



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 01:18 PM EDT

PDB ID : 6EXD  
Title : Crystal structure of DotM cytoplasmic domain (residues 153-380) SeMet derivative  
Authors : Meir, A.; Waksman, G.  
Deposited on : 2017-11-07  
Resolution : 2.14 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

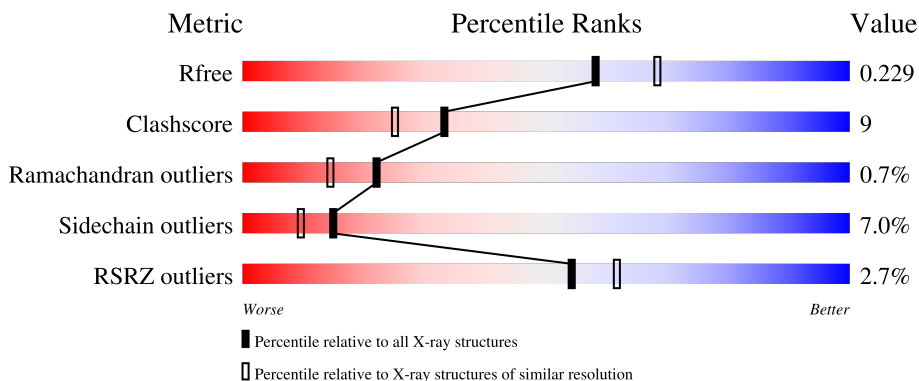
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	235	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	235	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>5%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3647 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 IcmP (DotM).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	Se	0	2	0
			1746	1111	311	311	2	11			
1	B	220	Total	C	N	O	S	Se	0	0	0
			1770	1127	312	318	2	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	GLY	-	expression tag	UNP Q5ZYC7
A	147	PRO	-	expression tag	UNP Q5ZYC7
A	148	SER	-	expression tag	UNP Q5ZYC7
A	149	GLY	-	expression tag	UNP Q5ZYC7
A	150	GLY	-	expression tag	UNP Q5ZYC7
A	151	GLY	-	expression tag	UNP Q5ZYC7
A	152	ALA	-	expression tag	UNP Q5ZYC7
B	146	GLY	-	expression tag	UNP Q5ZYC7
B	147	PRO	-	expression tag	UNP Q5ZYC7
B	148	SER	-	expression tag	UNP Q5ZYC7
B	149	GLY	-	expression tag	UNP Q5ZYC7
B	150	GLY	-	expression tag	UNP Q5ZYC7
B	151	GLY	-	expression tag	UNP Q5ZYC7
B	152	ALA	-	expression tag	UNP Q5ZYC7

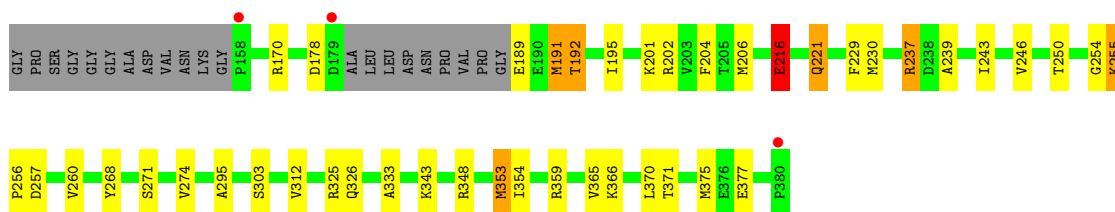
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	58	Total	O	0	0
			58	58		

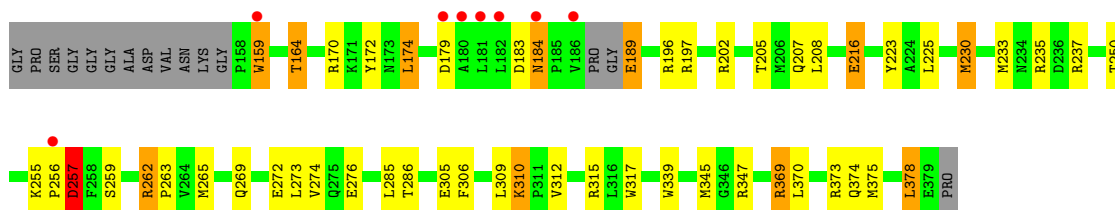
### 3 Residue-property plots [i](#)

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: IcmP (DotM)



#### • Molecule 1: IcmP (DotM)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.00Å 118.00Å 66.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 2.14 44.10 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.01-2.14) 99.6 (44.10-2.14)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.191 , 0.227 0.193 , 0.229	Depositor DCC
$R_{free}$ test set	1469 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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	0.91	1/1773 (0.1%)	1.09	7/2374 (0.3%)
1	B	0.94	2/1797 (0.1%)	1.05	8/2410 (0.3%)
All	All	0.92	3/3570 (0.1%)	1.07	15/4784 (0.3%)

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
1	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CB-CG	5.47	1.62	1.52
1	B	216	GLU	CD-OE1	-5.43	1.19	1.25
1	B	216	GLU	CB-CG	5.02	1.61	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	MSE	CG-SE-CE	11.61	124.44	98.90
1	A	237	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	202	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	197	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	257	ASP	CB-CG-OD1	6.56	124.21	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	GLY	Peptide
1	B	256	PRO	Peptide

## 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	1746	0	1760	35	1
1	B	1770	0	1782	27	1
2	A	73	0	0	7	0
2	B	58	0	0	2	0
All	All	3647	0	3542	61	1

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 9.

The worst 5 of 61 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:246:VAL:O	1:A:250:THR:HG22	1.71	0.91
1:A:370:LEU:HD12	1:A:375:MSE:HE2	1.62	0.80
1:A:370:LEU:HB2	1:A:375:MSE:HE2	1.63	0.80
1:A:326:GLN:HB3	2:A:466:HOH:O	1.82	0.77
1:A:216:GLU:HG3	2:A:422:HOH:O	1.87	0.75

All (1) 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:A:189:GLU:OE2	1:B:202:ARG:CZ[4_674]	2.15	0.05

## 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	212/235 (90%)	202 (95%)	8 (4%)	2 (1%)	17	10
1	B	216/235 (92%)	205 (95%)	10 (5%)	1 (0%)	29	22
All	All	428/470 (91%)	407 (95%)	18 (4%)	3 (1%)	22	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	ASN
1	A	303	SER
1	A	377	GLU

### 5.3.2 Protein sidechains

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	184/184 (100%)	174 (95%)	10 (5%)	22	17
1	B	187/184 (102%)	170 (91%)	17 (9%)	9	5
All	All	371/368 (101%)	344 (93%)	27 (7%)	15	8

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	179	ASP
1	B	230	MSE
1	B	312	VAL

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Mol	Chain	Res	Type
1	B	216	GLU
1	B	257	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	269	GLN
1	B	321	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 [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	203/235 (86%)	-0.14	3 (1%) 73 78	8, 26, 55, 89	0
1	B	209/235 (88%)	-0.07	8 (3%) 40 48	10, 28, 67, 100	0
All	All	412/470 (87%)	-0.10	11 (2%) 54 61	8, 27, 64, 100	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	TRP	4.6
1	B	181	LEU	4.4
1	B	179	ASP	4.0
1	B	186	VAL	3.6
1	A	179	ASP	3.4

### 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 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.