



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 02:07 PM JST

PDB ID : 8GU7
Title : Selective targeting of the Beclin 2-Atg14L coiled coil complex by stapled peptides promotes autophagy and endolysosomal trafficking of GPCRs
Authors : Qiu, X.; Zhao, Y.
Deposited on : 2022-09-11
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

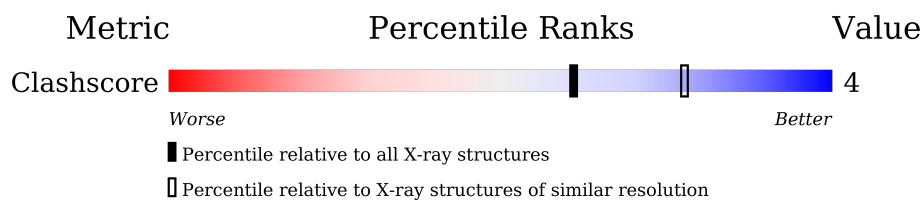
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1099 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 Beclin 1-associated autophagy-related key regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	37	308	192	57	56	3	0	0	0
1	B	36	307	193	57	54	3	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8CDJ3
A	0	PRO	-	expression tag	UNP Q8CDJ3
A	1	GLY	-	expression tag	UNP Q8CDJ3
A	2	SER	-	expression tag	UNP Q8CDJ3
A	3	GLY	-	expression tag	UNP Q8CDJ3
A	4	SER	-	expression tag	UNP Q8CDJ3
A	20	LEU	CYS	engineered mutation	UNP Q8CDJ3
A	32	SER	CYS	engineered mutation	UNP Q8CDJ3
A	34	LEU	GLY	engineered mutation	UNP Q8CDJ3
B	-1	GLY	-	expression tag	UNP Q8CDJ3
B	0	PRO	-	expression tag	UNP Q8CDJ3
B	1	GLY	-	expression tag	UNP Q8CDJ3
B	2	SER	-	expression tag	UNP Q8CDJ3
B	3	GLY	-	expression tag	UNP Q8CDJ3
B	4	SER	-	expression tag	UNP Q8CDJ3
B	20	LEU	CYS	engineered mutation	UNP Q8CDJ3
B	32	SER	CYS	engineered mutation	UNP Q8CDJ3
B	34	LEU	GLY	engineered mutation	UNP Q8CDJ3

- Molecule 2 is a protein called Beclin-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	31	251	149	46	56	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	28	227	137	41	49	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	expression tag	UNP A8MW95
C	2	PRO	-	expression tag	UNP A8MW95
C	3	GLY	-	expression tag	UNP A8MW95
C	4	SER	-	expression tag	UNP A8MW95
C	91	LEU	ARG	engineered mutation	UNP A8MW95
D	1	GLY	-	expression tag	UNP A8MW95
D	2	PRO	-	expression tag	UNP A8MW95
D	3	GLY	-	expression tag	UNP A8MW95
D	4	SER	-	expression tag	UNP A8MW95
D	91	LEU	ARG	engineered mutation	UNP A8MW95

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	D	4	Total	O	0	0
			4	4		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.50Å 72.50Å 68.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.11 – 2.60	Depositor
% Data completeness (in resolution range)	99.7 (41.11-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.11 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.217 , 0.240	Depositor
Wilson B-factor (Å ²)	41.2	Xtrriage
Anisotropy	0.243	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1099	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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.

4 Model quality [i](#)

4.1 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	1.06	0/309	0.88	0/406
1	B	0.84	0/308	0.96	0/404
2	C	1.03	0/250	0.94	0/336
2	D	0.98	0/226	1.01	0/303
All	All	0.98	0/1093	0.94	0/1449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	308	0	334	1	0
1	B	307	0	339	6	0
2	C	251	0	238	4	0
2	D	227	0	222	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	4	0	0	0	0
All	All	1099	0	1133	10	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 4.

The worst 5 of 10 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:23:ARG:HD2	2:D:21:GLU:OE2	1.94	0.68
2:D:28:LEU:O	2:D:31:VAL:HG12	1.97	0.63
2:C:35:ASN:OD1	2:C:35:ASN:N	2.32	0.61
1:B:23:ARG:HD3	2:C:21:GLU:OE2	2.11	0.51
1:B:23:ARG:HH21	1:B:26:GLN:NE2	2.09	0.51

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.