



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:37 PM BST

PDB ID : 6ZM3
Title : The structure of an E2 ubiquitin-conjugating complex (UBC2-UEV1) essential for Leishmania amastigote differentiation
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Deposited on : 2020-07-01
Resolution : 1.70 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

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	:	2.13.1
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)	:	2.13.1

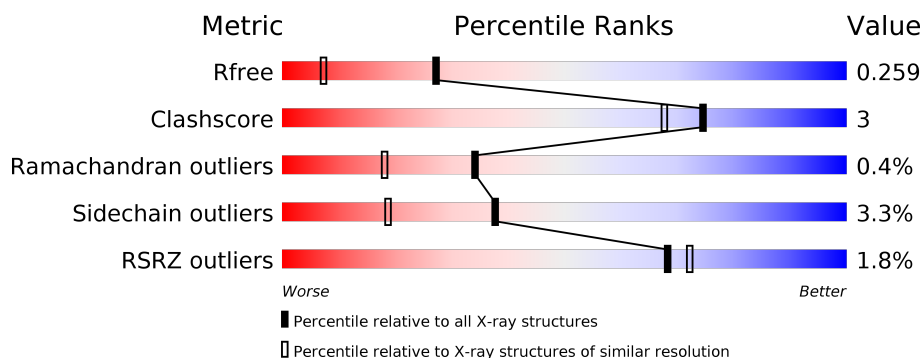
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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	AAA	151	<div> <div>%</div> <div> </div> <div>89% 8% .</div> </div>
1	CCC	151	<div> <div>3%</div> <div> </div> <div>87% 9% . .</div> </div>
2	BBB	141	<div> <div>%</div> <div> </div> <div>83% 11% . .</div> </div>
2	DDD	141	<div> <div>%</div> <div> </div> <div>88% 8% . .</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4921 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 Putative ubiquitin-conjugating enzyme e2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	147	Total	C	N	O	S	0	0	0
			1191	767	201	217	6			
1	CCC	146	Total	C	N	O	S	0	0	0
			1183	761	200	216	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	GLY	-	expression tag	UNP E9AK51
AAA	-1	PRO	-	expression tag	UNP E9AK51
AAA	0	ALA	-	expression tag	UNP E9AK51
CCC	-2	GLY	-	expression tag	UNP E9AK51
CCC	-1	PRO	-	expression tag	UNP E9AK51
CCC	0	ALA	-	expression tag	UNP E9AK51

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	138	Total	C	N	O	S	2	4	0
			1155	728	201	220	6			
2	DDD	136	Total	C	N	O	S	0	1	0
			1125	713	195	211	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-2	GLY	-	expression tag	UNP E9API2
BBB	-1	PRO	-	expression tag	UNP E9API2
BBB	0	ALA	-	expression tag	UNP E9API2
DDD	-2	GLY	-	expression tag	UNP E9API2
DDD	-1	PRO	-	expression tag	UNP E9API2
DDD	0	ALA	-	expression tag	UNP E9API2

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	85	Total 85	O 85	0	0
3	BBB	70	Total 70	O 70	0	0
3	CCC	43	Total 43	O 43	0	0
3	DDD	69	Total 69	O 69	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.

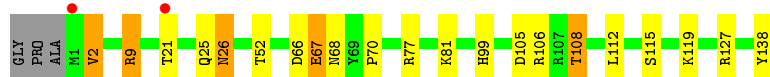
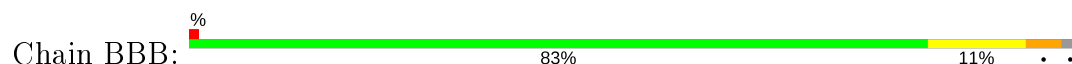
- Molecule 1: Putative ubiquitin-conjugating enzyme e2



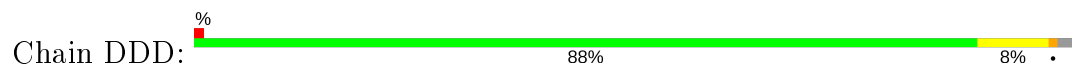
- Molecule 1: Putative ubiquitin-conjugating enzyme e2



- Molecule 2: Ubiquitin-conjugating enzyme-like protein



- Molecule 2: Ubiquitin-conjugating enzyme-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	32.52Å 72.57Å 120.09Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	46.25 – 1.70 46.25 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.25-1.70) 98.9 (46.25-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258, REFMAC 5.8.0258	Depositor
R, R_{free}	0.223 , 0.260 0.221 , 0.259	Depositor DCC
R_{free} test set	3255 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4921	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9473e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

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	AAA	0.41	0/1223	0.81	0/1662
1	CCC	0.38	0/1215	0.73	0/1651
2	BBB	0.48	1/1187 (0.1%)	0.82	3/1608 (0.2%)
2	DDD	0.41	0/1156	0.82	1/1565 (0.1%)
All	All	0.42	1/4781 (0.0%)	0.80	4/6486 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	119	LYS	CD-CE	6.45	1.67	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	26	ASN	CB-CA-C	5.63	121.66	110.40
2	BBB	67	GLU	CB-CA-C	-5.51	99.37	110.40
2	DDD	9	ARG	CG-CD-NE	-5.49	100.27	111.80
2	BBB	9	ARG	CG-CD-NE	-5.29	100.68	111.80

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	AAA	1191	0	1216	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	1183	0	1205	6	0
2	BBB	1155	0	1122	11	1
2	DDD	1125	0	1100	9	0
3	AAA	85	0	0	1	0
3	BBB	70	0	0	3	0
3	CCC	43	0	0	0	0
3	DDD	69	0	0	0	0
All	All	4921	0	4643	30	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 3.

All (30) 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)
2:BBB:105:ASP:O	2:BBB:108:THR:OG1	2.04	0.75
2:DDD:52:THR:HG23	2:DDD:54:PHE:H	1.59	0.67
2:BBB:77:ARG:HG2	3:BBB:203:HOH:O	1.99	0.61
2:BBB:108:THR:HG22	2:BBB:112:LEU:HD23	1.83	0.60
1:CCC:3:THR:CG2	1:CCC:6:ILE:HD13	2.34	0.58
2:DDD:52:THR:CG2	2:DDD:54:PHE:H	2.17	0.58
1:CCC:75:HIS:ND1	1:CCC:76:PRO:HD2	2.26	0.51
2:BBB:99:HIS:HE1	3:BBB:211:HOH:O	1.94	0.50
2:DDD:51:SER:O	2:DDD:51:SER:OG	2.29	0.48
1:CCC:3:THR:HG22	1:CCC:6:ILE:HD13	1.96	0.47
1:AAA:116:ASP:OD1	1:AAA:128:LYS:HD3	2.15	0.47
2:DDD:48:GLY:HA3	2:DDD:54:PHE:O	2.15	0.47
1:AAA:58:GLU:HG3	2:BBB:2:VAL:HB	1.96	0.46
1:CCC:41:PRO:O	1:CCC:42:GLN:HB2	2.16	0.46
1:AAA:28:GLU:CD	1:AAA:28:GLU:H	2.19	0.46
2:BBB:9:ARG:HG2	2:BBB:70:PRO:HG3	1.98	0.44
2:DDD:16:THR:HG23	2:DDD:21:THR:CG2	2.46	0.44
2:BBB:25[B]:GLN:HG2	2:BBB:25[B]:GLN:O	2.11	0.44
2:DDD:16:THR:HG23	2:DDD:21:THR:HG23	2.00	0.43
2:BBB:81:LYS:HA	2:BBB:138:TYR:CE2	2.53	0.43
1:CCC:28:GLU:H	1:CCC:28:GLU:CD	2.22	0.43
2:DDD:52:THR:O	2:DDD:55:GLU:HG2	2.19	0.42
1:AAA:59:GLU:HB2	1:AAA:63:LYS:HG3	2.02	0.42
2:BBB:21:THR:HG23	3:BBB:246:HOH:O	2.20	0.42
1:AAA:24:THR:HG23	3:AAA:249:HOH:O	2.19	0.41
2:DDD:52:THR:HG23	2:DDD:54:PHE:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:52:THR:HG22	2:BBB:127:ARG:HB2	2.02	0.41
1:CCC:74:TYR:HB2	1:CCC:141:TRP:CE3	2.56	0.41
2:DDD:98:PHE:CE2	2:DDD:100:VAL:HB	2.56	0.41
2:BBB:66[B]:ASP:OD1	2:BBB:68:ASN:N	2.37	0.40

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)
2:BBB:26:ASN:ND2	2:BBB:67:GLU:OE2[1_455]	2.13	0.07

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	AAA	145/151 (96%)	141 (97%)	4 (3%)	0	100	100
1	CCC	144/151 (95%)	139 (96%)	5 (4%)	0	100	100
2	BBB	140/141 (99%)	135 (96%)	3 (2%)	2 (1%)	11	2
2	DDD	133/141 (94%)	131 (98%)	2 (2%)	0	100	100
All	All	562/584 (96%)	546 (97%)	14 (2%)	2 (0%)	34	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BBB	106	ARG
2	BBB	2	VAL

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	AAA	134/136 (98%)	129 (96%)	5 (4%)	34	15
1	CCC	133/136 (98%)	126 (95%)	7 (5%)	22	7
2	BBB	132/129 (102%)	129 (98%)	3 (2%)	50	33
2	DDD	128/129 (99%)	125 (98%)	3 (2%)	50	33
All	All	527/530 (99%)	509 (97%)	18 (3%)	38	18

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	17	CYS
1	AAA	46	GLU
1	AAA	94	SER
1	AAA	127	TRP
1	AAA	129	GLU
2	BBB	108	THR
2	BBB	115[A]	SER
2	BBB	115[B]	SER
1	CCC	6	ILE
1	CCC	7	ILE
1	CCC	17	CYS
1	CCC	119	LEU
1	CCC	127	TRP
1	CCC	129	GLU
1	CCC	147	LYS
2	DDD	52	THR
2	DDD	77	ARG
2	DDD	106	ARG

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 monosaccharides 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, 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	AAA	147/151 (97%)	-0.15	2 (1%) 75 79	15, 25, 45, 53	0
1	CCC	146/151 (96%)	-0.03	4 (2%) 54 58	20, 34, 56, 67	0
2	BBB	138/141 (97%)	-0.05	2 (1%) 75 79	19, 29, 46, 74	1 (0%)
2	DDD	136/141 (96%)	-0.29	2 (1%) 73 77	18, 26, 45, 78	0
All	All	567/584 (97%)	-0.13	10 (1%) 68 72	15, 28, 50, 78	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	DDD	1	MET	3.4
2	BBB	21	THR	3.1
1	CCC	119	LEU	3.1
1	CCC	120	ALA	2.8
2	BBB	1	MET	2.7
1	CCC	7	ILE	2.6
1	AAA	120	ALA	2.6
2	DDD	20	GLY	2.3
1	AAA	119	LEU	2.1
1	CCC	3	THR	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.