Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 12:30 PM GMT

PDB ID	:	3VH3
Title	:	Crystal structure of Atg7CTD-Atg8 complex
Authors	:	Noda, N.N.; Satoo, K.; Inagaki, F.
Deposited on	:	2011-08-23
Resolution	:	2.00 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		12
Ramachandran outliers		0.5%
Sidechain outliers		5.0%
RSRZ outliers		10.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
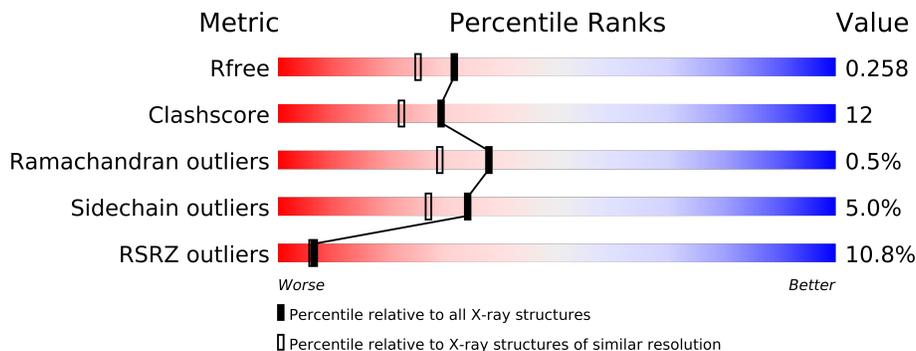
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	340	
2	B	119	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3459 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ubiquitin-like modifier-activating enzyme ATG7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total 2438	C 1560	N 415	O 448	S 15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLY	-	EXPRESSION TAG	UNP P38862
A	292	PRO	-	EXPRESSION TAG	UNP P38862
A	293	HIS	-	EXPRESSION TAG	UNP P38862
A	294	MET	-	EXPRESSION TAG	UNP P38862

- Molecule 2 is a protein called Autophagy-related protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total 852	C 557	N 137	O 155	S 3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP P38182
B	-1	PRO	-	EXPRESSION TAG	UNP P38182
B	0	HIS	-	EXPRESSION TAG	UNP P38182
B	26	PRO	LYS	ENGINEERED MUTATION	UNP P38182

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total O 140 140		0	0
4	B	28	Total O 28 28		0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Ubiquitin-like modifier-activating enzyme ATG7

Chain A:
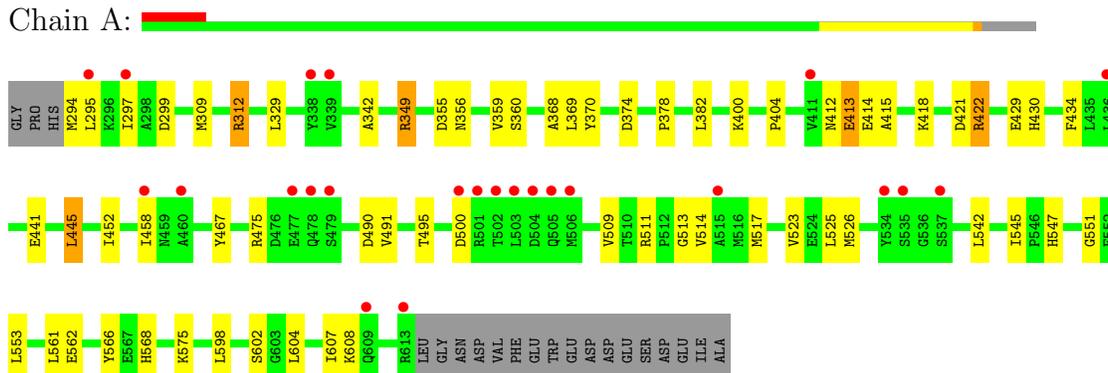
• Molecule 2: Autophagy-related protein 8

Chain B:
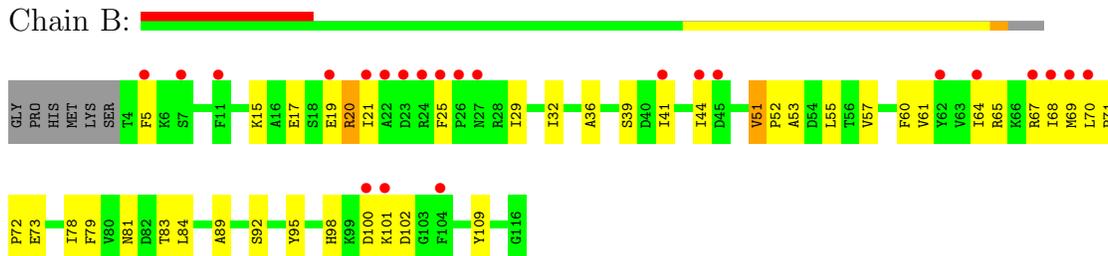
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	69.81Å 69.81Å 220.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.28 – 2.00 33.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.6 (33.28-2.00) 91.6 (33.28-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	5.30 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.257 0.230 , 0.258	Depositor DCC
R_{free} test set	3438 reflections (10.98%)	DCC
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 37843 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3459	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.34	0/2486	0.61	0/3379
2	B	0.32	0/874	0.53	0/1191
All	All	0.34	0/3360	0.60	0/4570

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2438	0	2415	40	0
2	B	852	0	797	41	0
3	A	1	0	0	0	0
4	A	140	0	0	3	0
4	B	28	0	0	0	0
All	All	3459	0	3212	80	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (80) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:PRO:HG2	1:A:445:LEU:HD12	1.57	0.86
2:B:53:ALA:HB1	2:B:92:SER:HB3	1.59	0.82
2:B:70:LEU:HD12	2:B:71:PRO:HD2	1.60	0.81
1:A:349:ARG:HH11	1:A:349:ARG:HG2	1.46	0.79
2:B:60:PHE:CE2	2:B:64:ILE:HD11	2.21	0.76
2:B:71:PRO:HB2	2:B:73:GLU:OE1	1.86	0.75
1:A:561:LEU:HD13	2:B:84:LEU:HD13	1.73	0.70
2:B:52:PRO:HG2	2:B:55:LEU:HB2	1.75	0.69
1:A:374:ASP:HB3	1:A:382:LEU:HD11	1.79	0.64
1:A:349:ARG:HG2	1:A:349:ARG:NH1	2.11	0.64
2:B:29:ILE:HD11	2:B:53:ALA:HA	1.82	0.61
1:A:441:GLU:CG	1:A:495:THR:O	2.49	0.61
2:B:79:PHE:CE1	2:B:84:LEU:HD12	2.37	0.59
1:A:604:LEU:O	1:A:608:LYS:HG3	2.03	0.59
2:B:5:PHE:CD1	2:B:32:ILE:HD13	2.38	0.58
1:A:441:GLU:HG3	1:A:495:THR:O	2.03	0.58
1:A:370:TYR:HD2	1:A:382:LEU:HD22	1.70	0.57
2:B:17:GLU:O	2:B:21:ILE:HG13	2.05	0.56
2:B:81:ASN:ND2	2:B:98:HIS:HB3	2.21	0.56
1:A:509:VAL:HA	4:A:815:HOH:O	2.04	0.56
1:A:356:ASN:HA	1:A:400:LYS:HG3	1.87	0.56
2:B:20:ARG:HG2	2:B:20:ARG:HH11	1.72	0.55
2:B:64:ILE:HG22	2:B:68:ILE:HD12	1.89	0.54
2:B:57:VAL:HG23	2:B:89:ALA:O	2.08	0.54
1:A:452:ILE:HA	1:A:475:ARG:HH21	1.73	0.54
1:A:412:ASN:HB3	1:A:415:ALA:HB3	1.91	0.52
2:B:79:PHE:HE1	2:B:84:LEU:HD12	1.75	0.52
1:A:517:MET:HE3	1:A:553:LEU:HD11	1.92	0.51
2:B:36:ALA:HB3	2:B:39:SER:HB2	1.91	0.51
1:A:413:GLU:HG3	1:A:414:GLU:N	2.24	0.51
2:B:68:ILE:O	2:B:68:ILE:HG22	2.11	0.51
1:A:404:PRO:HG2	1:A:445:LEU:CD1	2.37	0.51
2:B:61:VAL:O	2:B:65:ARG:HG2	2.11	0.50
1:A:370:TYR:CD2	1:A:382:LEU:HD22	2.47	0.49
2:B:65:ARG:NH2	2:B:72:PRO:HA	2.28	0.49
2:B:29:ILE:N	2:B:51:VAL:O	2.46	0.48
2:B:57:VAL:O	2:B:61:VAL:HG23	2.13	0.48
1:A:458:ILE:CD1	1:A:526:MET:HB2	2.43	0.48
2:B:20:ARG:HG2	2:B:20:ARG:NH1	2.28	0.48
2:B:41:ILE:HD11	2:B:109:TYR:CD1	2.49	0.48
2:B:70:LEU:CD1	2:B:71:PRO:HD2	2.38	0.47
2:B:65:ARG:HH21	2:B:72:PRO:HA	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:41:ILE:HD11	2:B:109:TYR:HD1	1.79	0.47
2:B:64:ILE:O	2:B:68:ILE:HG13	2.15	0.47
1:A:490:ASP:OD1	1:A:491:VAL:N	2.39	0.47
1:A:418:LYS:O	1:A:422:ARG:HB2	2.15	0.47
2:B:29:ILE:CD1	2:B:53:ALA:HA	2.45	0.46
2:B:60:PHE:O	2:B:64:ILE:HG13	2.15	0.46
1:A:378:PRO:HB2	4:A:820:HOH:O	2.14	0.46
2:B:17:GLU:HG3	2:B:20:ARG:NH1	2.30	0.46
1:A:429:GLU:HG3	1:A:430:HIS:ND1	2.31	0.46
2:B:73:GLU:CD	2:B:73:GLU:H	2.20	0.45
1:A:607:ILE:HD12	1:A:608:LYS:N	2.32	0.45
1:A:547:HIS:HD2	1:A:562:GLU:HA	1.82	0.45
2:B:72:PRO:HG2	2:B:73:GLU:OE2	2.17	0.44
1:A:517:MET:CE	1:A:553:LEU:HD11	2.48	0.44
1:A:342:ALA:HB3	1:A:523:VAL:HG21	1.99	0.44
2:B:57:VAL:CG1	2:B:78:ILE:HD11	2.48	0.43
1:A:467:TYR:CZ	1:A:551:GLY:HA3	2.53	0.43
1:A:359:VAL:HG21	1:A:382:LEU:HD13	1.99	0.43
1:A:355:ASP:O	1:A:400:LYS:HA	2.17	0.43
1:A:312:ARG:HG2	1:A:312:ARG:HH11	1.82	0.43
1:A:299:ASP:OD1	1:A:349:ARG:NH2	2.52	0.43
1:A:607:ILE:HD12	1:A:607:ILE:C	2.38	0.43
2:B:17:GLU:HA	2:B:20:ARG:HG2	2.01	0.43
2:B:44:ILE:HD12	2:B:67:ARG:O	2.19	0.43
2:B:29:ILE:HG23	2:B:95:TYR:CD2	2.54	0.42
1:A:545:ILE:O	1:A:545:ILE:HG13	2.19	0.42
2:B:15:LYS:O	2:B:19:GLU:HG3	2.19	0.42
1:A:511:ARG:O	1:A:514:VAL:HG22	2.19	0.42
1:A:566:TYR:CE2	1:A:568:HIS:HB2	2.55	0.41
1:A:513:GLY:O	1:A:517:MET:HG3	2.21	0.41
1:A:294:MET:O	1:A:297:ILE:HG22	2.20	0.41
2:B:100:ASP:HB3	2:B:102:ASP:OD1	2.20	0.41
2:B:64:ILE:CG2	2:B:68:ILE:HD12	2.51	0.41
1:A:329:LEU:HD23	1:A:434:PHE:HB2	2.03	0.41
1:A:575:LYS:HE2	1:A:602:SER:O	2.20	0.41
1:A:514:VAL:HG12	1:A:553:LEU:HD13	2.03	0.40
2:B:100:ASP:OD1	2:B:101:LYS:N	2.55	0.40
4:A:905:HOH:O	2:B:83:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	318/340 (94%)	307 (96%)	9 (3%)	2 (1%)	33	24
2	B	111/119 (93%)	105 (95%)	6 (5%)	0	100	100
All	All	429/459 (94%)	412 (96%)	15 (4%)	2 (0%)	38	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	ALA
1	A	413	GLU

5.3.2 Protein sidechains ⓘ

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	259/298 (87%)	246 (95%)	13 (5%)	34	27
2	B	82/106 (77%)	78 (95%)	4 (5%)	35	28
All	All	341/404 (84%)	324 (95%)	17 (5%)	34	27

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	LEU
1	A	309	MET
1	A	312	ARG
1	A	349	ARG
1	A	360	SER
1	A	369	LEU
1	A	421	ASP

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Mol	Chain	Res	Type
1	A	422	ARG
1	A	445	LEU
1	A	500	ASP
1	A	525	LEU
1	A	542	LEU
1	A	598	LEU
2	B	20	ARG
2	B	25	PHE
2	B	51	VAL
2	B	69	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	HIS
1	A	547	HIS
2	B	81	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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.

5.7 Other polymers ⓘ

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 ⓘ

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	320/340 (94%)	0.41	24 (7%)	14	13	28, 43, 74, 85	0
2	B	113/119 (94%)	1.10	23 (20%)	1	2	33, 71, 91, 96	0
All	All	433/459 (94%)	0.59	47 (10%)	6	6	28, 47, 84, 96	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	25	PHE	5.3
2	B	23	ASP	4.9
1	A	478	GLN	4.5
2	B	24	ARG	4.4
2	B	27	ASN	4.4
2	B	5	PHE	4.3
2	B	44	ILE	4.1
1	A	501	ARG	3.7
2	B	7	SER	3.7
1	A	504	ASP	3.6
1	A	506	MET	3.5
1	A	505	GLN	3.5
1	A	339	VAL	3.4
2	B	22	ALA	3.2
2	B	21	ILE	3.2
2	B	62	TYR	3.2
1	A	477	GLU	3.1
1	A	534	TYR	3.1
1	A	500	ASP	3.0
1	A	609	GLN	3.0
2	B	19	GLU	3.0
2	B	45	ASP	3.0
2	B	67	ARG	2.9
1	A	297	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	26	PRO	2.8
1	A	535	SER	2.7
2	B	104	PHE	2.7
2	B	41	ILE	2.6
2	B	101	LYS	2.6
1	A	460	ALA	2.6
1	A	502	THR	2.6
2	B	11	PHE	2.5
2	B	100	ASP	2.5
1	A	479	SER	2.5
1	A	338	TYR	2.5
2	B	69	MET	2.4
1	A	537	SER	2.4
2	B	64	ILE	2.4
1	A	503	LEU	2.4
1	A	458	ILE	2.3
1	A	515	ALA	2.3
1	A	295	LEU	2.3
2	B	70	LEU	2.2
1	A	436	LEU	2.2
1	A	613	ARG	2.2
1	A	411	VAL	2.1
2	B	68	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	701	1/1	0.10	-1.31	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.