



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:26 AM UTC

PDB ID : 5JJA / pdb_00005jja
Title : Crystal structure of a PP2A B56gamma/BubR1 complex
Authors : Wang, Z.; Wang, J.; Rao, Z.; Xu, W.
Deposited on : 2016-04-22
Resolution : 2.35 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

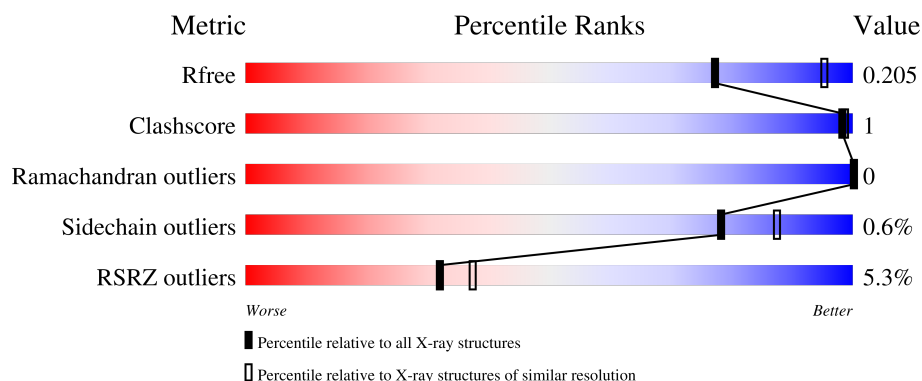
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	352	2% 93% 5%
1	B	352	7% 92% 5%
2	C	75	11% 89%
2	D	75	3% 11% 89%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5927 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 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2775	1831	448	484	12			
1	B	333	Total	C	N	O	S	0	0	0
			2782	1835	451	484	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q13362
B	29	GLY	-	expression tag	UNP Q13362

- Molecule 2 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			65	42	9	14			
2	D	8	Total	C	N	O	0	0	0
			65	42	9	14			

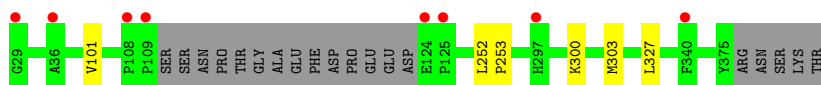
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	646	GLY	-	expression tag	UNP O60566
C	670	ASP	SER	engineered mutation	UNP O60566
C	676	ASP	SER	engineered mutation	UNP O60566
C	680	ASP	THR	engineered mutation	UNP O60566
D	646	GLY	-	expression tag	UNP O60566
D	670	ASP	SER	engineered mutation	UNP O60566
D	676	ASP	SER	engineered mutation	UNP O60566
D	680	ASP	THR	engineered mutation	UNP O60566

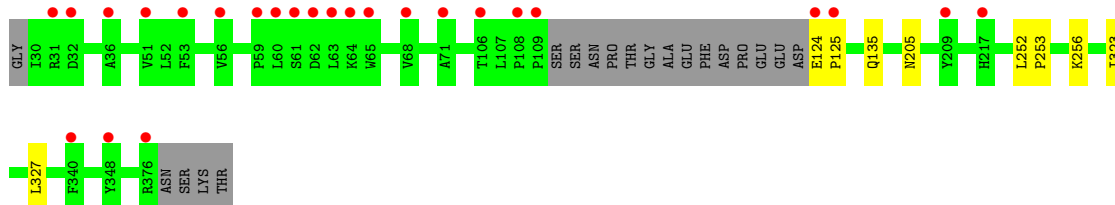
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0
3	B	105	Total 105	O 105	0	0
3	C	6	Total 6	O 6	0	0
3	D	6	Total 6	O 6	0	0

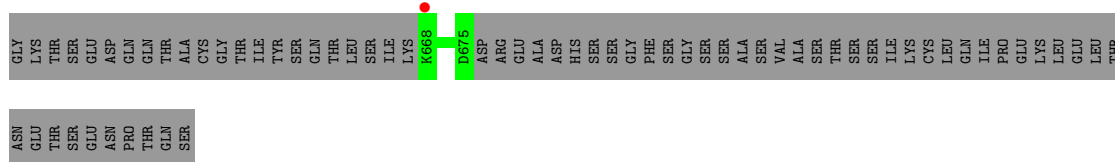
- Molecule 1: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform



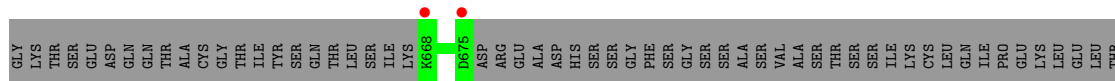
- Molecule 1: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform



- Molecule 2: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta



- Molecule 2: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta



ASN
GLU
THR
SER
GLU
ASN
PRO
THR
GLN
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.02Å 95.59Å 167.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 50.00 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.35) 99.5 (50.00-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.179 , 0.204 0.186 , 0.205	Depositor DCC
R_{free} test set	2882 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5927	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.53	0/2853	0.71	0/3871
1	B	0.52	0/2860	0.72	0/3880
2	C	0.50	0/65	0.59	0/87
2	D	0.50	0/65	0.73	0/87
All	All	0.52	0/5843	0.71	0/7925

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 [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	2775	0	2810	3	0
1	B	2782	0	2820	4	0
2	C	65	0	66	0	0
2	D	65	0	66	0	0
3	A	123	0	0	0	0
3	B	105	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
All	All	5927	0	5762	7	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 1.

All (7) 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:B:124:GLU:N	1:B:125:PRO:CD	2.66	0.58
1:A:252:LEU:HB2	1:A:253:PRO:HD3	1.96	0.47
1:B:327:LEU:HD23	1:B:327:LEU:C	2.39	0.47
1:A:300:LYS:O	1:A:303:MET:HG2	2.16	0.46
1:A:327:LEU:C	1:A:327:LEU:HD23	2.44	0.42
1:B:252:LEU:HB2	1:B:253:PRO:HD3	2.00	0.42
1:B:323:ILE:HD12	1:B:323:ILE:C	2.47	0.40

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	329/352 (94%)	326 (99%)	3 (1%)	0	100	100
1	B	329/352 (94%)	326 (99%)	3 (1%)	0	100	100
2	C	6/75 (8%)	6 (100%)	0	0	100	100
2	D	6/75 (8%)	6 (100%)	0	0	100	100
All	All	670/854 (78%)	664 (99%)	6 (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	310/327 (95%)	309 (100%)	1 (0%)	86	92
1	B	311/327 (95%)	308 (99%)	3 (1%)	68	81
2	C	8/67 (12%)	8 (100%)	0	100	100
2	D	8/67 (12%)	8 (100%)	0	100	100
All	All	637/788 (81%)	633 (99%)	4 (1%)	78	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	VAL
1	B	135	GLN
1	B	205	ASN
1	B	256	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	330	GLN
1	B	44	GLN
1	B	82	HIS
1	B	83	ASN
1	B	85	ASN
1	B	330	GLN
1	B	362	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	333/352 (94%)	-0.07	8 (2%) 59 66	29, 40, 61, 99	0
1	B	333/352 (94%)	0.13	25 (7%) 20 23	30, 42, 80, 104	0
2	C	8/75 (10%)	0.81	1 (12%) 8 9	42, 48, 77, 83	0
2	D	8/75 (10%)	0.78	2 (25%) 2 1	41, 47, 74, 78	0
All	All	682/854 (79%)	0.05	36 (5%) 32 37	29, 41, 73, 104	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	PRO	8.6
1	B	60	LEU	6.7
1	A	109	PRO	4.9
1	B	108	PRO	4.7
1	A	125	PRO	4.4
1	B	65	TRP	4.4
1	B	56	VAL	4.2
1	B	64	LYS	4.0
2	C	668	LYS	4.0
2	D	668	LYS	4.0
1	B	106	THR	3.8
1	B	376	ARG	3.7
1	A	124	GLU	3.6
1	B	59	PRO	3.6
1	B	209	TYR	3.4
1	B	125	PRO	3.4
1	B	63	LEU	3.3
1	B	68	VAL	3.3
1	B	53	PHE	3.1
1	B	31	ARG	3.0
1	A	29	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	51	VAL	2.8
1	B	124	GLU	2.6
2	D	675	ASP	2.6
1	B	71	ALA	2.6
1	A	36	ALA	2.4
1	A	340	PHE	2.3
1	B	340	PHE	2.3
1	B	348	TYR	2.3
1	B	36	ALA	2.3
1	B	61	SER	2.3
1	B	217	HIS	2.2
1	A	297	HIS	2.2
1	B	32	ASP	2.1
1	A	108	PRO	2.1
1	B	62	ASP	2.0

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 oligosaccharides 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.