



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:34 pm BST

PDB ID : 5NPW  
Title : Structure of human ATG5-ATG16L1(ATG5BD) complex (C2)  
Authors : Archana, A.; Scrima, A.  
Deposited on : 2017-04-19  
Resolution : 3.10 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](mailto: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  
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

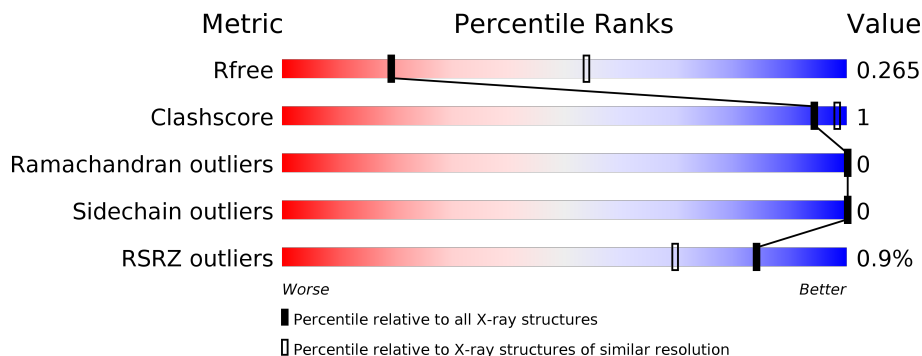
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	282	
1	C	282	
1	E	282	
1	G	282	
2	B	301	
2	D	301	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	301	 13% 87%
2	H	301	 % 13% 86%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 19441 atoms, of which 9489 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 Autophagy protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	266	4205	1406	2049	346	392	12	0	0	0
1	C	268	4253	1417	2076	351	396	13	0	0	0
1	E	266	4131	1388	1999	347	385	12	0	0	0
1	G	261	4084	1364	1984	342	381	13	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q9H1Y0
A	-5	ALA	-	expression tag	UNP Q9H1Y0
A	-4	HIS	-	expression tag	UNP Q9H1Y0
A	-3	MET	-	expression tag	UNP Q9H1Y0
A	-2	SER	-	expression tag	UNP Q9H1Y0
A	-1	GLY	-	expression tag	UNP Q9H1Y0
A	0	ARG	-	expression tag	UNP Q9H1Y0
C	-6	GLY	-	expression tag	UNP Q9H1Y0
C	-5	ALA	-	expression tag	UNP Q9H1Y0
C	-4	HIS	-	expression tag	UNP Q9H1Y0
C	-3	MET	-	expression tag	UNP Q9H1Y0
C	-2	SER	-	expression tag	UNP Q9H1Y0
C	-1	GLY	-	expression tag	UNP Q9H1Y0
C	0	ARG	-	expression tag	UNP Q9H1Y0
E	-6	GLY	-	expression tag	UNP Q9H1Y0
E	-5	ALA	-	expression tag	UNP Q9H1Y0
E	-4	HIS	-	expression tag	UNP Q9H1Y0
E	-3	MET	-	expression tag	UNP Q9H1Y0
E	-2	SER	-	expression tag	UNP Q9H1Y0
E	-1	GLY	-	expression tag	UNP Q9H1Y0
E	0	ARG	-	expression tag	UNP Q9H1Y0

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	expression tag	UNP Q9H1Y0
G	-5	ALA	-	expression tag	UNP Q9H1Y0
G	-4	HIS	-	expression tag	UNP Q9H1Y0
G	-3	MET	-	expression tag	UNP Q9H1Y0
G	-2	SER	-	expression tag	UNP Q9H1Y0
G	-1	GLY	-	expression tag	UNP Q9H1Y0
G	0	ARG	-	expression tag	UNP Q9H1Y0

- Molecule 2 is a protein called Autophagy-related protein 16-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	B	40	Total 652	C 209	H 320	N 65	O 58	0	0	0
2	D	40	Total 700	C 216	H 352	N 72	O 60	0	0	0
2	F	39	Total 673	C 212	H 335	N 67	O 59	0	0	0
2	H	41	Total 736	C 225	H 374	N 76	O 61	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	GLY	-	expression tag	UNP Q676U5
B	8	GLY	-	expression tag	UNP Q676U5
B	9	GLY	-	expression tag	UNP Q676U5
B	10	ARG	-	expression tag	UNP Q676U5
D	7	GLY	-	expression tag	UNP Q676U5
D	8	GLY	-	expression tag	UNP Q676U5
D	9	GLY	-	expression tag	UNP Q676U5
D	10	ARG	-	expression tag	UNP Q676U5
F	7	GLY	-	expression tag	UNP Q676U5
F	8	GLY	-	expression tag	UNP Q676U5
F	9	GLY	-	expression tag	UNP Q676U5
F	10	ARG	-	expression tag	UNP Q676U5
H	7	GLY	-	expression tag	UNP Q676U5
H	8	GLY	-	expression tag	UNP Q676U5
H	9	GLY	-	expression tag	UNP Q676U5
H	10	ARG	-	expression tag	UNP Q676U5

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	C	2	Total O 2 2	0	0
3	E	1	Total O 1 1	0	0
3	G	2	Total O 2 2	0	0







THR  
LEU  
LYS  
ASP  
GLU  
TYR  
ASP  
ALA  
LEU  
GLN  
ILE  
THR  
PHE  
THR  
ALA  
GLU  
GLY  
LYS  
LEU  
ARG  
GLN  
SER  
MET  
ALA  
GLU  
LYS  
ALA  
ASN  
ARG  
LEU  
ASN  
ALA  
GLU  
SER  
ASN  
GLN  
LYS  
ASP  
ASP  
ILE  
LEU  
GLU  
VAL  
ILE  
THR  
THR  
GLU  
GLU  
THR  
ASN  
GLN  
SER  
ASP  
GLU  
HIS  
LEU  
VAL  
THR  
GLU  
THR  
THR  
TRP  
SER  
MET  
ALA  
GLU  
LYS  
ALA  
ASN  
ARG  
ALA  
ASN  
ARG  
LEU  
ASN  
LYS  
ASN  
LYS  
LEU  
GLU  
SER  
GLY  
SER  
PRO  
VAL  
ARG  
ALA  
ILE  
SER  
GLU  
THR  
ALA  
THR  
LEU

GLN  
LYS  
GLU  
LEU  
ALA  
GLU  
TYR  
ASP  
ALA  
LEU  
GLN  
ILE  
THR  
PHE  
THR  
VAL  
GLU  
GLN  
ASP  
ASN  
VAL  
ASP  
ASP  
ILE  
LEU  
GLU  
VAL  
ILE  
THR  
THR  
GLU  
GLU  
THR  
THR  
TRP  
SER  
MET  
ALA  
GLU  
LYS  
ALA  
ASN  
ARG  
ALA  
ASN  
ARG  
LEU  
ASN  
LYS  
ASN  
LYS  
LEU  
GLU  
SER  
GLY  
SER  
PRO  
VAL  
ARG  
ALA  
ILE  
SER  
GLU  
THR  
ALA  
THR  
LEU

ASN  
ILE  
PHE  
GLY  
ARG  
SER  
VAL  
SER  
SER  
PHE  
SER  
PRO  
VAL  
PRO  
GLN  
ASP  
ASN  
VAL  
ASP  
THR  
THR  
HIS  
PRO  
GLY  
SER  
SER  
GLY  
LYS  
GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.86Å 75.99Å 142.44Å 90.00° 131.41° 90.00°	Depositor
Resolution (Å)	48.32 – 3.10 48.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.32-3.10) 99.6 (48.39-3.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.217 , 0.264 0.220 , 0.265	Depositor DCC
$R_{free}$ test set	1472 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtrriage
Anisotropy	0.502	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	19441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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	0.29	1/2222 (0.0%)	0.41	0/3026
1	C	0.31	1/2243 (0.0%)	0.42	0/3055
1	E	0.30	1/2198 (0.0%)	0.41	0/3001
1	G	0.31	1/2162 (0.0%)	0.41	0/2943
2	B	0.23	0/337	0.35	0/451
2	D	0.23	0/353	0.39	0/469
2	F	0.23	0/343	0.40	0/459
2	H	0.23	0/367	0.37	0/487
All	All	0.29	4/10225 (0.0%)	0.41	0/13891

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	107	PHE	C-N	9.36	1.52	1.34
1	C	107	PHE	C-N	8.50	1.50	1.34
1	A	107	PHE	C-N	7.82	1.49	1.34
1	E	107	PHE	C-N	7.75	1.49	1.34

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	2156	2049	2045	10	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2177	2076	2073	5	0
1	E	2132	1999	1998	6	0
1	G	2100	1984	1981	5	0
2	B	332	320	320	1	0
2	D	348	352	352	3	0
2	F	338	335	335	0	0
2	H	362	374	374	2	0
3	A	2	0	0	2	0
3	C	2	0	0	0	0
3	E	1	0	0	2	0
3	G	2	0	0	0	0
All	All	9952	9489	9478	26	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 1.

All (26) 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:275:ASP:OD2	2:H:26:ARG:NH1	2.10	0.85
1:E:99:ASN:OD1	3:E:301:HOH:O	2.06	0.73
1:A:24:GLN:OE1	1:A:24:GLN:N	2.23	0.71
1:A:99:ASN:ND2	3:A:302:HOH:O	2.24	0.66
1:G:6:ASP:OD1	2:H:10:ARG:NH2	2.39	0.55
1:G:237:GLN:NE2	1:G:244:GLU:OE2	2.41	0.54
1:E:95:ALA:O	3:E:301:HOH:O	2.18	0.53
1:A:112:LEU:O	3:A:301:HOH:O	2.19	0.51
1:E:227:ILE:O	1:E:227:ILE:HG22	2.13	0.49
1:A:188:ARG:NH1	1:C:25:ASP:OD2	2.49	0.46
1:A:133:ASP:OD2	1:A:142:ILE:N	2.38	0.46
1:C:69:TRP:CE2	1:C:103:HIS:HB2	2.52	0.45
1:E:116:PRO:HB2	1:E:120:ALA:HB3	2.00	0.43
1:A:109:GLU:OE1	1:A:114:HIS:NE2	2.51	0.43
1:G:184:TYR:OH	1:G:204:ARG:NH2	2.50	0.43
1:A:85:LEU:HD21	1:A:190:TYR:CZ	2.54	0.43
2:D:43:LEU:O	2:D:47:ASP:HB2	2.20	0.42
1:G:69:TRP:CE2	1:G:103:HIS:HB2	2.54	0.42
1:A:275:ASP:OD2	1:A:275:ASP:O	2.38	0.42
1:C:109:GLU:OE1	1:C:114:HIS:NE2	2.53	0.42
1:C:38:LEU:HD11	2:D:33:GLU:HA	2.02	0.42
2:D:31:ALA:HA	1:E:96:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TYR:HB3	2:B:36:ILE:CD1	2.50	0.41
1:E:88:ASP:HA	1:E:92:SER:HB3	2.02	0.41
1:G:23:TYR:HB3	1:G:26:GLU:HG2	2.03	0.41
1:C:66:SER:OG	1:C:67:GLU:N	2.54	0.41

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	262/282 (93%)	258 (98%)	4 (2%)	0	100	100
1	C	264/282 (94%)	258 (98%)	6 (2%)	0	100	100
1	E	262/282 (93%)	255 (97%)	7 (3%)	0	100	100
1	G	253/282 (90%)	245 (97%)	8 (3%)	0	100	100
2	B	38/301 (13%)	36 (95%)	2 (5%)	0	100	100
2	D	38/301 (13%)	36 (95%)	2 (5%)	0	100	100
2	F	37/301 (12%)	36 (97%)	1 (3%)	0	100	100
2	H	39/301 (13%)	37 (95%)	2 (5%)	0	100	100
All	All	1193/2332 (51%)	1161 (97%)	32 (3%)	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	228/258 (88%)	228 (100%)	0	100	100
1	C	232/258 (90%)	232 (100%)	0	100	100
1	E	223/258 (86%)	223 (100%)	0	100	100
1	G	222/258 (86%)	222 (100%)	0	100	100
2	B	32/267 (12%)	32 (100%)	0	100	100
2	D	36/267 (14%)	36 (100%)	0	100	100
2	F	35/267 (13%)	35 (100%)	0	100	100
2	H	38/267 (14%)	38 (100%)	0	100	100
All	All	1046/2100 (50%)	1046 (100%)	0	100	100

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

Some 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 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	266/282 (94%)	-0.23	1 (0%) 92 84	31, 57, 108, 151	0
1	C	268/282 (95%)	-0.25	3 (1%) 80 64	33, 55, 92, 121	0
1	E	266/282 (94%)	-0.10	4 (1%) 73 54	36, 65, 110, 171	0
1	G	261/282 (92%)	-0.19	1 (0%) 92 84	35, 59, 110, 160	0
2	B	40/301 (13%)	-0.12	0 100 100	40, 65, 107, 119	0
2	D	40/301 (13%)	-0.29	0 100 100	41, 54, 89, 99	0
2	F	39/301 (12%)	0.03	0 100 100	35, 62, 102, 110	0
2	H	41/301 (13%)	-0.06	2 (4%) 29 14	41, 58, 104, 126	0
All	All	1221/2332 (52%)	-0.18	11 (0%) 84 69	31, 59, 108, 171	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	116	PRO	4.3
1	E	3	ASP	4.0
1	C	274	THR	3.9
2	H	8	GLY	2.9
1	A	27	ILE	2.7
1	E	208	ALA	2.6
2	H	9	GLY	2.5
1	C	228	ASP	2.4
1	E	273	PRO	2.2
1	E	178	GLU	2.2
1	C	94	SER	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

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.