wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 05:37 AM EDT

PDB ID	:	7MU2
Title	:	Crystal Structure of WIPI2 in complex with W2IR of ATG16L1
Authors	:	Strong, L.M.; Flower, T.G.; Buffalo, C.Z.; Hurley, J.H.
Deposited on	:	2021-05-14
Resolution	:	1.85 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 (i)) were used in the production of this report:

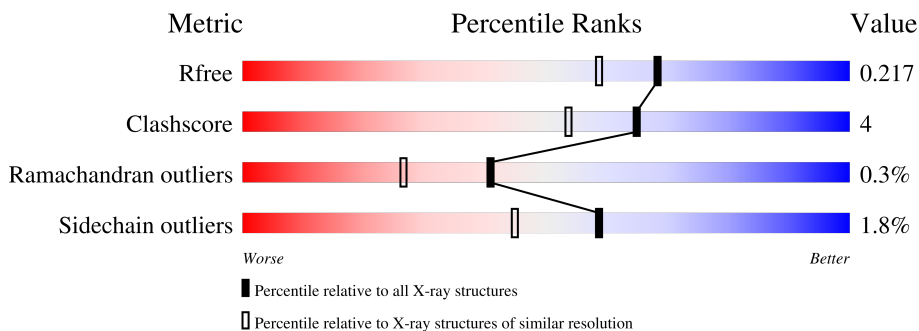|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.85 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		0.217
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		1.8%

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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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%

Mol	Chain	Length	Quality of chain
1	A	324	86% 8% · 5%
1	C	324	91% 6% ·
2	B	25	64% 12% 8% 16%
2	D	25	48% 52%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5665 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 WD repeat domain phosphoinositide-interacting protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2356	1494	402	443	17			
1	C	316	Total	C	N	O	S	0	0	0
			2422	1534	416	453	19			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	0	0	0
			170	100	35	35			
2	D	12	Total	C	N	O	0	0	0
			92	56	17	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	TYR	-	insertion	UNP E7EVC7
D	206	TYR	-	insertion	UNP E7EVC7

- Molecule 3 is water.

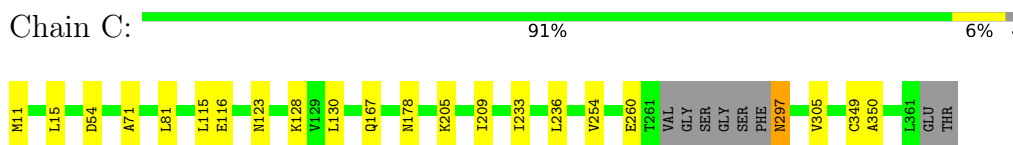| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	309	Total	O	0	0
			309	309		
3	B	18	Total	O	0	0
			18	18		
3	C	292	Total	O	0	0
			292	292		
3	D	6	Total	O	0	0
			6	6		

3 Residue-property plots ⓘ

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. 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. 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.
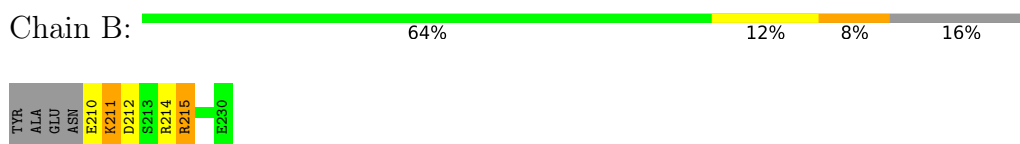
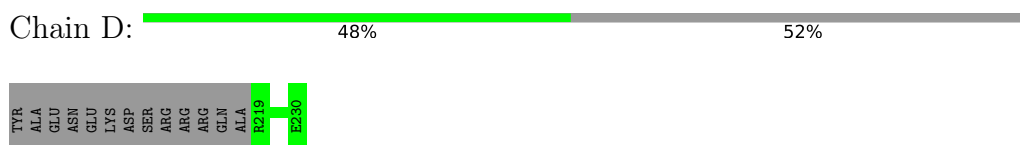• Molecule 1: WD repeat domain phosphoinositide-interacting protein 2
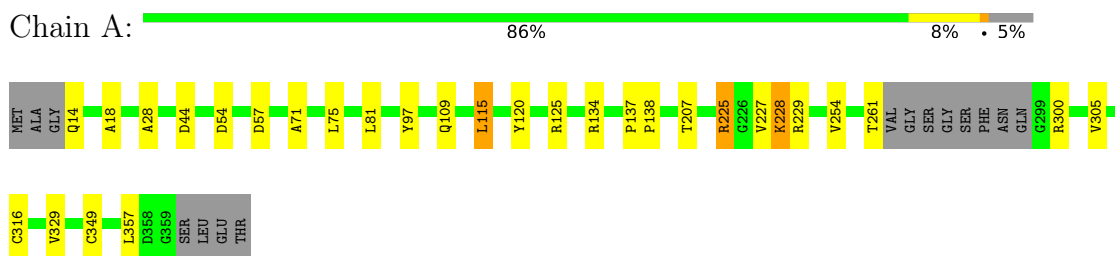
Chain A:

86%   8%   · 5%

MET ALA GLY Q14 A18 A28 D44 D54 D57 A71 L75 L81 Y97 Q109 L115 Y120 R125 R134 P137 P138 T207 R225 G226 V227 K228 R229 V254 T261 VAL GLY SER GLY SER PHE ASN GLN G299 R300 V305

C316 V329 C349 L357 D358 G359 SER LEU GLU THR

• Molecule 1: WD repeat domain phosphoinositide-interacting protein 2

Chain C:

91%   6%   ·

M11 L15 D54 A71 L81 L115 E116 N123 K128 V129 L130 Q167 N178 K205 I209 I233 L236 V254 E260 T261 VAL GLY SER GLY SER PHE N297 V305 C349 A350 L361 GLU THR

• Molecule 2: Autophagy-related protein 16-1

Chain B:

64%   12%   8%   16%

TYR ALA GLU ASN E210 K211 D212 S213 R214 R215 E230

• Molecule 2: Autophagy-related protein 16-1

Chain D:

48%   52%

TYR ALA GLU ASN GLU LYS ASP SER ARG ARG GLN ALA R219 E230

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.77Å 49.08Å 120.13Å 90.00° 95.86° 90.00°	Depositor
Resolution (Å)	38.94 – 1.85 38.95 – 1.27	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.94-1.85) 54.3 (38.95-1.27)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.51 (at 1.27Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.183 , 0.217 0.183 , 0.217	Depositor DCC
R_{free} test set	2001 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å^2)	9.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5665	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.39	0/2398	0.61	0/3243
1	C	0.38	0/2464	0.61	0/3330
2	B	0.35	0/169	0.42	0/220
2	D	0.33	0/91	0.51	0/120
All	All	0.38	0/5122	0.60	0/6913

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 ⓘ

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	2356	0	2342	22	1
1	C	2422	0	2431	16	0
2	B	170	0	170	4	0
2	D	92	0	90	0	0
3	A	309	0	0	9	4
3	B	18	0	0	1	1
3	C	292	0	0	8	1
3	D	6	0	0	0	0
All	All	5665	0	5033	41	5

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 41 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:134:ARG:NH1	3:A:403:HOH:O	2.09	0.85
1:A:229:ARG:O	3:A:401:HOH:O	1.96	0.84
1:C:54:ASP:OD1	3:C:401:HOH:O	1.99	0.81
1:A:228:LYS:O	3:A:402:HOH:O	2.04	0.74
1:A:225:ARG:NE	3:A:401:HOH:O	2.20	0.73

All (5) 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)
3:A:441:HOH:O	3:C:609:HOH:O[2_656]	1.91	0.29
3:A:634:HOH:O	3:A:675:HOH:O[4_556]	2.09	0.11
1:A:261:THR:OG1	1:A:261:THR:OG1[2_656]	2.11	0.09
3:A:453:HOH:O	3:A:634:HOH:O[4_546]	2.13	0.07
3:A:684:HOH:O	3:B:318:HOH:O[4_546]	2.14	0.06

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	305/324 (94%)	299 (98%)	4 (1%)	2 (1%)	22	9
1	C	312/324 (96%)	305 (98%)	7 (2%)	0	100	100
2	B	19/25 (76%)	18 (95%)	1 (5%)	0	100	100
2	D	10/25 (40%)	9 (90%)	1 (10%)	0	100	100
All	All	646/698 (93%)	631 (98%)	13 (2%)	2 (0%)	41	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	VAL
1	A	228	LYS

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	256/276 (93%)	251 (98%)	5 (2%)	55	40
1	C	266/276 (96%)	264 (99%)	2 (1%)	81	76
2	B	16/20 (80%)	13 (81%)	3 (19%)	1	0
2	D	8/20 (40%)	8 (100%)	0	100	100
All	All	546/592 (92%)	536 (98%)	10 (2%)	59	45

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	215	ARG
1	C	115	LEU
1	C	297	ASN
1	A	300	ARG
1	A	357	LEU

Sometimes 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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.