



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 01:35 AM EDT

PDB ID : 5TKZ  
Title : MEC-8 N-terminal RRM bound to tandem GCAC ligand  
Authors : Soufari, H.; Mackereth, C.D.  
Deposited on : 2016-10-10  
Resolution : 1.53 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](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	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

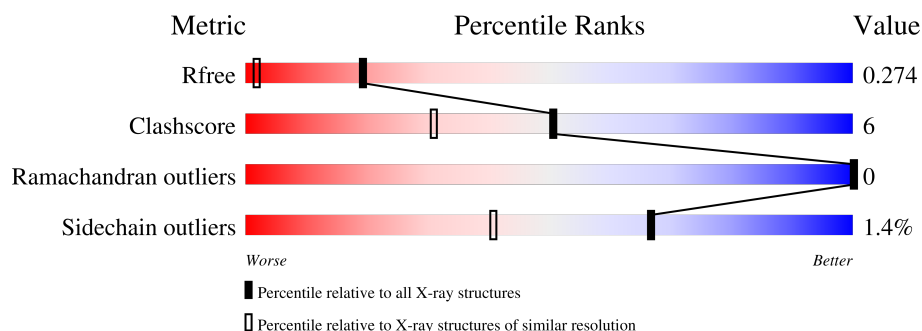
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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))
$R_{free}$	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)

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 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	94	
1	B	94	
2	C	20	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1740 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 Mec-8 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	1	0
			703	446	126	128	3			
1	B	89	Total	C	N	O	S	0	1	0
			697	442	125	128	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP Q22039
A	25	ALA	-	expression tag	UNP Q22039
A	26	MET	-	expression tag	UNP Q22039
A	27	ALA	-	expression tag	UNP Q22039
A	54	ALA	CYS	engineered mutation	UNP Q22039
A	102	ALA	CYS	engineered mutation	UNP Q22039
B	24	GLY	-	expression tag	UNP Q22039
B	25	ALA	-	expression tag	UNP Q22039
B	26	MET	-	expression tag	UNP Q22039
B	27	ALA	-	expression tag	UNP Q22039
B	54	ALA	CYS	engineered mutation	UNP Q22039
B	102	ALA	CYS	engineered mutation	UNP Q22039

- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*GP\*CP\*AP\*CP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*GP\*CP\*AP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	P	0	0	0
			206	96	42	58	10			


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	0	0
3	B	56	Total 56	O 56	0	0
3	C	10	Total 10	O 10	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. 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. 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.

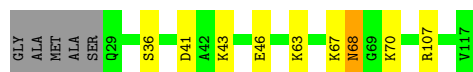
- Molecule 1: Mec-8 protein

Chain A: 

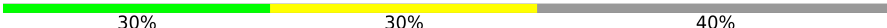


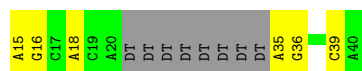
- Molecule 1: Mec-8 protein

Chain B: 



- Molecule 2: DNA (5'-D(\*AP\*GP\*CP\*AP\*CP\*AP\*TP\*TP\*TP\*TP\*TP\*TP\*TP\*AP\*GP\*CP\*AP\*CP\*A)-3')

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.19Å 52.19Å 156.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.74 – 1.53 25.74 – 1.53	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.74-1.53) 99.4 (25.74-1.53)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.53Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.233 , 0.271 0.234 , 0.274	Depositor DCC
$R_{free}$ test set	2009 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , -10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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

### 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	0.50	0/714	0.60	0/959
1	B	0.43	0/708	0.63	0/953
2	C	0.87	0/230	0.93	0/352
All	All	0.54	0/1652	0.67	0/2264

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	703	0	727	10	0
1	B	697	0	711	6	0
2	C	206	0	112	8	0
3	A	68	0	0	3	0
3	B	56	0	0	0	0
3	C	10	0	0	1	0
All	All	1740	0	1550	18	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 6.

All (18) 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)
2:C:35:DA:N7	3:C:101:HOH:O	2.17	0.77
1:A:67:LYS:O	3:A:201:HOH:O	2.13	0.66
1:A:104:GLN:OE1	3:A:203:HOH:O	2.14	0.66
1:A:107:ARG:NH2	2:C:36:DG:N7	2.46	0.64
1:B:63:LYS:HE3	2:C:18:DA:N3	2.19	0.57
2:C:15:DA:H2'	2:C:16:DG:C8	2.41	0.56
1:B:36:SER:OG	1:B:107:ARG:HG3	2.05	0.55
1:A:116:LYS:HD2	2:C:39:DC:C4	2.45	0.52
1:A:116:LYS:HG2	2:C:39:DC:C2	2.46	0.50
1:A:37:GLY:HA2	1:A:104:GLN:NE2	2.29	0.47
1:B:68:ASN:N	1:B:68:ASN:HD22	2.13	0.46
1:B:41:ASP:O	1:B:43:LYS:NZ	2.44	0.45
1:A:46:GLU:HG2	1:B:46:GLU:HG2	1.99	0.44
1:A:55:ARG:NE	3:A:204:HOH:O	2.31	0.43
1:A:70:LYS:HA	1:A:71:PRO:HD3	1.90	0.43
1:A:116:LYS:HG2	2:C:39:DC:N3	2.34	0.42
2:C:35:DA:H2''	2:C:36:DG:C8	2.55	0.42
1:B:67:LYS:O	1:B:70:LYS:HG3	2.20	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	88/94 (94%)	87 (99%)	1 (1%)	0	100	100
1	B	88/94 (94%)	88 (100%)	0	0	100	100
All	All	176/188 (94%)	175 (99%)	1 (1%)	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	Percentiles	
1	A	75/76 (99%)	74 (99%)	1 (1%)	69	43
1	B	73/76 (96%)	72 (99%)	1 (1%)	67	41
All	All	148/152 (97%)	146 (99%)	2 (1%)	67	41

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	B	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	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 monosaccharides 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

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.