

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 19, 2020 – 11:02 am BST

PDB ID : 5QQH

Title: PanDDA analysis group deposition - Crystal Structure of Kalirin/Rac1 in

complex with MolPort-020-096-465

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Deposited on : 2019-05-03

Resolution : 2.09 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.11

buster-report : 1.1.7 (2018)

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)

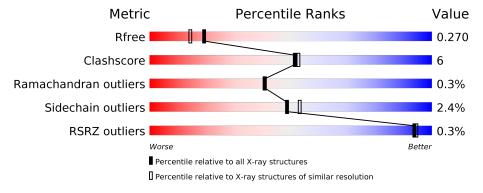
Validation Pipeline (wwPDB-VP) : 2.11

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.09 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	178	88%	10%	
2	В	182	86%	11%	



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3136 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 Ras-related C3 botulinum toxin substrate 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	177	Total	С	N	О	S	0	0	0
			1352	868	221	256	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Α	0	SER	_	expression tag	UNP P63000

• Molecule 2 is a protein called Kalirin.

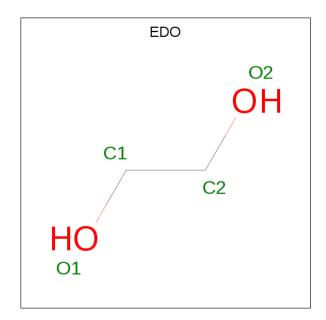
			Atoms			ZeroOcc	AltConf	Trace		
2	В	179	Total	C	N	0	S	0	0	0
Z	D	179	1421	916	230	265	10	U	U	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	1230	SER	_	expression tag	UNP O60229
В	1231	MET	_	expression tag	UNP O60229
В	1370	VAL	ILE	conflict	UNP O60229

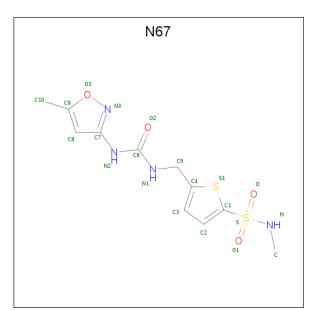
• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0

 $\bullet \ \ Molecule \ 4 \ is \ N-methyl-5-(\{[(5-methyl-1,2-oxazol-3-yl)carbamoyl]amino\}methyl)thiophene-2-sulfonamide (three-letter code: N67) (formula: $C_{11}H_{14}N_4O_4S_2$).$ 



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
1	Λ	1	Total	С	N	О	S	0	0
4	A	1	21	11	4	4	2	0	U

• Molecule 5 is water.



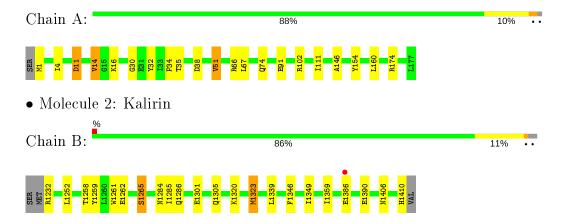
$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	185	Total O 185 185	0	0
5	В	153	Total O 153 153	0	0



# 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: Ras-related C3 botulinum toxin substrate 1





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	62.66Å 62.66Å 342.82Å	Danagitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.14 - 2.09	Depositor
Resolution (A)	57.14 - 2.09	EDS
% Data completeness	99.8 (57.14-2.09)	Depositor
(in resolution range)	99.9 (57.14-2.09)	EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.70 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
D D	0.200 , 0.263	Depositor
$R, R_{free}$	0.209 , $0.270$	DCC
$R_{free}$ test set	1229 reflections $(4.94\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31 , 45.0	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3136	wwPDB-VP
Average B, all atoms $(Å^2)$	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: N67, EDO

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		
MIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.84	0/1382	0.93	4/1890 (0.2%)	
2	В	0.80	0/1451	0.81	1/1964 (0.1%)	
All	All	0.82	0/2833	0.87	5/3854 (0.1%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	102	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	A	11	ASP	CB-CG-OD1	7.04	124.64	118.30
2	В	1323	MET	CA-CB-CG	6.52	124.38	113.30
1	A	102	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	174	ARG	NE-CZ-NH2	-5.13	117.74	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	1352	0	1325	13	1
2	В	1421	0	1367	23	1
3	A	4	0	6	0	0
4	A	21	0	0	1	0

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Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
5	A	185	0	0	1	1
5	В	153	0	0	8	1
All	All	3136	0	2698	31	4

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 6.

The worst 5 of 31 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	Clash overlap (Å)
1:A:66:ARG:H	2:B:1406:ASN:HD21	1.21	0.87
1:A:74:GLN:NE2	2:B:1339:LEU:HD11	2.13	0.64
2:B:1320:LYS:O	2:B:1323:MET:HG2	1.99	0.63
1:A:66:ARG:N	2:B:1406:ASN:HD21	1.93	0.62
2:B:1286:GLN:OE1	5:B:1501:HOH:O	2.16	0.60

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{array}{ll}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:A:91:GLU:OE2	1:A:91:GLU:OE2[10_665]	1.50	0.70
5:A:408:HOH:O	5:A:408:HOH:O[10_665]	1.88	0.32
5:B:1509:HOH:O	5:B:1513:HOH:O[8_555]	2.02	0.18
2:B:1305:GLN:NE2	2:B:1305:GLN:NE2[10_555]	2.12	0.08

### 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	Perce	$_{ m ntiles}$
1	A	175/178 (98%)	171 (98%)	3 (2%)	1 (1%)	25	21
2	В	177/182 (97%)	168 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	352/360 (98%)	339 (96%)	12 (3%)	1 (0%)	41 41	

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	${f Res}$	Type
1	Α	30	GLY

#### 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	144/154 (94%)	138 (96%)	6 (4%)	30 30		
2	В	148/166 (89%)	147 (99%)	1 (1%)	84 88		
All	All	292/320 (91%)	285 (98%)	7 (2%)	49 53		

#### 5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
2	В	1265	SER
1	A	111	ILE
1	A	14	VAL
1	A	160	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	1406	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Tuno	Chain	Res Link		Во	nd leng	$_{ m ths}$	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	201	-	3,3,3	0.43	0	2,2,2	0.79	0
4	N67	A	202	-	17,22,22	3.12	9 (52%)	14,31,31	2.85	6 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	201	_	_	0/1/1/1	-
4	N67	A	202	-	-	0/8/18/18	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(A)
4	A	202	N67	C1-S	-8.81	1.62	1.76
4	A	202	N67	C6-N1	4.60	1.44	1.35
4	A	202	N67	C6-N2	4.05	1.45	1.37
4	A	202	N67	C10-C9	-3.40	1.44	1.48
4	A	202	N67	C4-S1	-2.72	1.68	1.73

The worst 5 of 6 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	202	N67	C7-N2-C6	-6.21	121.69	130.41
4	A	202	N67	C1-S-N	-5.88	99.63	107.74
4	A	202	N67	C7-C8-C9	-3.94	103.17	107.23
4	A	202	N67	O2-C6-N2	-2.62	119.20	123.62
4	A	202	N67	C10-C9-C8	2.40	135.44	129.02

There are no chirality outliers.

There are no torsion outliers.

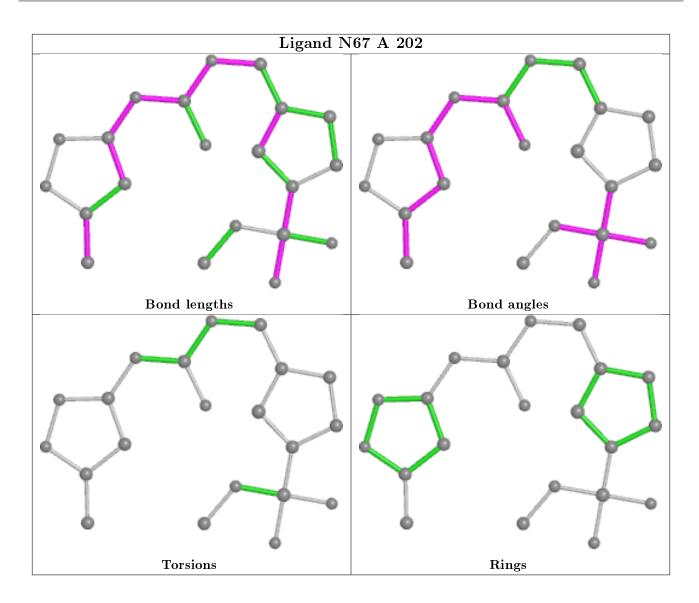
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	N67	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	177/178 (99%)	-0.56	0 100 100	26, 36, 62, 91	0
2	В	179/182 (98%)	-0.41	1 (0%) 89 91	27, 41, 76, 97	0
All	All	356/360 (98%)	-0.48	1 (0%) 94 94	26, 39, 71, 97	0

#### All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	1386	GLU	2.4

### 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)

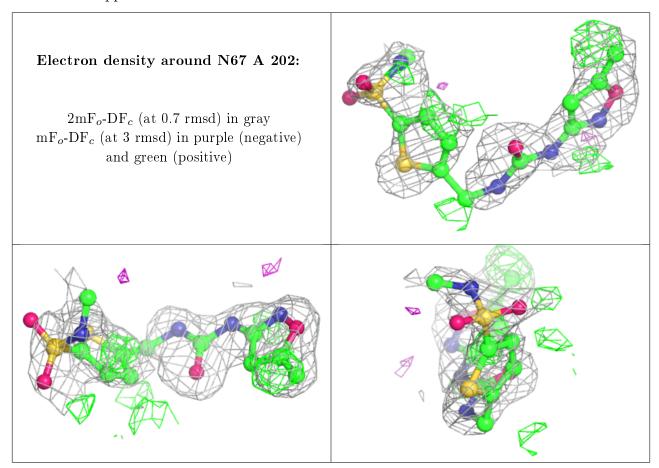
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	N67	A	202	21/21	0.73	0.23	27,35,55,65	21
3	EDO	A	201	4/4	0.86	0.13	62,65,67,75	0

The following is a graphical depiction of the model fit to experimental electron density of all



instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers (i)

There are no such residues in this entry.

