



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2017 – 08:27 AM EDT

PDB ID : 2O8A
Title : rat PP1cgamma complexed with mouse inhibitor-2
Authors : Hurley, T.D.
Deposited on : unknown
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

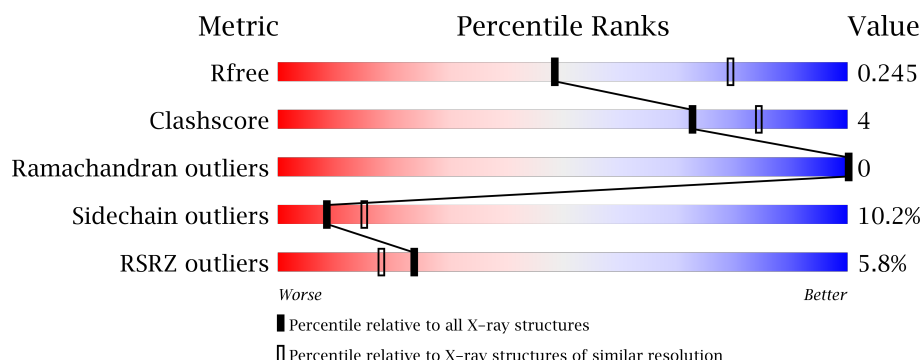
1 Overall quality at a glance

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}	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (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 ≥ 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 10%, orange 10%, orange 20%, yellow 20%, yellow 74%, green 74%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 74% 13% • 10% </div> </div>
1	B	329	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 20%, yellow 20%, yellow 74%, green 74%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 74% 15% • 10% </div> </div>
2	I	206	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 11%, orange 11%, orange 18%, yellow 18%, yellow 10%, green 10%, green 71%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 11% 18% 10% 71% </div> </div>
2	J	206	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 7%, orange 7%, orange 20%, yellow 20%, yellow 8%, green 8%, green 72%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 7% 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	I	5	Total 5	O 5	0	0
3	B	38	Total 38	O 38	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 HIS ILE K12 K16 M17 LYS THR SER ALA ALA SER PRO PRO VAL VAL PRO SER SER ALA GLU GLN PRO ARG PRO PRO ILE VAL VAL GLU GLU GLU LEU SER SER LYS K44 K47 M51 L54 A55 T56 TYR HIS PRO ALA ASP LYS ASP TYR LEU

MET LYS ILE ASP PRO ASN THR PRO TYR HIS ASN MET ILE GLY ASP ASP GLU ASP ALA TYR SER SER PRO SER SER GLY ASN GLU VAL MET THR PRO ASP ILE LEU ALA LYS LYS LEU ALA ALA LYS K44 K47 M51 L54 A55 T56 TYR ARG THR ARG GLN SER GLY LYS

ASP ASN ASP L130 S131 P132 E133 E134 R135 E136 K137 K138 R139 E142 M143 K144 K156 S163 K164 D165 L166 H167 D168 ASP ASP GLU ASP GLU MET ALA THR ALA ASP GLY ASP SER MET ASN VAL GLU SER GLN GLY SER THR THR ASP HIS LEU HIS LYS

SER
GLN
SER
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.61Å)	Xtriage
Refinement program	REFMAC	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 ²)	45.7	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5842	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.47	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
1:A:284:SER:HB2	1:A:294:GLN:HE22	1.61	0.64
2:I:131:SER:HB2	2:I:134:GLU:HB2	1.78	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 [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	261/291 (90%)	238 (91%)	23 (9%)	12	21
1	B	261/291 (90%)	242 (93%)	19 (7%)	16	32
2	I	54/181 (30%)	42 (78%)	12 (22%)	1	1
2	J	53/181 (29%)	43 (81%)	10 (19%)	2	2
All	All	629/944 (67%)	565 (90%)	64 (10%)	8	15

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 [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 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, 95th 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 ²)	Q<0.9
1	A	295/329 (89%)	-0.24	1 (0%) 93 93	30, 42, 59, 73	0
1	B	295/329 (89%)	-0.37	3 (1%) 82 79	30, 42, 59, 73	0
2	I	59/206 (28%)	1.45	22 (37%) 0 0	36, 62, 82, 85	0
2	J	58/206 (28%)	1.01	15 (25%) 1 0	35, 63, 82, 85	0
All	All	707/1070 (66%)	-0.05	41 (5%) 24 18	30, 44, 71, 85	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	167	HIS	5.7
2	J	168	ASP	5.6
2	I	51	MET	5.6
2	I	167	HIS	5.5
2	I	54	LEU	5.4

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 carbohydrates 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.