wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 09:13 AM UTC

PDB ID	:	8Y1U / pdb_00008y1u
Title	:	Crystal structure of ASB7-Elongin B/C bound to the LZTS1-degron
Authors	:	Dong, C.; Yan, X.; Zhou, M.
Deposited on	:	2024-01-25
Resolution	:	2.41 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 (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:

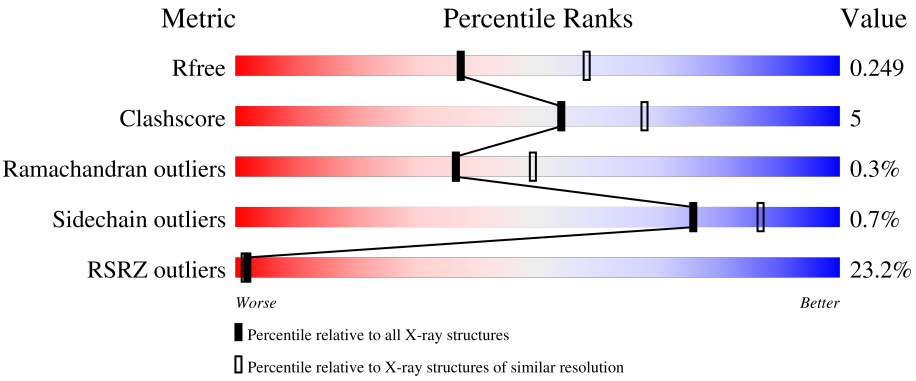
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	309	13% 84% 14%
2	B	23	4% 83% 17%
3	C	104	26% 28% 6% 66%
4	D	96	31% 59% 38%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3191 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 Ankyrin repeat and SOCS box protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2324	1447	431	435	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP Q9H672

- Molecule 2 is a protein called Peptide from Leucine zipper putative tumor suppressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	S	0	0	0
			201	123	36	41	1			

- Molecule 3 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	S	0	0	0
			201	121	36	43	1			

- Molecule 4 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	60	Total	C	N	O	S	0	0	0
			380	235	70	74	1			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	64	Total	O	0	0
			64	64		

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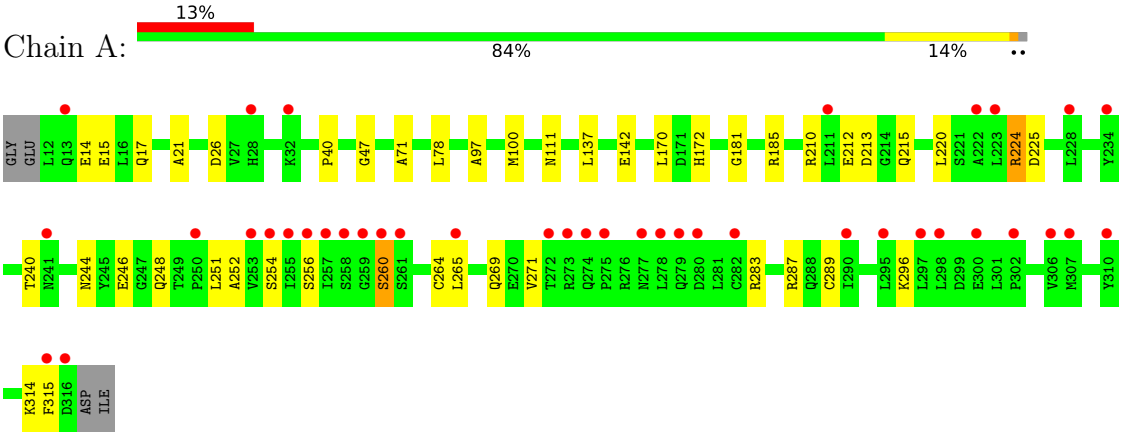
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	14	Total O 14 14	0	0
5	C	6	Total O 6 6	0	0
5	D	1	Total O 1 1	0	0

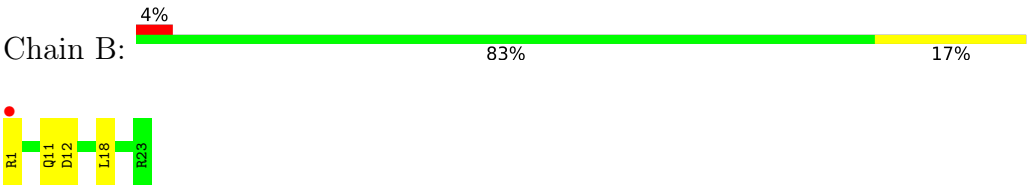
3 Residue-property plots (i)

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.

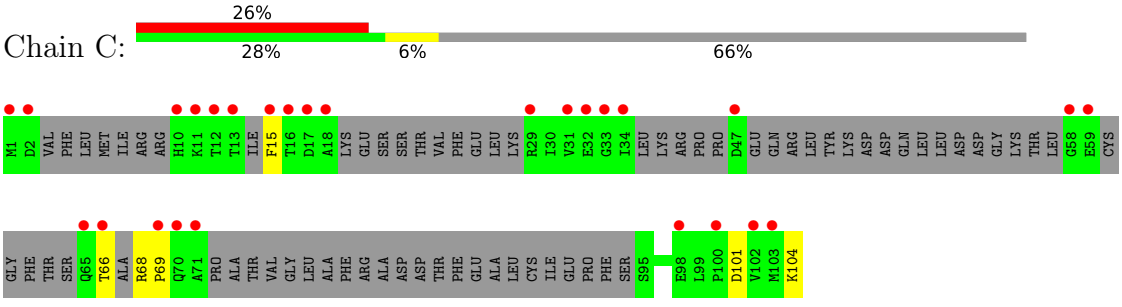
• Molecule 1: Ankyrin repeat and SOCS box protein 7



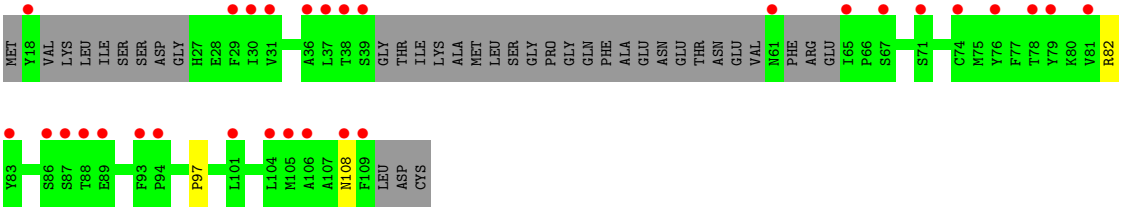
• Molecule 2: Peptide from Leucine zipper putative tumor suppressor 1



• Molecule 3: Elongin-B



• Molecule 4: Elongin-C


MET
Y18
VAL
LYS
LEU
ILE
SER
SER
ASP
GLY
H27
E28
F29
I30
V31
A36
L37
T38
S39
GLY
THR
ILE
LYS
ALA
MET
LEU
SER
GLY
PRO
GLY
GLN
PHE
ALA
GLU
ASN
GLU
THR
ASN
GLU
VAL
N61
PHE
ARG
GLU
I65
P66
S67
S71
C74
M75
Y76
F77
T78
Y79
K80
V81
R82
Y83
S86
S87
T88
E89
F93
P94
P97
L101
L104
M105
A106
A107
N108
F109
LEU
ASP
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.15Å 43.72Å 159.23Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	48.12 – 2.41 48.12 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.12-2.41) 99.5 (48.12-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.215 , 0.243 0.227 , 0.249	Depositor DCC
R_{free} test set	1999 reflections (7.65%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 81.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3191	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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	0.44	0/2366	0.70	2/3206 (0.1%)
2	B	0.44	0/201	0.69	0/265
3	C	0.53	0/196	0.87	0/258
4	D	0.68	0/386	1.14	1/529 (0.2%)
All	All	0.48	0/3149	0.78	3/4258 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	108	ASN	N-CA-C	-12.45	98.07	113.38
1	A	296	LYS	N-CA-C	-7.46	104.21	113.38
1	A	224	ARG	CA-C-O	-5.01	115.09	120.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2324	0	2217	23	1
2	B	201	0	207	4	0
3	C	201	0	126	4	0
4	D	380	0	267	2	0
5	A	64	0	0	0	0
5	B	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	6	0	0	1	0
5	D	1	0	0	0	0
All	All	3191	0	2817	29	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 5.

The worst 5 of 29 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:283:ARG:O	1:A:287:ARG:HG3	1.93	0.69
3:C:101:ASP:HA	3:C:104:LYS:HG2	1.74	0.68
1:A:260:SER:HA	1:A:265:LEU:HD21	1.80	0.63
1:A:14:GLU:HA	1:A:17:GLN:HG2	1.79	0.63
3:C:66:THR:C	3:C:68:ARG:N	2.62	0.58

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-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLU:OE2	1:A:224:ARG:NH1[2_456]	1.78	0.42

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	303/309 (98%)	291 (96%)	11 (4%)	1 (0%)	36 49
2	B	21/23 (91%)	21 (100%)	0	0	100 100
3	C	18/104 (17%)	15 (83%)	3 (17%)	0	100 100
4	D	54/96 (56%)	47 (87%)	7 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	396/532 (74%)	374 (94%)	21 (5%)	1 (0%)	36 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	SER

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	232/262 (88%)	230 (99%)	2 (1%)	70 84
2	B	23/23 (100%)	23 (100%)	0	100 100
3	C	11/92 (12%)	11 (100%)	0	100 100
4	D	25/85 (29%)	25 (100%)	0	100 100
All	All	291/462 (63%)	289 (99%)	2 (1%)	76 87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	256	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	293	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 oligosaccharides 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, 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>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	305/309 (98%)	0.76	40 (13%) 7 5	31, 65, 144, 170	0
2	B	23/23 (100%)	0.34	1 (4%) 40 35	35, 47, 79, 116	0
3	C	35/104 (33%)	2.83	27 (77%) 0 0	109, 161, 225, 259	0
4	D	60/96 (62%)	2.29	30 (50%) 0 0	110, 151, 185, 195	0
All	All	423/532 (79%)	1.13	98 (23%) 2 1	31, 77, 178, 259	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	109	PHE	6.6
4	D	18	TYR	6.2
4	D	61	ASN	5.3
1	A	222	ALA	5.3
3	C	18	ALA	5.3

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.