

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

#### Oct 2, 2021 – 09:06 PM EDT

PDB ID	:	3LH1
Title	:	Q191A mutant of the DegS-deltaPDZ $$
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Deposited on		
Resolution	:	2.51  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 following versions of software and data (see references (1)) were used in the production of this report:

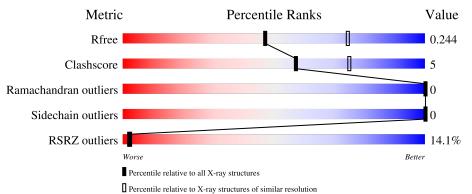
MolProbity Xtriage (Phenix) EDS	:	
		20191225.v01 (using entries in the PDB archive December 25th 2019)
		5.8.0158
		7.0.044 (Gargrove)
Ideal geometry (proteins)		
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 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	$\begin{array}{l} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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				
			12%				
1	А	241	74%	8%	17%		



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2894 atoms, of which 1453 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 Protease degS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	199	Total 2884	C 900	Н 1453	N 257	0 271	${ m S} { m 3}$	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	16	MET	-	expression tag	UNP P0AEE3
А	17	ARG	-	expression tag	UNP P0AEE3
A	18	GLY	-	expression tag	UNP P0AEE3
А	19	SER	-	expression tag	UNP P0AEE3
А	20	HIS	-	expression tag	UNP P0AEE3
A	21	HIS	-	expression tag	UNP P0AEE3
А	22	HIS	-	expression tag	UNP P0AEE3
А	23	HIS	-	expression tag	UNP P0AEE3
А	24	HIS	-	expression tag	UNP P0AEE3
А	25	HIS	-	expression tag	UNP P0AEE3
А	26	GLY	-	expression tag	UNP P0AEE3
А	191	ALA	GLN	engineered mutation	UNP P0AEE3

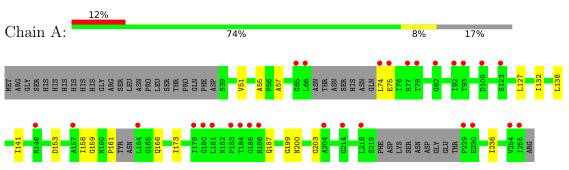
• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	10	Total O 10 10	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: Protease degS



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	70.89Å $70.89$ Å $120.84$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	27.37 - 2.51	Depositor
nesolution (A)	27.37 - 2.51	EDS
% Data completeness	$85.4\ (27.37-2.51)$	Depositor
(in resolution range)	85.5 (27.37-2.51)	EDS
R <sub>merge</sub>	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.81 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
$R, R_{free}$	0.222 , $0.258$	Depositor
II, Ilfree	0.216 , $0.244$	DCC
$R_{free}$ test set	644 reflections $(9.69%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	48.1	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, $61.0$	EDS
L-test for $twinning^2$	$<  L  > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2894	wwPDB-VP
Average B, all atoms $(Å^2)$	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.41% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



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

# 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	
IVI01	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.26	0/1445	0.47	0/1964

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	А	1431	1453	1452	14	0
2	А	10	0	0	1	0
All	All	1441	1453	1452	14	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.

All (14) 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:161:PRO:HB3	1:A:199:GLY:HA3	1.95	0.48
1:A:159:GLY:HA3	1:A:200:ASN:HA	1.95	0.47
1:A:141:ILE:HG23	1:A:141:ILE:O	2.16	0.44
1:A:127:LEU:HD21	1:A:236:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HD11	1:A:138:LEU:HD11	2.00	0.43
1:A:55:ALA:HB1	1:A:166:GLN:OE1	2.18	0.43
1:A:74:LEU:HD23	1:A:74:LEU:N	2.34	0.43
1:A:51:VAL:O	1:A:55:ALA:HB3	2.19	0.43
1:A:153:ASP:HB2	1:A:173:ILE:HD12	2.01	0.43
1:A:187:GLN:O	1:A:187:GLN:HG3	2.20	0.42
1:A:57:ALA:HB2	2:A:3:HOH:O	2.21	0.41
1:A:158:ILE:O	1:A:203:GLY:HA3	2.22	0.40
1:A:75:GLU:HG3	1:A:75:GLU:O	2.22	0.40
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.87	0.40

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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	А	$191/241 \ (79\%)$	188 (98%)	3~(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	А	148/197~(75%)	148 (100%)	0	100 100



There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	А	94	ASN
1	А	96	HIS

#### 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)

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,  $95^{th}$  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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	199/241~(82%)	0.94	28 (14%) 2 2	54, 76, 122, 150	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	74	LEU	9.0
1	А	229	PRO	6.3
1	А	181	LEU	5.5
1	А	183	PRO	5.3
1	А	184	THR	4.4
1	А	180	GLY	4.4
1	А	186	ARG	4.2
1	А	78	THR	4.0
1	А	66	LEU	3.4
1	А	230	GLU	3.4
1	А	65	GLY	3.3
1	А	179	ILE	3.2
1	А	77	ARG	3.1
1	А	75	GLU	3.1
1	А	218	LEU	3.0
1	А	82	GLY	2.8
1	А	214	GLY	2.8
1	А	92	ILE	2.8
1	А	146	ARG	2.7
1	А	164	LEU	2.6
1	А	204	ALA	2.6
1	А	254	VAL	2.5
1	А	185	GLY	2.5
1	А	255	ILE	2.4
1	А	100	ASP	2.3
1	А	123	SER	2.3
1	A	157	ALA	2.2

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Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	93	THR	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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

