	107 (95%)	4 (4%)	2 (2%)	7	9
1	F	113/133 (85%)	110 (97%)	2 (2%)	1 (1%)	14	22
1	I	113/133 (85%)	111 (98%)	2 (2%)	0	100	100
1	K	113/133 (85%)	109 (96%)	4 (4%)	0	100	100
1	M	113/133 (85%)	108 (96%)	4 (4%)	1 (1%)	14	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	113/133 (85%)	109 (96%)	2 (2%)	2 (2%)	7	9
2	B	4/6 (67%)	4 (100%)	0	0	100	100
2	E	4/6 (67%)	4 (100%)	0	0	100	100
2	G	4/6 (67%)	4 (100%)	0	0	100	100
2	H	4/6 (67%)	4 (100%)	0	0	100	100
2	J	4/6 (67%)	4 (100%)	0	0	100	100
2	L	4/6 (67%)	4 (100%)	0	0	100	100
2	N	4/6 (67%)	4 (100%)	0	0	100	100
2	P	4/6 (67%)	4 (100%)	0	0	100	100
All	All	936/1112 (84%)	905 (97%)	23 (2%)	8 (1%)	14	22

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	F	24	SER
1	M	23	GLN
1	C	24	SER
1	O	24	SER

### 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	94/110 (86%)	90 (96%)	4 (4%)	25	42
1	C	94/110 (86%)	92 (98%)	2 (2%)	48	69
1	D	94/110 (86%)	90 (96%)	4 (4%)	25	42
1	F	94/110 (86%)	86 (92%)	8 (8%)	8	14
1	I	94/110 (86%)	91 (97%)	3 (3%)	34	54
1	K	94/110 (86%)	93 (99%)	1 (1%)	70	84
1	M	94/110 (86%)	92 (98%)	2 (2%)	48	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	94/110 (86%)	91 (97%)	3 (3%)	34	54
2	B	6/6 (100%)	6 (100%)	0	100	100
2	E	6/6 (100%)	6 (100%)	0	100	100
2	G	6/6 (100%)	5 (83%)	1 (17%)	2	2
2	H	6/6 (100%)	5 (83%)	1 (17%)	2	2
2	J	6/6 (100%)	5 (83%)	1 (17%)	2	2
2	L	6/6 (100%)	6 (100%)	0	100	100
2	N	6/6 (100%)	6 (100%)	0	100	100
2	P	6/6 (100%)	4 (67%)	2 (33%)	0	0
All	All	800/928 (86%)	768 (96%)	32 (4%)	27	45

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	69	ARG
1	O	74	LYS
1	F	6	SER
1	F	5	LEU
2	P	116	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	54	HIS
1	M	108	GLN
1	O	23	GLN
1	O	3	HIS
1	I	97	ASN

### 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 oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	115/133 (86%)	-0.75	0 100 100	45, 65, 92, 120	0
1	C	115/133 (86%)	-0.76	0 100 100	57, 69, 109, 125	0
1	D	115/133 (86%)	-0.93	0 100 100	48, 63, 94, 124	0
1	F	115/133 (86%)	-0.80	0 100 100	49, 66, 99, 120	0
1	I	115/133 (86%)	-0.80	0 100 100	48, 66, 96, 125	0
1	K	115/133 (86%)	-0.74	0 100 100	55, 69, 104, 126	0
1	M	115/133 (86%)	-0.73	0 100 100	55, 71, 107, 124	0
1	O	115/133 (86%)	-0.81	0 100 100	49, 70, 103, 127	0
2	B	6/6 (100%)	-0.53	0 100 100	74, 82, 95, 96	0
2	E	6/6 (100%)	-0.72	0 100 100	66, 71, 97, 101	0
2	G	6/6 (100%)	-0.75	0 100 100	59, 67, 85, 96	0
2	H	6/6 (100%)	-0.73	0 100 100	68, 75, 89, 94	0
2	J	6/6 (100%)	-0.34	0 100 100	67, 77, 96, 96	0
2	L	6/6 (100%)	-0.79	0 100 100	64, 79, 95, 98	0
2	N	6/6 (100%)	-0.59	0 100 100	73, 77, 102, 107	0
2	P	6/6 (100%)	-0.44	0 100 100	75, 81, 93, 107	0
All	All	968/1112 (87%)	-0.78	0 100 100	45, 68, 103, 127	0

There are no RSRZ outliers to report.

### 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 monosaccharides 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.