

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

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PDB ID : 6K86

Title: The closed state of RGLG1 mutant-E378A

Authors : Wang, Q.; Wu, Y.

Deposited on : 2019-06-11

Resolution : 1.59 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 (i) 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 (1)) were used in the production of this report:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$ 

EDS : 2.36

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)

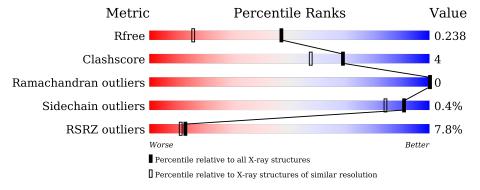
Validation Pipeline (wwPDB-VP) : 2.36

## 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 1.59 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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 <=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		
			7%		
1	В	301	85%	8%	7%



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2380 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 E3 ubiquitin-protein ligase RGLG1.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	В	281	Total 2195	C 1391	N 372	O 424	S 8	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual Comment		Reference
В	119	GLY	-	expression tag	UNP Q9SS90
В	120	THR	-	expression tag	UNP Q9SS90
В	121	SER	-	expression tag	UNP Q9SS90
В	122	SER	-	expression tag	UNP Q9SS90
В	123	MET	-	expression tag	UNP Q9SS90
В	124	ALA	-	expression tag	UNP Q9SS90
В	125	ASP	-	expression tag	UNP Q9SS90
В	126	ILE	-	expression tag	UNP Q9SS90
В	127	GLY	-	expression tag	UNP Q9SS90
В	128	SER	-	expression tag	UNP Q9SS90
В	378	ALA	GLU	engineered mutation	UNP Q9SS90

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Mg	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Na 1 1	0	0



#### • Molecule 4 is water.

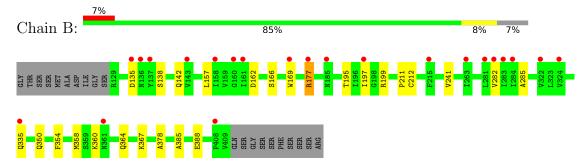
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	183	Total O 183 183	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: E3 ubiquitin-protein ligase RGLG1





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	45.59Å 72.56Å 80.85Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.39 - 1.59	Depositor
Resolution (A)	28.39 - 1.59	EDS
% Data completeness	95.2 (28.39-1.59)	Depositor
(in resolution range)	96.7 (28.39-1.59)	EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.02 (at 1.59Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D D.	0.197 , 0.233	Depositor
$R, R_{free}$	0.205 , $0.238$	DCC
$R_{free}$ test set	1716 reflections $(4.85\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 44.1	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	0.96	EDS
Total number of atoms	2380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.55% 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: NA, MG

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	$\mathbf{lengths}$	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	В	0.38	0/2244	0.51	0/3049	

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	В	2195	0	2153	16	0
2	В	1	0	0	0	0
3	В	1	0	0	0	0
4	В	183	0	0	4	0
All	All	2380	0	2153	16	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.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:B:360:LYS:O	1:B:367:LYS:NZ	2.12	0.80
1:B:335:GLN:NE2	4:B:606:HOH:O	2.35	0.60
1:B:135:ASP:OD1	4:B:601:HOH:O	2.18	0.51
1:B:350:GLN:OE1	4:B:602:HOH:O	2.20	0.50
1:B:354:PHE:CZ	1:B:358:MET:HG3	2.48	0.47
1:B:166:SER:HA	1:B:169:TRP:CZ2	2.50	0.47
1:B:177:ARG:HH11	1:B:177:ARG:HG3	1.82	0.45
1:B:195:THR:O	1:B:199:ARG:HG3	2.17	0.44
1:B:364:GLN:HB2	4:B:750:HOH:O	2.17	0.43
1:B:138:SER:N	1:B:142:GLN:OE1	2.37	0.43
1:B:385:ALA:HA	1:B:388:GLU:HG2	1.99	0.43
1:B:350:GLN:CD	1:B:378:ALA:HB3	2.40	0.41
1:B:162:ASP:CB	1:B:285:ALA:HA	2.51	0.41
1:B:212:CYS:SG	1:B:241:VAL:HG22	2.62	0.41
1:B:197:ILE:HG21	1:B:282:VAL:HG21	2.02	0.40
1:B:157:LEU:O	1:B:211:PRO:HD2	2.22	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	В	279/301 (93%)	273 (98%)	6 (2%)	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	В	243/259 (94%)	242 (100%)	1 (0%)	91 84		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	177	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 $>$	# RSRZ > 2		$OWAB(A^2)$	Q<0.9
1	В	281/301 (93%)	0.38	22 (7%) 13 11		25, 35, 50, 64	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	169	TRP	5.3
1	В	361	ASN	5.0
1	В	161	ILE	4.9
1	В	158	ILE	4.2
1	В	284	ILE	4.2
1	В	281	LEU	3.8
1	В	135	ASP	3.3
1	В	408	PRO	3.1
1	В	263	ILE	3.1
1	В	177	ARG	2.9
1	В	197	ILE	2.7
1	В	324	VAL	2.7
1	В	282	VAL	2.6
1	В	283	ILE	2.5
1	В	215	PHE	2.4
1	В	335	GLN	2.3
1	В	160	GLY	2.3
1	В	143	VAL	2.2
1	В	322	VAL	2.1
1	В	136	ASN	2.1
1	В	137	TYR	2.1
1	В	185	ASN	2.1

## 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 monosaccharides 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.

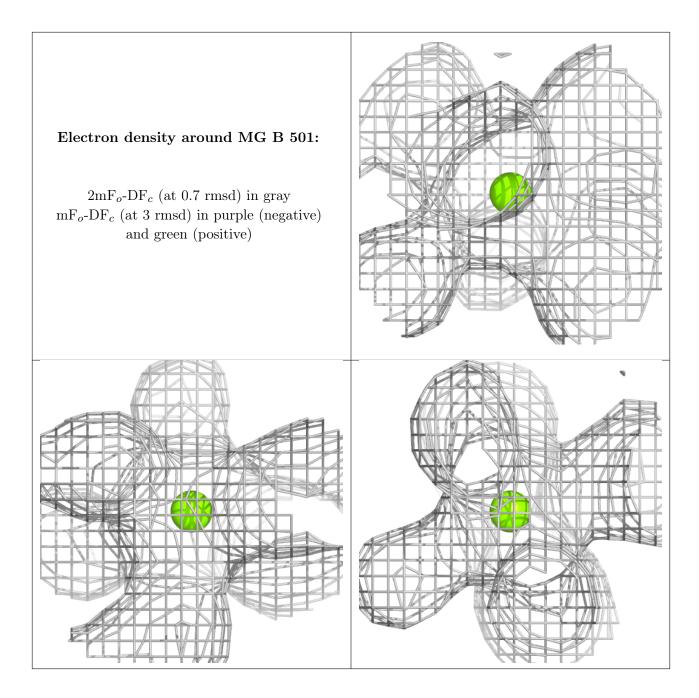
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	NA	В	502	1/1	0.93	0.05	39,39,39,39	0
2	MG	В	501	1/1	0.97	0.07	40,40,40,40	0

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.



# Electron density around NA B 502: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)





## 6.5 Other polymers (i)

There are no such residues in this entry.

