

# wwPDB X-ray Structure Validation Summary Report (i)

#### Feb 4, 2024 – 03:20 PM EST

PDB ID	:	1RJF
Title	:	Structure of PPM1, a leucine carboxy methyltransferase involved in the regu-
		lation of protein phosphatase 2A activity
Authors	:	Leulliot, N.; Quevillon-Cheruel, S.; Sorel, I.; de La Sierra-Gallay, I.L.; Collinet,
		B.; Graille, M.; Blondeau, K.; Bettache, N.; Poupon, A.; Janin, J.; van
		Tilbeurgh, H.
Deposited on	:	2003-11-19
Resolution	:	2.25  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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

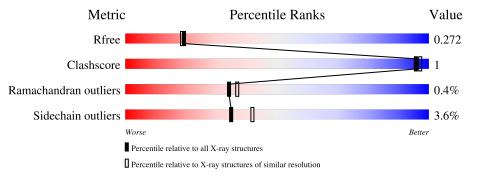
MolProbity		4 02b-467
5		
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.25 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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 >=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%

Mol	Chain	Length	Quality of chain		
1	А	334	90%	6%	·
1	В	334	92%	6%	·
1	С	334	89%	8%	••



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8150 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 carboxy methyl transferase for protein phosphatase 2A catalytic subunit.

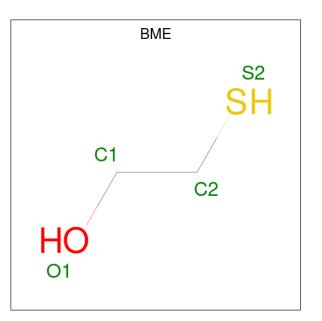
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	321	Total	С	Ν	0	S	0	0	0
	А	521	2583	1644	439	482	18	0		0
1	В	327	Total	С	Ν	0	S	0	1	0
	D	321	2640	1679	449	494	18	0	1	0
1	С	295	Total	С	Ν	0	S	0	0	0
	I C	C 325	2619	1665	448	488	18	U	U	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	329	HIS	-	expression tag	UNP Q04081
А	330	HIS	-	expression tag	UNP Q04081
А	331	HIS	-	expression tag	UNP Q04081
A	332	HIS	-	expression tag	UNP Q04081
A	333	HIS	-	expression tag	UNP Q04081
А	334	HIS	-	expression tag	UNP Q04081
В	329	HIS	-	expression tag	UNP Q04081
В	330	HIS	-	expression tag	UNP Q04081
В	331	HIS	-	expression tag	UNP Q04081
В	332	HIS	-	expression tag	UNP Q04081
В	333	HIS	-	expression tag	UNP Q04081
В	334	HIS	-	expression tag	UNP Q04081
С	329	HIS	-	expression tag	UNP Q04081
С	330	HIS	-	expression tag	UNP Q04081
С	331	HIS	-	expression tag	UNP Q04081
С	332	HIS	-	expression tag	UNP Q04081
С	333	HIS	-	expression tag	UNP Q04081
С	334	HIS	-	expression tag	UNP Q04081

• Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).

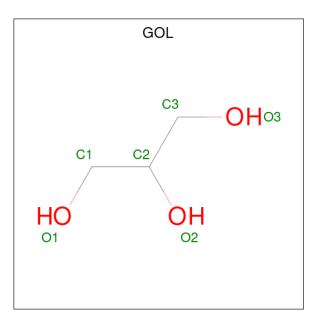




Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{O} & \text{S} \\ 4 & 2 & 1 & 1 \end{array}$	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	119	Total O 119 119	0	0
4	В	103	Total O 103 103	0	0
4	С	50	$\begin{array}{cc} \text{Total} & \text{O} \\ 50 & 50 \end{array}$	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: carboxy methyl transferase for protein phosphatase 2A catalytic subunit

Chain A:	90%	6% •
MET ARC ARC ARC ARC ARC CLN GLN GLN CLN GLN D11 D11 D11 D64 C B64 C B64 C B64 C B64 C B64 C B64 C B64 C B64 C B70 C B70 C B70 C B70 A A A A A A A A A A A A A A A A A A A	R111 M112 M112 8165 8166 P161 6201 E201 R242 R242 R242	L251 L255 L255 L255 L255 H15 H15 H15 H15 H15 H15 H15
• Molecule 1: carboxy methy	'l transferase for prote	ein phosphatase 2A catalytic subunit
Chain B:	92%	6% ·
MET GLU GLU ARC D9 D9 R46 R46 R46 R46 R46 B64 D64 D64 D64 V101	M112 0117 1122 1122 1156 1156 1156 1156 1156 1156 1156 1156 1156 1156 1156 1156 1157 1161 1172	1251 1251 1285 1309 HIS HIS HIS HIS
• Molecule 1: carboxy methy	'l transferase for prote	ein phosphatase 2A catalytic subunit
Chain C:	89%	8% ••
MET MET GLU GLU GLU TLE G TB D11 D11 M68 F40 F40 F40 F64	V73 D86 M12 M12 M147 K154 E155 D156 K159	8160 P161 P161 E200 E200
LEEH SIH SIH		



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	112.39Å 112.39Å 162.85Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	30.00 - 2.25	Depositor
Resolution (A)	28.18 - 2.25	EDS
% Data completeness	97.6 (30.00-2.25)	Depositor
(in resolution range)	$97.6\ (28.18-2.25)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.16 (at 2.24 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.1.24$	Depositor
$R, R_{free}$	0.183 , $0.239$	Depositor
II, IIfree	0.258 , $0.272$	DCC
$R_{free}$ test set	2738 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	21.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.36 , $10.0$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.245 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8150	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 4.90% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

# 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BME

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		
MOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.31	1/2633~(0.0%)	0.59	5/3557~(0.1%)	
1	В	0.31	1/2694~(0.0%)	0.60	6/3640~(0.2%)	
1	С	0.31	1/2671~(0.0%)	0.60	9/3609~(0.2%)	
All	All	0.31	3/7998~(0.0%)	0.60	20/10806~(0.2%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	В	201	GLU	CD-OE2	7.57	1.33	1.25
1	А	201	GLU	CD-OE2	7.36	1.33	1.25
1	С	201	GLU	CD-OE2	6.93	1.33	1.25

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	С	11	ASP	CB-CG-OD2	5.29	123.06	118.30
1	С	285	ASP	CB-CG-OD2	5.26	123.04	118.30
1	В	9	ASP	CB-CG-OD2	5.25	123.02	118.30
1	С	9	ASP	CB-CG-OD2	5.20	122.98	118.30
1	В	285	ASP	CB-CG-OD2	5.17	122.95	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2583	0	2608	6	0
1	В	2640	0	2663	7	0
1	С	2619	0	2637	5	0
2	А	8	0	12	0	0
2	В	8	0	12	0	0
2	С	8	0	12	0	0
3	А	12	0	16	0	0
4	А	119	0	0	0	0
4	В	103	0	0	0	0
4	С	50	0	0	0	0
All	All	8150	0	7960	17	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 1.

The worst 5 of 17 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:160:SER:CB	1:A:161:PRO:CD	2.80	0.59
1:C:160:SER:HB2	1:C:161:PRO:CD	2.40	0.52
1:C:160:SER:CB	1:C:161:PRO:CD	2.88	0.51
1:A:160:SER:HB3	1:A:161:PRO:HD3	1.93	0.50
1:A:160:SER:CB	1:A:161:PRO:HD3	2.42	0.49

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	А	319/334~(96%)	304~(95%)	14 (4%)	1 (0%)	41 46

Continued on next page...



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	В	326/334~(98%)	314 (96%)	11 (3%)	1 (0%)	41	46
1	С	323/334~(97%)	308~(95%)	13 (4%)	2(1%)	25	25
All	All	968/1002~(97%)	926 (96%)	38 (4%)	4 (0%)	34	37

Continued from previous page...

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	160	SER
1	С	160	SER
1	С	256	ASN
1	В	160	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	А	290/303~(96%)	280~(97%)	10 (3%)	37	45	
1	В	297/303~(98%)	291~(98%)	6 (2%)	55	64	
1	С	294/303~(97%)	278~(95%)	16 (5%)	22	22	
All	All	881/909~(97%)	849 (96%)	32 (4%)	35	42	

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

Mol	Chain	Res	Type
1	С	247	MET
1	С	255	ARG
1	В	154	LYS
1	В	112	MET
1	С	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:



Mol	Chain	Res	Type
1	В	209	ASN
1	В	210	ASN
1	С	330	HIS
1	С	177	ASN
1	А	209	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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Turne	Chain	Res	Link	B	Bond lengths			Bond angles		
	Type	Ullaili			Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	BME	С	336	-	3,3,3	0.25	0	$1,\!2,\!2$	0.24	0	
2	BME	А	336	-	3,3,3	0.28	0	1,2,2	0.27	0	
2	BME	В	335	-	3,3,3	0.27	0	1,2,2	0.25	0	
2	BME	А	335	-	3,3,3	0.27	0	1,2,2	0.25	0	
2	BME	С	335	-	3,3,3	0.28	0	1,2,2	0.24	0	
3	GOL	А	337	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.24	0	
2	BME	В	336	-	3,3,3	0.29	0	1,2,2	0.12	0	
3	GOL	А	338	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.16	0	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	С	336	-	-	0/1/1/1	-
2	BME	А	336	-	-	0/1/1/1	-
2	BME	В	335	-	-	1/1/1/1	-
2	BME	А	335	-	-	1/1/1/1	-
2	BME	С	335	-	-	0/1/1/1	-
3	GOL	А	337	-	-	2/4/4/4	-
2	BME	В	336	-	-	0/1/1/1	-
3	GOL	А	338	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	335	BME	O1-C1-C2-S2
2	В	335	BME	O1-C1-C2-S2
3	А	337	GOL	O1-C1-C2-C3
3	А	337	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

### 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)

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

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

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

## 6.3 Carbohydrates (i)

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

## 6.4 Ligands (i)

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

### 6.5 Other polymers (i)

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

