



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 11:35 am BST

PDB ID : 6IQU
Title : Crystal structure of Prc with PDZ domain deletion in complex with NlpI
Authors : Chueh, C.K.; Chang, C.I.
Deposited on : 2018-11-08
Resolution : 2.90 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

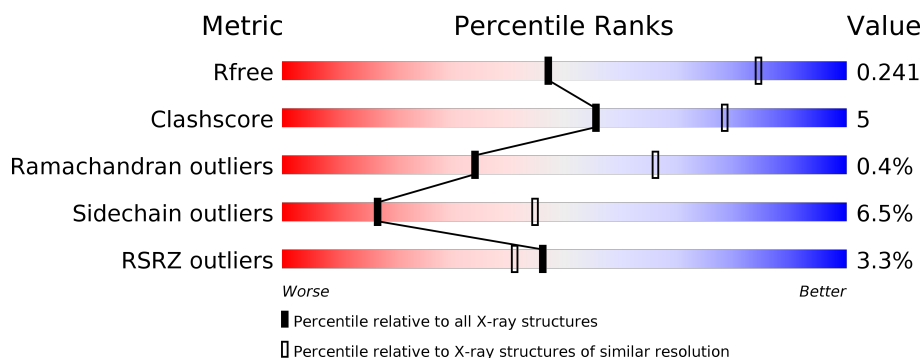
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	278	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>• 7%</div> </div> </div>
2	B	596	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 10%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6445 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 Lipoprotein NlpI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2099	1340	347	409	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	-	expression tag	UNP P0AFB1
A	18	HIS	-	expression tag	UNP P0AFB1
A	19	MET	-	expression tag	UNP P0AFB1

- Molecule 2 is a protein called Tail-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	539	Total	C	N	O	S	0	0	0
			4335	2729	755	843	8			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	ALA	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	LEU	deletion	UNP P23865
B	?	-	GLN	deletion	UNP P23865
B	?	-	MET	deletion	UNP P23865
B	?	-	ASP	deletion	UNP P23865
B	?	-	ASP	deletion	UNP P23865
B	?	-	ASP	deletion	UNP P23865
B	?	-	TYR	deletion	UNP P23865
B	?	-	THR	deletion	UNP P23865

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	?	-	ASN	deletion	UNP P23865
B	?	-	SER	deletion	UNP P23865
B	?	-	MET	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	ALA	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	PRO	deletion	UNP P23865
B	?	-	ALA	deletion	UNP P23865
B	?	-	ALA	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	SER	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	ALA	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	?	-	SER	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	ASP	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	GLN	deletion	UNP P23865
B	?	-	THR	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	PRO	deletion	UNP P23865
B	?	-	MET	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	ASP	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	TRP	deletion	UNP P23865
B	?	-	ARG	deletion	UNP P23865
B	?	-	LEU	deletion	UNP P23865
B	?	-	ASP	deletion	UNP P23865

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	ALA	deletion	UNP P23865
B	?	-	LEU	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	PRO	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	SER	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	ARG	deletion	UNP P23865
B	?	-	LEU	deletion	UNP P23865
B	?	-	GLU	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	?	-	LEU	deletion	UNP P23865
B	?	-	PRO	deletion	UNP P23865
B	?	-	ALA	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	GLY	deletion	UNP P23865
B	?	-	THR	deletion	UNP P23865
B	?	-	LYS	deletion	UNP P23865
B	?	-	THR	deletion	UNP P23865
B	?	-	ARG	deletion	UNP P23865
B	?	-	THR	deletion	UNP P23865
B	?	-	VAL	deletion	UNP P23865
B	?	-	THR	deletion	UNP P23865
B	?	-	LEU	deletion	UNP P23865
B	?	-	THR	deletion	UNP P23865
B	?	-	ARG	deletion	UNP P23865
B	?	-	GLU	deletion	UNP P23865
B	?	-	ARG	deletion	UNP P23865
B	?	-	ILE	deletion	UNP P23865
B	247	PHE	ARG	linker	UNP P23865
B	591	HIS	-	expression tag	UNP P23865
B	592	HIS	-	expression tag	UNP P23865
B	593	HIS	-	expression tag	UNP P23865
B	594	HIS	-	expression tag	UNP P23865

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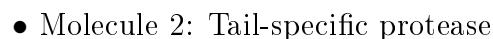
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Chain	Residue	Modelled	Actual	Comment	Reference
B	595	HIS	-	expression tag	UNP P23865
B	596	HIS	-	expression tag	UNP P23865

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	8	Total O 8 8	0	0

- Molecule 1: Lipoprotein NlpI



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.83Å 151.08Å 148.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.80 – 2.90 38.77 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.9 (38.80-2.90) 88.9 (38.77-2.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.95 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.192 , 0.233 0.195 , 0.241	Depositor DCC
R_{free} test set	1192 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6445	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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	0.78	0/2143	0.97	0/2909
2	B	0.77	0/4413	0.96	3/5959 (0.1%)
All	All	0.77	0/6556	0.96	3/8868 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	B	83	ASN	CB-CA-C	-5.39	99.62	110.40
2	B	403	ARG	NE-CZ-NH1	5.08	122.84	120.30

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2099	0	2026	15	0
2	B	4335	0	4300	51	0
3	A	3	0	0	0	0
3	B	8	0	0	0	0
All	All	6445	0	6326	65	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 65 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:B:85:LEU:HD21	2:B:119:ALA:HB2	1.43	1.01
2:B:119:ALA:HA	2:B:122:ARG:HB2	1.46	0.96
2:B:429:ARG:HD2	2:B:450:LYS:HA	1.46	0.96
2:B:117:ASN:O	2:B:120:GLN:HB2	1.76	0.85
1:A:286:ASP:OD1	1:A:286:ASP:N	2.29	0.64

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	257/278 (92%)	240 (93%)	16 (6%)	1 (0%)	34	66
2	B	535/596 (90%)	493 (92%)	40 (8%)	2 (0%)	34	66
All	All	792/874 (91%)	733 (93%)	56 (7%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	509	LYS
2	B	320	PRO
1	A	48	GLU

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	220/237 (93%)	215 (98%)	5 (2%)	50	80
2	B	471/518 (91%)	431 (92%)	40 (8%)	10	31
All	All	691/755 (92%)	646 (94%)	45 (6%)	17	45

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	232	ARG
2	B	255	MET
2	B	531	ARG
2	B	234	THR
2	B	262	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
2	B	558	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	259/278 (93%)	-0.04	6 (2%) 60 58	24, 42, 74, 121	0
2	B	539/596 (90%)	0.07	20 (3%) 41 37	28, 54, 90, 140	0
All	All	798/874 (91%)	0.03	26 (3%) 46 41	24, 49, 88, 140	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	234	THR	6.2
2	B	233	ASN	5.9
2	B	248	LEU	5.7
2	B	249	GLU	5.4
2	B	250	ASP	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.