



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 07:18 am BST

PDB ID : 6KIP
Title : Crystal structure of PTPRD phosphatase domain in complex with Liprin-alpha3 tandem SAM domains
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Deposited on : 2019-07-19
Resolution : 1.91 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

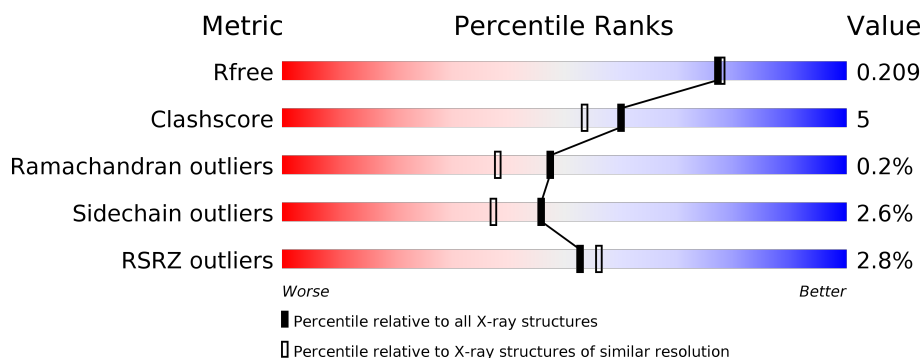
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 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	305	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> <div></div> </div>
2	B	331	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div></div> </div> <div></div> </div> <div>18%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5016 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 Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2391	1516	416	443	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1212	MET	-	expression tag	UNP Q64487
A	1509	LEU	-	expression tag	UNP Q64487
A	1510	GLU	-	expression tag	UNP Q64487
A	1511	HIS	-	expression tag	UNP Q64487
A	1512	HIS	-	expression tag	UNP Q64487
A	1513	HIS	-	expression tag	UNP Q64487
A	1514	HIS	-	expression tag	UNP Q64487
A	1515	HIS	-	expression tag	UNP Q64487
A	1516	HIS	-	expression tag	UNP Q64487

- Molecule 2 is a protein called Liprin-alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	272	Total	C	N	O	S	0	0	0
			2197	1386	395	403	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	803	LEU	-	expression tag	UNP P60469
B	804	GLY	-	expression tag	UNP P60469
B	805	SER	-	expression tag	UNP P60469
B	1128	THR	-	expression tag	UNP P60469
B	1129	ARG	-	expression tag	UNP P60469
B	1130	ALA	-	expression tag	UNP P60469
B	1131	ALA	-	expression tag	UNP P60469

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1132	ALA	-	expression tag	UNP P60469
B	1133	SER	-	expression tag	UNP P60469

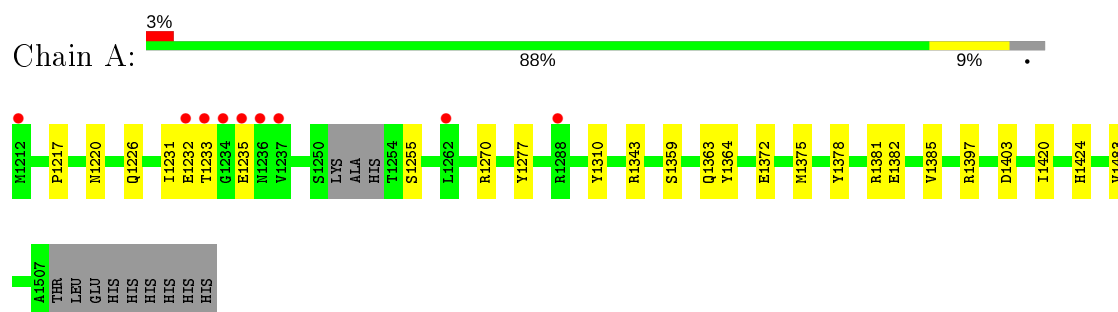
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	231	Total O 231 231	0	0
3	B	197	Total O 197 197	0	0

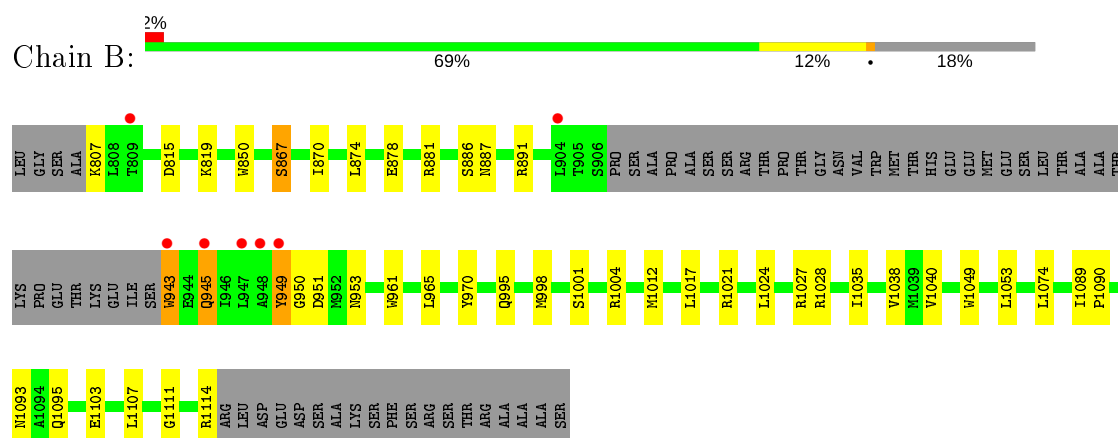
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Receptor-type tyrosine-protein phosphatase delta



- Molecule 2: Liprin-alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.01Å 98.01Å 140.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 1.91 49.25 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.25-1.91) 97.4 (49.25-1.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.162 , 0.208 0.168 , 0.209	Depositor DCC
R_{free} test set	2583 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5016	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.39	0/2446	0.52	0/3304
2	B	0.33	0/2241	0.49	0/3026
All	All	0.36	0/4687	0.51	0/6330

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	2391	0	2328	11	0
2	B	2197	0	2187	31	0
3	A	231	0	0	1	0
3	B	197	0	0	8	0
All	All	5016	0	4515	42	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 5.

The worst 5 of 42 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:1232:GLU:HG2	1:A:1233:THR:HG23	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1004:ARG:NH2	3:B:1202:HOH:O	2.16	0.76
2:B:950:GLY:HA2	2:B:953:ASN:HB3	1.68	0.75
2:B:1024:LEU:HD12	2:B:1040:VAL:HG13	1.69	0.74
2:B:807:LYS:N	3:B:1205:HOH:O	2.22	0.73

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	289/305 (95%)	278 (96%)	10 (4%)	1 (0%)	41	31
2	B	268/331 (81%)	262 (98%)	6 (2%)	0	100	100
All	All	557/636 (88%)	540 (97%)	16 (3%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1483	VAL

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	257/268 (96%)	250 (97%)	7 (3%)	44	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	236/284 (83%)	230 (98%)	6 (2%)	47	39
All	All	493/552 (89%)	480 (97%)	13 (3%)	46	37

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1385	VAL
1	A	1403	ASP
2	B	945	GLN
1	A	1359	SER
2	B	943	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1432	GLN
2	B	1095	GLN
2	B	1068	HIS
1	A	1261	ASN
2	B	1093	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 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	293/305 (96%)	-0.10	9 (3%) 49 52	13, 28, 67, 108	0
2	B	272/331 (82%)	-0.29	7 (2%) 56 59	18, 34, 62, 101	0
All	All	565/636 (88%)	-0.19	16 (2%) 53 56	13, 31, 67, 108	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1234	GLY	8.9
2	B	945	GLN	6.8
1	A	1233	THR	5.3
1	A	1236	ASN	4.7
2	B	943	TRP	4.4

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.