

Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 12:21 PM JST

PDB ID	:	7YW1
Title	:	crystal structure of UBE2O
Authors	:	Fu, Z.; Zhu, W.; Huang, H.
Deposited on	:	2022-08-20
Resolution	:	3.27 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 (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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.27 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1177 (3.32 - 3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	А	928	3% 65%	12%	22%	
1	В	928	5% 60%	9% •	30%	



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2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10032 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 (E3-independent) E2 ubiquitin-conjugating enzyme UBE2O.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	793	Total	С	Ν	0	\mathbf{S}	0	0	0
1	Π	120	5350	3390	932	1014	14	0	0	0
1	р	648	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	D	040	4682	2969	806	897	10	0	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: (E3-independent) E2 ubiquitin-conjugating enzyme UBE2O









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	115.32Å 132.53Å 155.04Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	54.04 - 3.27	Depositor
Resolution (A)	100.74 - 3.27	EDS
% Data completeness	76.6 (54.04-3.27)	Depositor
(in resolution range)	76.7(100.74-3.27)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.60 (at 3.26 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1-3660	Depositor
P. P.	0.249 , 0.300	Depositor
n, n_{free}	0.249 , 0.300	DCC
R_{free} test set	1351 reflections (4.72%)	wwPDB-VP
Wilson B-factor $(Å^2)$	87.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , 53.7	EDS
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	10032	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 3.25% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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	
	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.23	0/5459	0.41	0/7457
1	В	0.23	0/4770	0.41	0/6524
All	All	0.23	0/10229	0.41	0/13981

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 (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	А	5350	0	4977	62	0
1	В	4682	0	4224	49	0
All	All	10032	0	9201	109	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 6.

All (109) 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:378:SER:HB3	1:A:381:GLU:HG3	1.83	0.61
1:A:384:PRO:O	1:A:385:HIS:ND1	2.34	0.60



	loue page	Interatomic	omic Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:644:PHE:HB3	1:B:680:GLN:HG2	1.83	0.60	
1:A:114:HIS:HD2	1:A:281:PRO:HB2	1.67	0.59	
1:B:32:LEU:H	1:B:32:LEU:HD23	1.68	0.59	
1:A:404:ARG:NH2	1:A:493:ASP:OD1	2.36	0.58	
1:A:666:ARG:HH21	1:B:526:GLN:HA	1.68	0.58	
1:A:36:GLN:HA	1:A:803:LYS:HD3	1.84	0.58	
1:B:682:SER:HB2	1:B:779:LEU:HD21	1.86	0.58	
1:A:31:ILE:H	1:A:62:VAL:HG23	1.70	0.57	
1:A:687:ILE:HG23	1:A:703:ILE:HG12	1.87	0.57	
1:A:255:LEU:HB2	1:A:476:LYS:HG2	1.86	0.56	
1:A:865:ILE:HD12	1:A:894·ILE:HG23	1.88	0.56	
1:A:463:GLN:HG3	1:A:469:SER:HB3	1.88	0.55	
1:B:408:VAL:HG12	1:B:519:ABG:HA	1.87	0.55	
1:A:833:LEU:HB2	1:A:907:LEU:HD13	1.88	0.55	
1:A:257:THR:HG23	1:A:476:LYS:HB3	1.88	0.54	
1:A:351:HIS:ND1	1:A:422:PRO:HG3	2.23	0.54	
1:A:352:VAL:HG12	1:A:368:VAL:HA	1.90	0.54	
1:A:780:GLN:HA	1:A:783:VAL:HG22	1.90	0.53	
1:B:17:ASP:HB2	1:B:83:ARG:HA	1.91	0.53	
1:A:425:PRO:HB2	1:A:518:THR:HG23	1.89	0.53	
1:B:56:VAL:HG13	1:B:58:GLY:H	1.74	0.53	
1:B:411:HIS:NE2	1:B:518:THR:OG1	2.37	0.52	
1:A:153:GLU:OE1	1:A:450:ARG:NH1	2.42	0.52	
1:A:87:PRO:HD2	1:A:262:ALA:HA	1.92	0.51	
1:A:792:LYS:O	1:A:818:ASN:ND2	2.43	0.51	
1:A:448:GLY:O	1:A:451:SER:OG	2.28	0.51	
1:B:59:GLU:HA	1:B:74:PRO:HA	1.93	0.51	
1:B:156:ASP:HA	1:B:218:HIS:HA	1.92	0.50	
1:B:352:VAL:HB	1:B:366:VAL:HB	1.92	0.50	
1:B:341:VAL:HG12	1:B:384:PRO:HB3	1.93	0.50	
1:B:354:VAL:HA	1:B:366:VAL:HG12	1.93	0.50	
1:B:413:GLU:OE2	1:B:516:ARG:NH1	2.45	0.49	
1:A:17:ASP:N	1:A:17:ASP:OD1	2.45	0.49	
1:A:18:ILE:HG12	1:A:268:VAL:HG21	1.94	0.49	
1:A:225:TRP:O	1:A:242:ARG:NH2	2.39	0.49	
1:A:341:VAL:HG21	1:A:382:LEU:HD13	1.95	0.49	
1:B:654:HIS:HB3	1:B:657:TYR:HB2	1.94	0.49	
1:A:421:ALA:HB1	1:A:422:PRO:HD2	1.96	0.48	
1:B:417:ASN:N	1:B:515:GLU:O	2.46	0.48	
1:B:351:HIS:CE1	1:B:422:PRO:HG3	2.49	0.48	
1:B:93:ARG:NH1	1:B:317:GLU:OE2	2.47	0.48	



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:872:GLN:HA	1:A:888:ABG:HH21	1.79	0.47
1:A:746:ASN:ND2	1:A:789:VAL:O	2.47	0.47
1:A:697:ASP:HA	1:A:722:LEU:HD12	1.97	0.47
1:A:141:TYB:HB2	1:A:258:ILE:HB	1.96	0.47
1:A:260:ARG:HG2	1:A:407:PHE:CE2	2.49	0.47
1:A:683:LEU:HD23	1:A:684:PRO:HD2	1.95	0.47
1:A:522:ASP:OD1	1:A:523:SER:N	2.48	0.47
1:A:779:LEU:HA	1:A:782:LEU:HD12	1.97	0.47
1:B:37:ASP:HA	1:B:803:LYS:HD2	1.96	0.46
1:A:156:ASP:OD1	1:A:156:ASP:N	2.44	0.46
1:A:380:LEU:HD12	1:A:893:GLY:HA2	1.96	0.46
1:B:512:VAL:HG21	1:B:517:LEU:HD21	1.97	0.46
1:B:428:GLY:HA3	1:B:521:TYR:HB3	1.97	0.46
1:B:775:ARG:NH1	1:B:780:GLN:OE1	2.48	0.46
1:B:56:VAL:HG22	1:B:57:GLN:H	1.80	0.46
1:A:130:ILE:HG22	1:A:274:LEU:HD23	1.97	0.46
1:B:685:ASP:N	1:B:685:ASP:OD1	2.48	0.46
1:A:846:TRP:HA	1:A:850:THR:HB	1.98	0.45
1:B:352:VAL:HG12	1:B:368:VAL:HA	1.97	0.45
1:B:705:GLY:HA3	1:B:711:TYR:O	2.17	0.45
1:B:411:HIS:O	1:B:516:ARG:NH2	2.42	0.45
1:B:368:VAL:O	1:B:372:GLY:N	2.44	0.45
1:B:149:GLY:HA2	1:B:226:LEU:HG	1.98	0.45
1:B:112:LEU:HB2	1:B:300:VAL:HA	1.99	0.45
1:B:56:VAL:H	1:B:59:GLU:HG2	1.82	0.44
1:A:360:GLN:HE22	1:A:875:ALA:HA	1.82	0.44
1:A:260:ARG:HG2	1:A:407:PHE:HE2	1.82	0.44
1:B:847:PHE:O	1:B:851:SER:OG	2.35	0.44
1:A:711:TYR:HE1	1:A:745:VAL:HG22	1.82	0.44
1:B:651:PRO:HB3	1:B:838:GLY:HA3	1.99	0.44
1:B:503:ILE:HD11	1:B:507:ALA:HA	2.00	0.44
1:A:180:GLY:H	1:A:213:VAL:HB	1.83	0.43
1:A:666:ARG:NH2	1:B:526:GLN:HA	2.33	0.43
1:A:512:VAL:HG21	1:A:517:LEU:HD21	2.01	0.43
1:A:416:THR:OG1	1:A:417:ASN:N	2.52	0.43
1:A:861:ALA:O	1:A:865:ILE:HG12	2.19	0.43
1:B:726:PHE:CG	1:B:727:PRO:HA	2.54	0.43
1:B:848:TYR:HA	1:B:853:LYS:HB2	2.00	0.43
1:A:726:PHE:CG	1:A:727:PRO:HA	2.54	0.42
1:A:711:TYR:HB3	1:A:716:PHE:CZ	2.53	0.42
1:A:772:SER:H	1:A:776:SER:HB2	1.85	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:A:819:GLU:HG3	1:A:889:LEU:HD23	2.01	0.42
1:B:38:ALA:H	1:B:803:LYS:HD3	1.84	0.42
1:A:108:VAL:HG12	1:A:266:MET:HE3	2.00	0.42
1:A:427:ILE:HD13	1:A:427:ILE:HA	1.95	0.42
1:B:890:SER:C	1:B:892:GLY:H	2.23	0.42
1:B:327:TYR:CZ	1:B:330:PRO:HA	2.55	0.42
1:A:91:LEU:HD21	1:A:309:VAL:HG13	2.02	0.41
1:B:515:GLU:N	1:B:515:GLU:OE1	2.53	0.41
1:B:252:LEU:HD23	1:B:252:LEU:H	1.85	0.41
1:B:809:ASP:OD1	1:B:809:ASP:N	2.39	0.41
1:B:493:ASP:OD1	1:B:494:LEU:N	2.53	0.41
1:A:95:VAL:HG13	1:A:325:VAL:HG11	2.03	0.41
1:A:139:GLY:O	1:A:150:GLN:NE2	2.54	0.41
1:A:672:MET:HA	1:A:675:GLU:HB2	2.02	0.41
1:A:702:LEU:HD22	1:A:840:LEU:HD13	2.03	0.41
1:B:665:THR:OG1	1:B:666:ARG:N	2.50	0.41
1:B:670:ALA:O	1:B:674:LYS:HG2	2.20	0.41
1:A:847:PHE:O	1:A:853:LYS:HB2	2.21	0.41
1:B:98:VAL:HG12	1:B:359:ALA:HB1	2.03	0.40
1:B:255:LEU:HB2	1:B:256:THR:H	1.67	0.40
1:A:506:SER:O	1:A:506:SER:OG	2.38	0.40
1:A:654:HIS:HB3	1:A:657:TYR:HB2	2.03	0.40
1:B:296:ASP:OD1	1:B:296:ASP:N	2.54	0.40
1:A:156:ASP:HB3	1:A:218:HIS:HA	2.03	0.40
1:A:739:THR:HG22	1:A:740:ASN:H	1.86	0.40

There are no symmetry-related clashes.

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	А	701/928~(76%)	635 (91%)	62 (9%)	4 (1%)	25 58



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	611/928~(66%)	554 (91%)	52 (8%)	5(1%)	19	52
All	All	1312/1856~(71%)	1189 (91%)	114 (9%)	9(1%)	22	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	31	ILE
1	А	422	PRO
1	В	422	PRO
1	В	524	VAL
1	В	402	VAL
1	А	484	SER
1	А	477	GLN
1	В	648	PRO
1	В	241	PRO

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	Percer	ntiles
1	А	521/786~(66%)	514 (99%)	7 (1%)	69	82
1	В	438/786~(56%)	428~(98%)	10 (2%)	50	73
All	All	959/1572~(61%)	942~(98%)	17~(2%)	59	78

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

Mol	Chain	Res	Type
1	А	35	TRP
1	А	89	ASP
1	А	145	ASN
1	А	251	ASP
1	А	266	MET
1	А	666	ARG
1	А	815	ARG



Mol	Chain	Res	Type
1	В	64	TYR
1	В	155	PHE
1	В	316	ARG
1	В	317	GLU
1	В	351	HIS
1	В	432	GLU
1	В	497	ASP
1	В	775	ARG
1	В	780	GLN
1	В	888	ARG

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	# RSRZ >	÷2	$OWAB(Å^2)$	Q < 0.9
1	А	723/928~(77%)	0.41	30 (4%) 37	35	39, 80, 118, 143	0
1	В	648/928~(69%)	0.41	47 (7%) 15	15	48, 91, 142, 174	0
All	All	1371/1856~(73%)	0.41	77 (5%) 24	23	39, 84, 132, 174	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	143	ILE	5.5
1	В	488	PHE	4.3
1	В	223	VAL	4.3
1	В	494	LEU	4.0
1	В	222	ALA	3.6
1	В	220	VAL	3.6
1	В	221	LEU	3.3
1	А	848	TYR	3.3
1	В	237	ALA	3.2
1	В	307	VAL	3.2
1	А	732	ILE	3.1
1	В	218	HIS	3.0
1	А	778	LEU	3.0
1	А	721	MET	3.0
1	В	335	CYS	3.0
1	В	219	THR	3.0
1	В	722	LEU	2.9
1	А	847	PHE	2.9
1	А	759	ILE	2.9
1	В	106	THR	2.8
1	В	142	VAL	2.8
1	А	221	LEU	2.8
1	В	720	TRP	2.8
1	А	294	GLU	2.8



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Mol	Chain	Res	Type	RSRZ
1	В	677	LYS	2.7
1	В	248	TYR	2.7
1	А	168	VAL	2.7
1	А	222	ALA	2.7
1	А	297	THR	2.7
1	В	493	ASP	2.7
1	А	232	LEU	2.6
1	В	154	MET	2.6
1	А	722	LEU	2.6
1	В	733	ALA	2.6
1	В	150	GLN	2.6
1	В	152	VAL	2.6
1	А	410	ILE	2.6
1	В	716	PHE	2.6
1	В	151	VAL	2.6
1	В	760	LEU	2.6
1	В	840	LEU	2.5
1	В	327	TYR	2.5
1	В	226	LEU	2.5
1	В	699	LEU	2.5
1	А	492	LEU	2.5
1	В	85	TYR	2.5
1	А	119	PHE	2.5
1	А	689	VAL	2.4
1	В	731	PRO	2.4
1	А	785	ILE	2.4
1	В	224	ALA	2.4
1	А	857	VAL	2.4
1	А	295	VAL	2.4
1	А	342	LEU	2.3
1	В	258	ILE	2.3
1	В	735	PHE	2.3
1	A	748	ASN	2.3
1	A	35	TRP	2.3
1	A	283	THR	2.2
1	В	301	GLN	2.2
1	В	112	LEU	2.2
1	A	760	LEU	2.2
1	A	819	GLU	2.2
1	В	698	LEU	2.1
1	А	858	LEU	2.1
1	В	407	PHE	2.1



Mol	Chain	Res	Type	RSRZ
1	В	309	VAL	2.1
1	В	672	MET	2.1
1	А	337	PRO	2.1
1	А	897	LEU	2.1
1	В	155	PHE	2.1
1	В	133	ALA	2.1
1	А	894	ILE	2.1
1	В	409	PHE	2.1
1	В	828	PHE	2.0
1	В	819	GLU	2.0
1	В	749	LEU	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 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.

