



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:47 AM GMT

PDB ID : 2O8A  
Title : rat PP1cgamma complexed with mouse inhibitor-2  
Authors : Hurley, T.D.  
Deposited on : 2006-12-12  
Resolution : 2.61 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

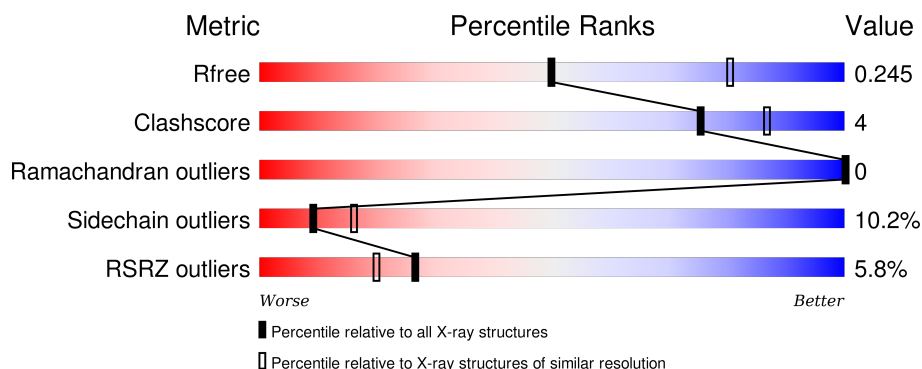
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	329	<div> <div></div> <div>74% 13% • 10%</div> </div>
1	B	329	<div> <div></div> <div>74% 15% • 10%</div> </div>
2	I	206	<div> <div>11%</div> <div>18% 10% 71%</div> </div>
2	J	206	<div> <div>7%</div> <div>20% 8% 72%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5842 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 Serine/threonine-protein phosphatase PP1-gamma catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2380	1527	399	436	18			
1	B	295	Total	C	N	O	S	0	0	0
			2380	1527	399	436	18			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	INITIATING METHIONINE	UNP P63088
A	-4	HIS	-	EXPRESSION TAG	UNP P63088
A	-3	HIS	-	EXPRESSION TAG	UNP P63088
A	-2	HIS	-	EXPRESSION TAG	UNP P63088
A	-1	HIS	-	EXPRESSION TAG	UNP P63088
A	0	HIS	-	EXPRESSION TAG	UNP P63088
A	1	HIS	-	EXPRESSION TAG	UNP P63088
B	-5	MET	-	INITIATING METHIONINE	UNP P63088
B	-4	HIS	-	EXPRESSION TAG	UNP P63088
B	-3	HIS	-	EXPRESSION TAG	UNP P63088
B	-2	HIS	-	EXPRESSION TAG	UNP P63088
B	-1	HIS	-	EXPRESSION TAG	UNP P63088
B	0	HIS	-	EXPRESSION TAG	UNP P63088
B	1	HIS	-	EXPRESSION TAG	UNP P63088

- Molecule 2 is a protein called Protein phosphatase inhibitor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	59	Total	C	N	O	S	0	0	0
			495	309	93	91	2			
2	J	58	Total	C	N	O	S	0	0	0
			487	305	92	88	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	38	Total 38	O 38	0	0
3	I	5	Total 5	O 5	0	0
3	J	10	Total 10	O 10	0	0



HIS  
LYS  
SER  
GLN  
SER  
SER

● Molecule 2: Protein phosphatase inhibitor 2



MET  
ALA  
ALA  
SER  
THR  
ALA  
SER  
HIS  
ARG  
PRO  
ILE  
K12  
K16  
M17  
LYS  
THR  
SER  
ALA  
ALA  
SER  
PRO  
PRO  
VAL  
VAL  
PRO  
SER  
ALA  
GLU  
GLN  
PRO  
ARG  
PRO  
ILE  
VAL  
GLU  
GLU  
GLU  
LEU  
SER  
LYS  
K44  
K47  
M51  
L54  
A55  
T56  
TYR  
HIS  
PRO  
ALA  
ASP  
LYS  
ASP  
TYR  
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MET  
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ASN  
ASP  
L130  
S131  
P132  
E133  
E134  
R135  
E136  
K137  
K138  
R139  
E142  
M143  
K144  
K156  
S163  
K164  
D165  
L166  
H167  
D168  
ASP  
GLU  
ASP  
GLU  
GLU  
MET  
ALA  
GLU  
THR  
ALA  
ASP  
GLY  
ASP  
SER  
MET  
ASN  
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SER  
THR  
THR  
ASP  
HIS  
LEU  
GLN  
HIS  
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SER  
GLN  
SER  
SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.46Å 103.81Å 151.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 2.61 41.69 – 2.61	Depositor EDS
% Data completeness (in resolution range)	95.4 (41.70-2.61) 95.4 (41.69-2.61)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.216 , 0.254 0.208 , 0.245	Depositor DCC
$R_{free}$ test set	2248 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.7	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44466 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/2434	0.76	8/3286 (0.2%)
1	B	0.47	0/2434	0.77	9/3286 (0.3%)
2	I	0.51	0/499	0.71	1/658 (0.2%)
2	J	0.51	0/491	0.75	2/647 (0.3%)
All	All	0.48	0/5858	0.76	20/7877 (0.3%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ASP	CB-CG-OD2	7.43	124.99	118.30
1	B	208	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	138	ASP	CB-CG-OD2	6.28	123.96	118.30
1	B	240	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	138	ASP	CB-CG-OD2	6.03	123.72	118.30

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	2380	0	2351	17	0
1	B	2380	0	2351	16	0
2	I	495	0	507	8	0
2	J	487	0	503	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	47	0	0	1	0
3	B	38	0	0	0	0
3	I	5	0	0	0	0
3	J	10	0	0	2	0
All	All	5842	0	5712	45	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.

The worst 5 of 45 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:J:131:SER:HB3	2:J:134:GLU:HB2	1.73	0.69
1:B:286:ASP:OD1	1:B:290:MET:HB3	1.97	0.65
2:I:131:SER:HB2	2:I:134:GLU:HB2	1.78	0.64
1:A:284:SER:HB2	1:A:294:GLN:HE22	1.61	0.64
2:I:52:ASN:O	2:I:56:THR:HG23	1.99	0.61

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	A	293/329 (89%)	277 (94%)	16 (6%)	0	100	100
1	B	293/329 (89%)	276 (94%)	17 (6%)	0	100	100
2	I	53/206 (26%)	51 (96%)	2 (4%)	0	100	100
2	J	52/206 (25%)	52 (100%)	0	0	100	100
All	All	691/1070 (65%)	656 (95%)	35 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	261/291 (90%)	238 (91%)	23 (9%)	12	23
1	B	261/291 (90%)	242 (93%)	19 (7%)	17	34
2	I	54/181 (30%)	42 (78%)	12 (22%)	1	2
2	J	53/181 (29%)	43 (81%)	10 (19%)	2	2
All	All	629/944 (67%)	565 (90%)	64 (10%)	9	16

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	138	LYS
1	B	6	LYS
2	J	156	LYS
2	I	142	GLU
2	I	166	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	B	99	GLN
1	B	239	HIS
2	J	140	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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<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	295/329 (89%)	-0.21	1 (0%) 94 93	30, 42, 59, 73	0
1	B	295/329 (89%)	-0.34	3 (1%) 84 81	30, 42, 59, 73	0
2	I	59/206 (28%)	1.50	22 (37%) 0 0	36, 62, 82, 85	0
2	J	58/206 (28%)	1.06	15 (25%) 1 0	35, 63, 82, 85	0
All	All	707/1070 (66%)	-0.02	41 (5%) 26 20	30, 44, 71, 85	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	167	HIS	5.8
2	J	168	ASP	5.8
2	I	51	MET	5.8
2	I	167	HIS	5.6
2	I	54	LEU	5.5

### 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 ⓘ

There are no such residues in this entry.