



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 AM UTC

PDB ID : 3L1Z / pdb_00003l1z
Title : Crystal structure of the U-BOX domain of human E4B ubiquitin ligase in complex with UBCH5C E2 ubiquitin conjugating enzyme
Authors : Benirschke, R.; Thompson, J.R.; Mer, G.
Deposited on : 2009-12-14
Resolution : 3.17 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 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	:	4-5-2 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

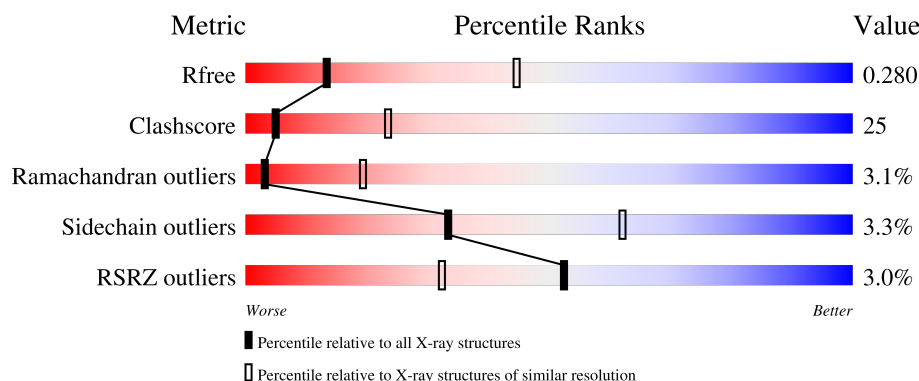
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

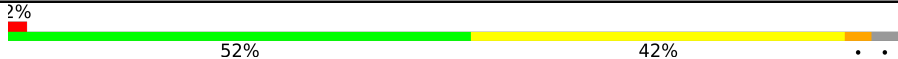
The reported resolution of this entry is 3.17 Å.

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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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 $\leq 5\%$. 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	A	157	
2	B	100	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1865 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 Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	26	0	0
			1216	775	210	222	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP P61077
A	-8	HIS	-	expression tag	UNP P61077
A	-7	HIS	-	expression tag	UNP P61077
A	-6	HIS	-	expression tag	UNP P61077
A	-5	HIS	-	expression tag	UNP P61077
A	-4	HIS	-	expression tag	UNP P61077
A	-3	HIS	-	expression tag	UNP P61077
A	-2	MET	-	expression tag	UNP P61077
A	-1	ASN	-	expression tag	UNP P61077
A	0	SER	-	expression tag	UNP P61077

- Molecule 2 is a protein called Ubiquitin conjugation factor E4 B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	S	20	0	0
			634	395	108	126	5			

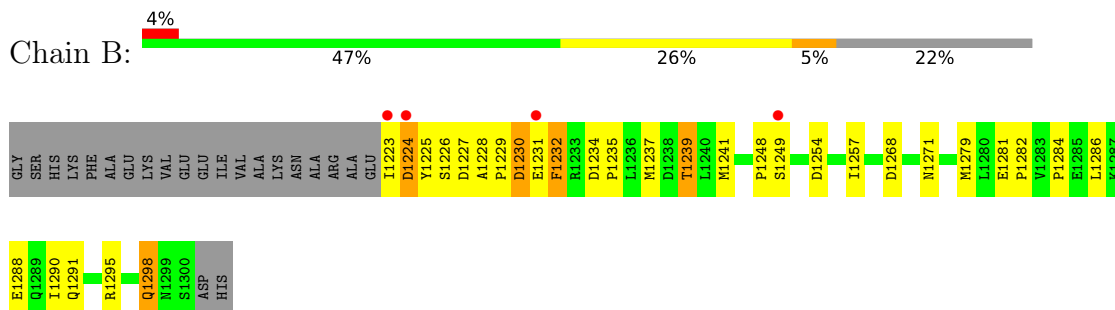
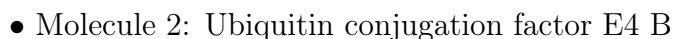
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1203	GLY	-	expression tag	UNP O95155
B	1204	SER	-	expression tag	UNP O95155
B	1205	HIS	-	expression tag	UNP O95155
B	1206	LYS	-	expression tag	UNP O95155
B	1207	PHE	-	expression tag	UNP O95155

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total 11	O 11	0	0
3	B	4	Total 4	O 4	0	0

- Molecule 1: Ubiquitin-conjugating enzyme E2 D3



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	142.71Å 142.71Å 83.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.78 – 3.17 32.78 – 3.17	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.78-3.17) 92.0 (32.78-3.17)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.18 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.232 , 0.279 0.230 , 0.280	Depositor DCC
R_{free} test set	963 reflections (9.22%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 116.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1865	wwPDB-VP
Average B, all atoms (Å ²)	93.0	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.*

¹Intensities estimated from amplitudes.

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.

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	A	0.40	0/1253	0.81	2/1706 (0.1%)
2	B	0.37	0/647	0.83	0/879
All	All	0.39	0/1900	0.82	2/2585 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	LYS	CA-C-N	7.37	125.04	119.66
1	A	63	LYS	C-N-CA	7.37	125.04	119.66

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	A	1216	0	1195	59	0
2	B	634	0	623	30	0
3	A	11	0	0	0	0
3	B	4	0	0	0	0
All	All	1865	0	1818	89	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 25.

All (89) 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:B:1226:SER:HA	2:B:1227:ASP:HB3	1.25	1.09
2:B:1229:PRO:O	2:B:1230:ASP:O	1.78	0.99
2:B:1229:PRO:O	2:B:1230:ASP:C	2.11	0.92
2:B:1234:ASP:HA	2:B:1241:MET:HE3	1.65	0.79
1:A:111:CYS:C	1:A:112:ASP:OD1	2.26	0.79
1:A:88:ILE:HD12	1:A:88:ILE:H	1.50	0.76
1:A:21:CYS:HB3	1:A:103:LEU:HD23	1.67	0.76
2:B:1226:SER:CA	2:B:1227:ASP:HB3	2.12	0.74
1:A:94:SER:H	1:A:97:LEU:HD12	1.53	0.74
1:A:5:ARG:HH11	1:A:61:PRO:HG3	1.52	0.74
2:B:1230:ASP:O	2:B:1232:PHE:N	2.21	0.73
1:A:13:LEU:HD11	1:A:100:SER:HB2	1.71	0.73
2:B:1249:SER:HB2	2:B:1268:ASP:OD2	1.89	0.72
2:B:1226:SER:HA	2:B:1227:ASP:CB	2.07	0.69
1:A:57:PRO:HD3	1:A:65:PRO:HA	1.74	0.69
2:B:1254:ASP:HB3	2:B:1257:ILE:HD13	1.76	0.67
1:A:113:PRO:O	1:A:115:PRO:HD3	1.93	0.67
2:B:1241:MET:HG2	2:B:1254:ASP:HB2	1.77	0.66
1:A:113:PRO:C	1:A:115:PRO:HD3	2.20	0.66
2:B:1226:SER:HB2	2:B:1228:ALA:H	1.60	0.65
1:A:87:ASP:O	1:A:92:GLN:HB3	1.96	0.65
1:A:-4:HIS:CE1	1:A:-2:MET:HE2	2.32	0.63
1:A:144:LYS:HE3	1:A:145:TYR:CZ	2.34	0.62
2:B:1232:PHE:N	2:B:1232:PHE:HD1	1.97	0.62
2:B:1232:PHE:HD1	2:B:1232:PHE:H	1.49	0.61
2:B:1229:PRO:C	2:B:1230:ASP:O	2.41	0.60
2:B:1232:PHE:N	2:B:1232:PHE:CD1	2.68	0.60
1:A:5:ARG:NH2	1:A:98:THR:HG22	2.17	0.59
1:A:18:PRO:HB2	1:A:21:CYS:HB2	1.85	0.59
2:B:1237:MET:HB2	2:B:1239:THR:HG23	1.85	0.58
1:A:112:ASP:OD1	1:A:112:ASP:N	2.32	0.58
1:A:142:THR:O	1:A:147:MET:HG2	2.04	0.57
2:B:1268:ASP:HB3	2:B:1271:ASN:OD1	2.03	0.57
1:A:25:PRO:C	1:A:27:GLY:H	2.12	0.57
2:B:1284:PRO:O	2:B:1288:GLU:HG2	2.05	0.57
1:A:60:TYR:CD1	1:A:61:PRO:HA	2.42	0.55
1:A:18:PRO:HB3	1:A:104:LEU:HD11	1.89	0.55
2:B:1226:SER:HB2	2:B:1228:ALA:N	2.22	0.54
2:B:1232:PHE:CD2	2:B:1290:ILE:HG12	2.43	0.54
1:A:126:ILE:HG22	1:A:134:TYR:HB2	1.90	0.53
1:A:9:GLU:O	1:A:13:LEU:HD13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ARG:HH11	1:A:61:PRO:CG	2.22	0.53
1:A:107:CYS:C	1:A:109:LEU:H	2.18	0.52
1:A:21:CYS:HB3	1:A:103:LEU:CD2	2.39	0.52
1:A:88:ILE:HG23	1:A:97:LEU:HD13	1.91	0.51
1:A:88:ILE:H	1:A:88:ILE:CD1	2.23	0.51
2:B:1291:GLN:O	2:B:1295:ARG:HG3	2.11	0.51
1:A:44:PRO:O	1:A:139:ARG:HG2	2.11	0.49
2:B:1286:LEU:O	2:B:1290:ILE:HG13	2.13	0.49
1:A:144:LYS:HE3	1:A:145:TYR:CE2	2.46	0.49
1:A:10:LEU:HD23	1:A:30:MET:HE1	1.95	0.49
1:A:133:LYS:HD2	1:A:136:ARG:HH22	1.78	0.48
1:A:35:ALA:HB3	1:A:52:LEU:HB2	1.94	0.48
2:B:1248:PRO:HG2	2:B:1279:MET:HE2	1.94	0.48
2:B:1225:TYR:CE2	2:B:1227:ASP:HB2	2.49	0.48
1:A:133:LYS:HD2	1:A:136:ARG:NH2	2.29	0.48
1:A:91:SER:O	1:A:92:GLN:HB2	2.13	0.48
1:A:44:PRO:HB2	1:A:138:SER:HB2	1.94	0.47
1:A:20:GLN:HB3	1:A:38:MET:HB2	1.96	0.47
1:A:121:PRO:O	1:A:125:ARG:HG3	2.15	0.47
1:A:51:PHE:C	1:A:52:LEU:HD12	2.39	0.47
1:A:136:ARG:O	1:A:140:GLU:HG3	2.15	0.47
1:A:49:VAL:O	1:A:49:VAL:HG23	2.14	0.47
2:B:1295:ARG:O	2:B:1298:GLN:HB2	2.13	0.46
1:A:143:GLN:O	1:A:147:MET:HG3	2.16	0.46
1:A:7:ASN:OD1	1:A:30:MET:HE2	2.17	0.45
1:A:36:THR:HG22	1:A:51:PHE:CD1	2.51	0.45
2:B:1223:ILE:O	2:B:1224:ASP:O	2.34	0.45
2:B:1226:SER:HB2	2:B:1228:ALA:HB2	2.00	0.44
1:A:88:ILE:HD12	1:A:88:ILE:N	2.26	0.44
1:A:58:THR:HG23	1:A:59:ASP:OD1	2.18	0.44
1:A:13:LEU:HA	1:A:16:ASP:O	2.18	0.43
1:A:72:ARG:HH11	1:A:72:ARG:HA	1.83	0.43
1:A:72:ARG:HA	1:A:72:ARG:NH1	2.33	0.43
1:A:18:PRO:HG3	1:A:100:SER:OG	2.19	0.42
1:A:22:SER:HB3	1:A:36:THR:OG1	2.19	0.42
1:A:74:TYR:HB3	1:A:138:SER:HA	2.01	0.42
1:A:90:ARG:HB3	1:A:91:SER:H	1.64	0.42
1:A:5:ARG:HH22	1:A:98:THR:HG22	1.84	0.42
2:B:1281:GLU:HA	2:B:1282:PRO:HD3	1.91	0.42
2:B:1234:ASP:HA	2:B:1235:PRO:HD3	1.89	0.42
1:A:25:PRO:C	1:A:27:GLY:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:HB2	1:A:54:ILE:HB	2.02	0.41
1:A:86:LEU:HD22	1:A:88:ILE:HD13	2.03	0.41
1:A:21:CYS:SG	1:A:103:LEU:HB3	2.62	0.40
1:A:75:HIS:NE2	1:A:113:PRO:HG3	2.36	0.40
2:B:1232:PHE:CE2	2:B:1290:ILE:HA	2.56	0.40
1:A:106:ILE:O	1:A:109:LEU:HB3	2.20	0.40
1:A:48:GLY:HA2	1:A:147:MET:HE3	2.02	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	A	150/157 (96%)	135 (90%)	11 (7%)	4 (3%)	4	22
2	B	76/100 (76%)	63 (83%)	10 (13%)	3 (4%)	2	15
All	All	226/257 (88%)	198 (88%)	21 (9%)	7 (3%)	3	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
2	B	1224	ASP
2	B	1230	ASP
1	A	26	VAL
1	A	39	GLY
2	B	1231	GLU
1	A	91	SER

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	A	137/142 (96%)	133 (97%)	4 (3%)	37	64
2	B	75/92 (82%)	72 (96%)	3 (4%)	28	58
All	All	212/234 (91%)	205 (97%)	7 (3%)	33	62

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	67	VAL
1	A	104	LEU
1	A	112	ASP
2	B	1232	PHE
2	B	1239	THR
2	B	1298	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 [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, 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	A	152/157 (96%)	0.03	3 (1%) 65 44	34, 87, 125, 166	6 (3%)
2	B	78/100 (78%)	0.28	4 (5%) 33 20	35, 85, 153, 158	6 (7%)
All	All	230/257 (89%)	0.11	7 (3%) 52 32	34, 86, 144, 166	12 (5%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1223	ILE	5.2
2	B	1249	SER	3.1
1	A	-4	HIS	2.7
1	A	38	MET	2.6
2	B	1224	ASP	2.2
2	B	1231	GLU	2.2
1	A	1	MET	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 oligosaccharides 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.