

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 02:19 PM JST

PDB ID : 5ILB

Title : Crystal structure of protease domain of Deg2 linked with the PDZ domain of

Deg9

Authors: Ouyang, M.; Liu, L.; Li, X.Y.; Zhao, S.; Zhang, L.X.

Deposited on : 2016-03-04

Resolution : 1.85 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:

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

EDS: 2.36

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)

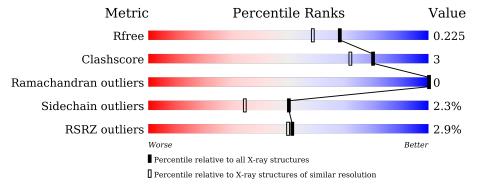
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	
1	A	474	93%	5% •
1	В	474	89%	7% ••



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8263 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 Protease Do-like 2, chloroplastic, Protease Do-like 9.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	466	Total 3621	C 2312	N 606	O 689	S 14	0	9	0
1	В	463	Total 3597	C 2290	N 612	O 681	S 14	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
A	109	GLY	-	expression tag	UNP O82261	
В	109	GLY	-	expression tag	UNP O82261	

• Molecule 2 is water.

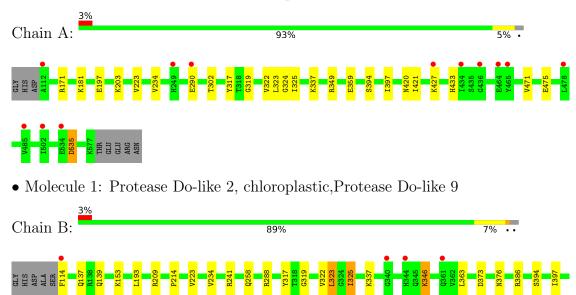
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	519	Total O 519 519	0	0
2	В	526	Total O 526 526	0	0



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 Do-like 2, chloroplastic, Protease Do-like 9





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	H 3	Depositor	
Cell constants	106.09Å 106.09Å 255.96Å	Donositon	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	26.52 - 1.85	Depositor	
Resolution (A)	26.52 - 1.85	EDS	
% Data completeness	96.0 (26.52-1.85)	Depositor	
(in resolution range)	96.0 (26.52-1.85)	EDS	
R_{merge}	0.08	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.46 (at 1.85Å)	Xtriage	
Refinement program	PHENIX 1.8.1_1168	Depositor	
R, R_{free}	0.190 , 0.225	Depositor	
it, it free	0.190 , 0.225	DCC	
R_{free} test set	4396 reflections $(5.01%)$	wwPDB-VP	
Wilson B-factor (\mathring{A}^2)	18.3	Xtriage	
Anisotropy	0.078	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 57.9	EDS	
L-test for twinning ²	$< L > = 0.51, < L^2> = 0.35$	Xtriage	
Estimated twinning fraction	0.000 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.002 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.004 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.000 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3* k-1/3*l 0.003 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.000 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 *k-1/3*l 0.020 for h,-h-k,-l	Xtriage	
F_o, F_c correlation	0.95	EDS	
Total number of atoms	8263	wwPDB-VP	
Average B, all atoms (Å ²)	22.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.26	0/3720	0.48	0/5050	
1	В	0.27	0/3679	0.48	0/4993	
All	All	0.26	0/7399	0.48	0/10043	

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)

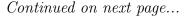
In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3621	0	3623	16	0
1	В	3597	0	3596	24	0
2	A	519	0	0	7	1
2	В	526	0	0	10	1
All	All	8263	0	7219	39	1

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 3.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-1 Atom-2		$egin{array}{c} \operatorname{Clash} \ \operatorname{overlap}\ (ext{\AA}) \end{array}$	
1:B:214:PRO:O	1:B:386:ARG:NH2	2.13	0.81	





Continued from previous page...

Atom 1		Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)	
1:B:346:LYS:HE3	1:B:376:ASN:HB3	1.74	0.68	
1:A:203:LYS:NZ	2:A:615:HOH:O	2.34	0.61	
1:A:223:VAL:HG22	1:A:234[B]:VAL:HG12	1.82	0.61	
1:B:139:GLN:NE2	2:B:601:HOH:O	2.21	0.60	
1:B:223:VAL:HG22	1:B:234[B]:VAL:HG12	1.85	0.59	
1:B:337:LYS:NZ	2:B:622:HOH:O	2.36	0.58	
1:A:317:TYR:CZ	1:A:319:GLY:HA2	2.41	0.56	
1:A:181:LYS:NZ	2:A:626:HOH:O	2.43	0.51	
1:B:524:LYS:NZ	2:B:616:HOH:O	2.32	0.51	
1:A:535:ASP:OD2	1:A:535:ASP:N	2.42	0.51	
1:A:181:LYS:NZ	2:A:602:HOH:O	2.43	0.51	
1:B:288:ARG:NH2	2:B:632:HOH:O	2.43	0.50	
1:B:317:TYR:CZ	1:B:319:GLY:HA2	2.47	0.50	
1:A:324:GLY:N	1:A:359:GLU:OE2	2.45	0.49	
1:A:359:GLU:HB3	1:A:421:ILE:HG21	1.93	0.49	
1:B:539:LYS:NZ	2:B:644:HOH:O	2.46	0.48	
1:A:349:ARG:NH2	2:A:632:HOH:O	2.46	0.48	
1:A:197:GLU:OE2	2:A:602:HOH:O	2.20	0.47	
1:B:137:GLN:NE2	2:B:646:HOH:O	2.48	0.47	
1:A:394:SER:HA	1:A:397:ILE:HD12	1.97	0.47	
1:B:437:LYS:O	2:B:602:HOH:O	2.21	0.46	
1:A:337:LYS:HE3	1:A:337:LYS:HB2	1.71	0.45	
1:B:323:LEU:HD13	1:B:325:ILE:HG12	1.98	0.45	
1:B:394:SER:HA	1:B:397:ILE:HD12	1.99	0.44	
1:B:153:LYS:HD3	1:B:193:LEU:HD13	2.00	0.43	
1:A:471[B]:VAL:HG21	1:B:478:LEU:HD12	2.00	0.43	
1:B:241:ARG:HD2	1:B:258:GLN:OE1	2.18	0.42	
1:B:402:THR:HG21	1:B:425:ILE:HG23	2.01	0.42	
1:B:461:TYR:CZ	1:B:470:PRO:HD3	2.55	0.42	
1:A:171:ARG:HD3	2:A:625:HOH:O	2.19	0.42	
1:B:539:LYS:HE3	1:B:547:ILE:HD13	2.02	0.42	
1:B:209:ARG:NH1	2:B:608:HOH:O	2.26	0.42	
1:A:302:THR:HG23	2:A:601:HOH:O	2.19	0.41	
1:B:373:ASP:OD1	2:B:603:HOH:O	2.22	0.41	
1:B:337:LYS:HB2	1:B:337:LYS:HE2	1.82	0.41	
1:A:427:LYS:HD2	1:A:427:LYS:HA	1.84	0.40	
1:B:427:LYS:HD2	1:B:427:LYS:HA	1.89	0.40	
1:B:498:SER:OG	2:B:604:HOH:O	2.22	0.40	

All (1) 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-1 Atom-2		Clash overlap (Å)
2:A:983:HOH:O	2:B:1045:HOH:O[9_544]	2.10	0.10

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	entiles
1	A	473/474 (100%)	463 (98%)	10 (2%)	0	100	100
1	В	$464/474 \ (98\%)$	452 (97%)	12 (3%)	0	100	100
All	All	937/948 (99%)	915 (98%)	22 (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	A	400/410 (98%)	392 (98%)	8 (2%)	55	40
1	В	397/410 (97%)	387 (98%)	10 (2%)	47	31
All	All	797/820 (97%)	779 (98%)	18 (2%)	50	34

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	GLU
1	A	322	VAL
1	A	323	LEU

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	A	325	ILE
1	A	420	ASN
1	A	433	HIS
1	A	475	GLU
1	A	535	ASP
1	В	114	PHE
1	В	322	VAL
1	В	323	LEU
1	В	325	ILE
1	В	346	LYS
1	В	363	LEU
1	В	437	LYS
1	В	466	GLU
1	В	521	LYS
1	В	560	LEU

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)

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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	466/474 (98%)	0.07	12 (2%) 56 54	2, 19, 42, 56	0
1	В	463/474 (97%)	0.06	15 (3%) 47 45	2, 20, 42, 58	0
All	All	929/948 (97%)	0.06	27 (2%) 51 50	2, 20, 42, 58	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	436	GLY	6.4
1	В	436	GLY	4.7
1	В	114	PHE	4.1
1	В	560	LEU	3.5
1	В	463	LYS	3.5
1	A	434	ILE	3.2
1	В	427	LYS	3.1
1	В	464	GLU	3.0
1	В	534	GLU	2.8
1	В	574	ASP	2.8
1	A	112	ALA	2.8
1	A	465	TYR	2.7
1	В	340	GLY	2.6
1	В	565	THR	2.5
1	A	485	VAL	2.5
1	A	464	GLU	2.5
1	A	290	GLU	2.5
1	A	502	ILE	2.5
1	В	435	SER	2.4
1	В	485	VAL	2.4
1	A	534	GLU	2.3
1	A	249	HIS	2.3
1	A	478	LEU	2.2
1	В	576	LEU	2.2

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	В	344	HIS	2.2
1	В	361	GLN	2.2
1	A	427	LYS	2.0

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.

