



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 07:57 am BST

PDB ID : 6A9E
Title : Crystal structure of the N-terminal domain of Atg2
Authors : Osawa, T.; Noda, N.N.
Deposited on : 2018-07-13
Resolution : 3.21 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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
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

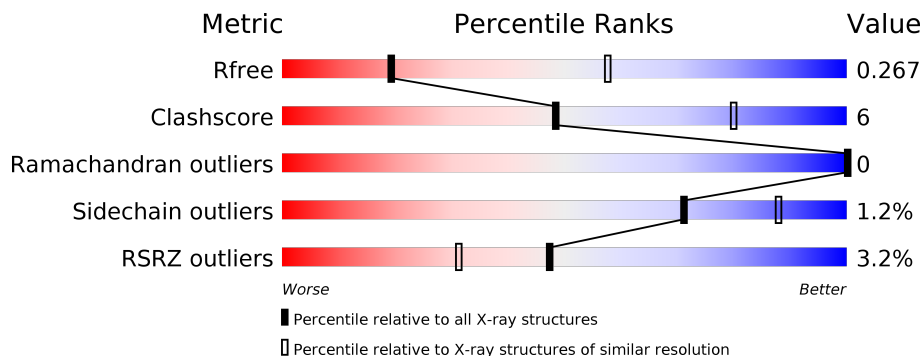
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	389	 4% 71% 15% 13%
1	B	389	 2% 76% 11% 13%

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 5023 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 Endolysin, Autophagy-related protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	339	2513	1598	434	469	2	10	0	0	0
1	B	339	2510	1595	439	463	2	11	0	0	0

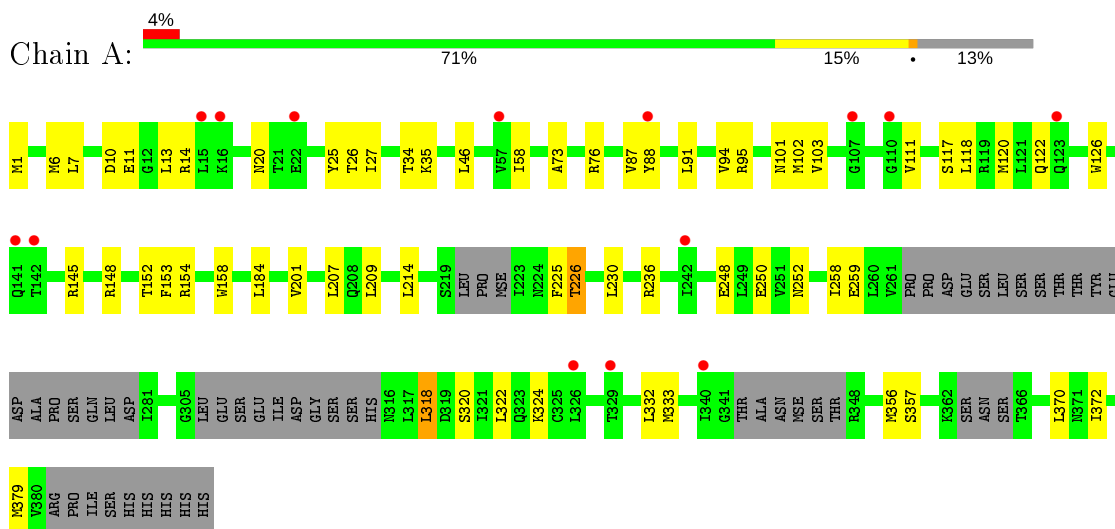
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ASN	ASP	engineered mutation	UNP A0A097J809
A	54	THR	CYS	engineered mutation	UNP A0A097J809
A	97	ALA	CYS	engineered mutation	UNP A0A097J809
A	162	ALA	-	linker	UNP A0A097J809
A	163	ALA	-	linker	UNP A0A097J809
A	164	ALA	-	linker	UNP A0A097J809
A	385	HIS	-	expression tag	UNP O94649
A	386	HIS	-	expression tag	UNP O94649
A	387	HIS	-	expression tag	UNP O94649
A	388	HIS	-	expression tag	UNP O94649
A	389	HIS	-	expression tag	UNP O94649
B	20	ASN	ASP	engineered mutation	UNP A0A097J809
B	54	THR	CYS	engineered mutation	UNP A0A097J809
B	97	ALA	CYS	engineered mutation	UNP A0A097J809
B	162	ALA	-	linker	UNP A0A097J809
B	163	ALA	-	linker	UNP A0A097J809
B	164	ALA	-	linker	UNP A0A097J809
B	385	HIS	-	expression tag	UNP O94649
B	386	HIS	-	expression tag	UNP O94649
B	387	HIS	-	expression tag	UNP O94649
B	388	HIS	-	expression tag	UNP O94649
B	389	HIS	-	expression tag	UNP O94649

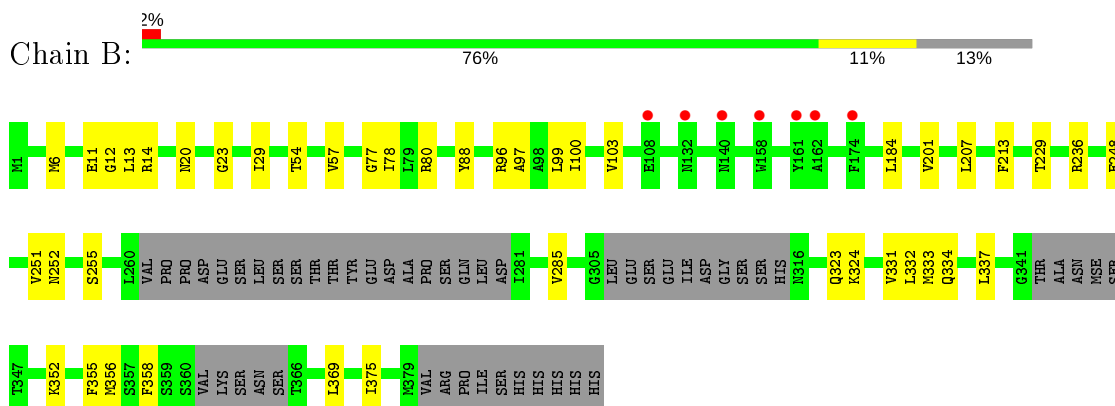
3 Residue-property plots [i](#)

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: Endolysin, Autophagy-related protein 2



- Molecule 1: Endolysin, Autophagy-related protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.45Å 62.70Å 86.32Å 90.00° 91.83° 90.00°	Depositor
Resolution (Å)	44.10 – 3.21 44.10 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.10-3.21) 99.4 (44.10-3.21)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.16 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.266 0.224 , 0.267	Depositor DCC
R_{free} test set	741 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 12.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -l,k,h 0.036 for -h,-k,l 0.447 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5023	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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	0.24	0/2529	0.41	0/3414
1	B	0.23	0/2527	0.39	0/3411
All	All	0.24	0/5056	0.40	0/6825

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	2513	0	2459	38	0
1	B	2510	0	2448	26	0
All	All	5023	0	4907	60	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 6.

All (60) 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:1:MSE:HE1	1:A:6:MSE:HB3	1.76	0.66
1:A:73:ALA:HA	1:A:76:ARG:HE	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD13	1:A:214:LEU:HD11	1.78	0.64
1:A:356:MSE:HE3	1:A:370:LEU:HD11	1.81	0.62
1:A:88:TYR:HE2	1:B:96:ARG:HH12	1.49	0.60
1:A:10:ASP:OD1	1:A:148:ARG:NH2	2.29	0.59
1:A:87:VAL:HG21	1:A:118:LEU:HB3	1.86	0.57
1:B:88:TYR:HD1	1:B:99:LEU:HD23	1.69	0.57
1:A:14:ARG:HH21	1:A:320:SER:HB2	1.69	0.56
1:B:11:GLU:O	1:B:14:ARG:NH2	2.41	0.53
1:A:20:ASN:ND2	1:A:26:THR:OG1	2.42	0.52
1:B:213:PHE:HZ	1:B:285:VAL:HG13	1.75	0.51
1:A:201:VAL:HG11	1:B:355:PHE:HZ	1.77	0.50
1:B:236:ARG:HB2	1:B:248:GLU:HB2	1.92	0.50
1:A:318:LEU:HG	1:A:322:LEU:HD13	1.95	0.49
1:A:126:TRP:HB3	1:A:154:ARG:HA	1.93	0.49
1:A:6:MSE:SE	1:A:101:ASN:HD22	2.46	0.48
1:A:236:ARG:HB2	1:A:248:GLU:HB2	1.95	0.48
1:B:77:GLY:HA2	1:B:80:ARG:HD2	1.96	0.48
1:A:102:MSE:SE	1:A:153:PHE:HE2	2.47	0.48
1:A:46:LEU:HD11	1:A:58:ILE:HG21	1.96	0.47
1:A:333:MSE:HB2	1:A:356:MSE:HG3	1.96	0.47
1:A:209:LEU:HG	1:A:230:LEU:HD22	1.96	0.47
1:A:252:ASN:ND2	1:B:334:GLN:OE1	2.47	0.47
1:A:103:VAL:HA	1:A:111:VAL:HG21	1.97	0.47
1:A:25:TYR:HB2	1:A:34:THR:HG22	1.95	0.47
1:A:11:GLU:OE2	1:A:145:ARG:NH1	2.44	0.47
1:A:184:LEU:HD13	1:A:207:LEU:HD13	1.96	0.47
1:A:94:VAL:HG12	1:A:152:THR:HG23	1.97	0.46
1:A:357:SER:OG	1:B:201:VAL:HG21	2.15	0.46
1:A:46:LEU:HD21	1:A:58:ILE:HG23	1.98	0.46
1:B:375:ILE:HD12	1:B:375:ILE:H	1.81	0.46
1:B:14:ARG:HA	1:B:323:GLN:HG2	1.98	0.46
1:A:117:SER:HA	1:A:120:MSE:HE3	1.98	0.46
1:B:78:ILE:HG12	1:B:103:VAL:HG21	1.98	0.46
1:A:225:PHE:CD1	1:A:258:ILE:HG12	2.52	0.45
1:B:13:LEU:HB3	1:B:324:LYS:HG3	1.98	0.45
1:B:251:VAL:HB	1:B:333:MSE:HG2	1.99	0.44
1:B:337:LEU:HD21	1:B:352:LYS:HG2	2.00	0.44
1:A:356:MSE:HB3	1:A:372:ILE:HG23	1.99	0.43
1:A:91:LEU:HD13	1:A:95:ARG:HB3	2.01	0.43
1:B:96:ARG:O	1:B:100:ILE:HG13	2.19	0.43
1:B:6:MSE:HE1	1:B:97:ALA:HB1	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HG2	1:A:153:PHE:HD1	1.84	0.43
1:B:251:VAL:O	1:B:333:MSE:HA	2.19	0.43
1:A:6:MSE:HE3	1:A:158:TRP:HZ3	1.84	0.42
1:A:13:LEU:HB3	1:A:324:LYS:HG3	2.01	0.42
1:B:331:VAL:HB	1:B:358:PHE:HB3	2.00	0.42
1:B:184:LEU:HD13	1:B:207:LEU:HD13	2.00	0.42
1:A:250:GLU:HA	1:A:332:LEU:O	2.20	0.42
1:B:252:ASN:HD22	1:B:334:GLN:HB2	1.85	0.42
1:B:229:THR:OG1	1:B:255:SER:HB3	2.20	0.42
1:A:87:VAL:HA	1:A:122:GLN:HG2	2.01	0.41
1:A:27:ILE:HG21	1:A:46:LEU:HD13	2.02	0.41
1:A:226:THR:HB	1:A:259:GLU:OE2	2.20	0.41
1:B:12:GLY:O	1:B:29:ILE:HG23	2.20	0.41
1:A:6:MSE:HG3	1:A:7:LEU:N	2.36	0.41
1:B:331:VAL:O	1:B:332:LEU:HD23	2.21	0.41
1:B:20:ASN:OD1	1:B:23:GLY:N	2.54	0.40
1:B:54:THR:HB	1:B:57:VAL:O	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	A	327/389 (84%)	315 (96%)	12 (4%)	0	100	100
1	B	329/389 (85%)	315 (96%)	14 (4%)	0	100	100
All	All	656/778 (84%)	630 (96%)	26 (4%)	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	251/330 (76%)	247 (98%)	4 (2%)	62	84
1	B	247/330 (75%)	245 (99%)	2 (1%)	81	93
All	All	498/660 (76%)	492 (99%)	6 (1%)	71	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	226	THR
1	A	318	LEU
1	A	379	MSE
1	B	356	MSE
1	B	369	LEU

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

Mol	Chain	Res	Type
1	B	323	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

6.1 Protein, DNA and RNA chains

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	329/389 (84%)	0.16	14 (4%) 35 22	25, 65, 94, 119	0
1	B	328/389 (84%)	0.06	7 (2%) 63 49	27, 61, 101, 126	0
All	All	657/778 (84%)	0.11	21 (3%) 47 31	25, 63, 97, 126	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	GLY	6.2
1	B	132	ASN	4.4
1	B	140	ASN	4.3
1	A	57	VAL	4.1
1	A	123	GLN	3.7
1	A	326	LEU	3.6
1	A	22	GLU	2.9
1	A	16	LYS	2.8
1	A	88	TYR	2.7
1	A	141	GLN	2.7
1	A	107	GLY	2.6
1	B	108	GLU	2.6
1	A	15	LEU	2.5
1	B	162	ALA	2.5
1	A	329	THR	2.5
1	A	142	THR	2.5
1	B	161	TYR	2.4
1	B	158	TRP	2.2
1	B	174	PHE	2.1
1	A	242	ILE	2.0
1	A	340	ILE	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 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.