



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:13 PM UTC

PDB ID : 6K9N / pdb_00006k9n
Title : Rice_OTUB_like_catalytic domain
Authors : Lu, L.N.; Liu, L.; Wang, F.
Deposited on : 2019-06-17
Resolution : 2.27 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 ⓘ 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

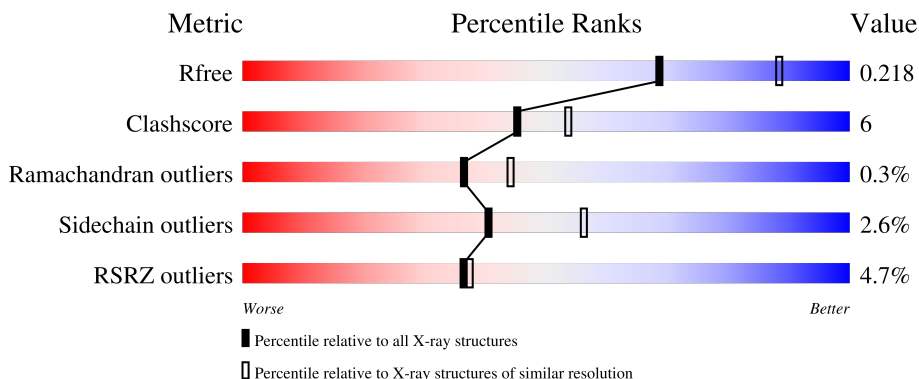
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	251	2% 84% 12% .
1	B	251	6% 81% 13% ..
1	C	251	4% 78% 17% .
1	D	251	6% 81% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8278 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 thioesterase.

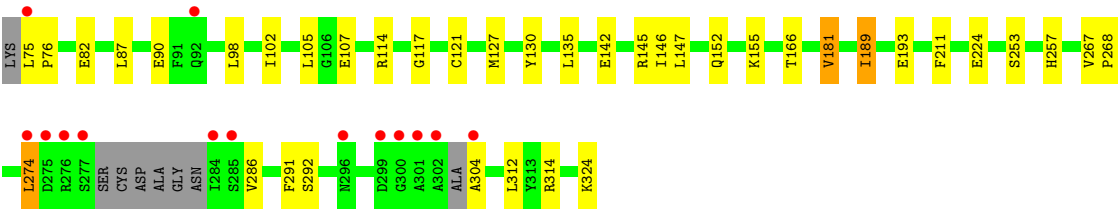
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1955	1249	321	377	8			
1	B	241	Total	C	N	O	S	0	0	0
			1951	1247	320	376	8			
1	C	240	Total	C	N	O	S	0	0	0
			1943	1243	319	373	8			
1	D	243	Total	C	N	O	S	0	0	0
			1957	1251	321	377	8			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	146	Total	O	0	0
			146	146		
2	B	106	Total	O	0	0
			106	106		
2	C	108	Total	O	0	0
			108	108		
2	D	112	Total	O	0	0
			112	112		

- Molecule 1: Ubiquitin thioesterase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.69Å 144.81Å 155.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.27 47.38 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.38-2.27) 98.0 (47.38-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.73 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.217 0.189 , 0.218	Depositor DCC
R_{free} test set	3033 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8278	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.19	0/1997	0.42	0/2693
1	B	0.18	0/1993	0.42	0/2688
1	C	0.18	0/1985	0.37	0/2677
1	D	0.18	0/1999	0.38	0/2696
All	All	0.18	0/7974	0.40	0/10754

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	A	1955	0	1897	19	0
1	B	1951	0	1894	23	0
1	C	1943	0	1890	25	0
1	D	1957	0	1901	25	0
2	A	146	0	0	6	1
2	B	106	0	0	7	0
2	C	108	0	0	5	0
2	D	112	0	0	6	1
All	All	8278	0	7582	91	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 6.

All (91) 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:B:196:GLU:OE1	2:B:401:HOH:O	1.82	0.95
1:B:276:ARG:O	2:B:402:HOH:O	1.83	0.95
1:C:100:GLU:OE2	2:C:401:HOH:O	1.84	0.93
1:C:176:ASP:OD2	2:C:402:HOH:O	1.89	0.87
1:D:82:GLU:OE1	2:D:401:HOH:O	1.94	0.84
1:D:224:GLU:OE2	2:D:402:HOH:O	1.97	0.83
1:D:314:ARG:NH2	2:D:403:HOH:O	2.17	0.77
1:B:82:GLU:OE2	1:B:114:ARG:NH1	2.23	0.71
1:B:136:GLU:OE1	2:B:403:HOH:O	2.10	0.70
1:B:127:MET:HG3	1:B:207:VAL:HG11	1.76	0.68
1:D:155:LYS:HE3	2:D:406:HOH:O	1.96	0.65
1:A:151:GLU:OE1	2:A:401:HOH:O	2.13	0.65
1:C:154:LYS:NZ	2:C:404:HOH:O	2.24	0.64
1:D:274:LEU:HB3	1:D:314:ARG:HG2	1.79	0.62
1:B:108:GLN:NE2	2:B:407:HOH:O	2.32	0.62
1:C:163:ILE:HD12	1:C:165:PHE:HB3	1.83	0.60
1:B:189:ILE:HG23	1:B:193:GLU:HB3	1.83	0.59
1:C:97:ILE:HD11	1:C:276:ARG:HG2	1.84	0.59
1:D:142:GLU:OE1	2:D:404:HOH:O	2.17	0.58
1:C:239:VAL:O	1:C:243:LYS:HG2	2.03	0.57
1:C:233:LEU:HD11	1:C:255:HIS:CE1	2.40	0.57
1:D:90:GLU:OE1	1:D:114:ARG:NH2	2.34	0.56
1:D:146:ILE:HD12	1:D:147:LEU:N	2.22	0.55
1:C:135:LEU:HB2	1:C:181:VAL:HG22	1.89	0.54
1:A:144:GLU:OE1	2:A:402:HOH:O	2.18	0.54
1:B:289:HIS:HE1	2:B:413:HOH:O	1.91	0.54
1:A:233:LEU:HD11	1:A:255:HIS:CE1	2.44	0.53
1:D:75:LEU:HG	1:D:76:PRO:HD3	1.91	0.53
1:D:135:LEU:HB2	1:D:181:VAL:HG22	1.90	0.53
1:C:176:ASP:OD1	2:C:403:HOH:O	2.18	0.52
1:D:105:LEU:HD21	1:D:312:LEU:HD13	1.91	0.52
1:C:237:THR:OG1	1:C:240:GLN:HG3	2.09	0.52
1:A:75:LEU:O	1:A:116:ARG:NH2	2.41	0.52
1:B:75:LEU:N	1:B:76:PRO:HD2	2.25	0.52
1:A:152:GLN:O	1:A:156:THR:HG23	2.09	0.51
1:D:145:ARG:NH2	1:D:146:ILE:HG23	2.25	0.51
1:D:82:GLU:OE2	1:D:114:ARG:NH1	2.43	0.51
1:C:202:MET:O	1:C:206:TYR:HD1	1.93	0.50
1:B:140:LYS:O	1:B:143:VAL:N	2.43	0.50
1:B:144:GLU:O	1:B:148:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:N	1:A:76:PRO:HD2	2.28	0.49
1:B:152:GLN:O	1:B:156:THR:HG23	2.13	0.48
1:C:152:GLN:O	1:C:156:THR:HG23	2.13	0.48
1:C:77:TYR:OH	1:C:201:GLN:HG3	2.13	0.48
1:B:229:PHE:O	1:B:233:LEU:HB2	2.14	0.48
1:A:215:THR:HG23	1:A:260:ALA:HB3	1.96	0.47
1:D:107:GLU:O	1:D:324:LYS:HD3	2.13	0.47
1:D:152:GLN:HG2	1:D:155:LYS:NZ	2.29	0.47
1:C:274:LEU:HD23	1:C:314:ARG:HD3	1.97	0.47
1:A:201:GLN:HG2	1:A:202:MET:HE2	1.97	0.47
1:C:187:SER:HB2	2:C:437:HOH:O	2.15	0.47
1:A:135:LEU:HB2	1:A:181:VAL:HG22	1.96	0.47
1:C:147:LEU:O	1:C:151:GLU:HG2	2.15	0.46
1:D:87:LEU:HG	1:D:102:ILE:HD13	1.97	0.45
1:D:130:TYR:OH	1:D:146:ILE:HG12	2.17	0.45
1:B:75:LEU:HD23	1:B:76:PRO:HD3	1.99	0.45
1:A:127:MET:HE3	1:A:198:THR:HB	2.00	0.44
1:B:234:THR:HG22	1:B:235:ASN:H	1.81	0.44
1:D:253:SER:HB3	1:D:257:HIS:HB2	1.99	0.44
1:D:127:MET:HB2	1:D:211:PHE:HE2	1.81	0.44
1:B:274:LEU:HB2	1:B:312:LEU:HD11	2.00	0.44
1:B:135:LEU:HB2	1:B:181:VAL:HG22	2.00	0.44
1:C:132:GLU:O	1:C:136:GLU:HG3	2.18	0.44
1:A:116:ARG:HD3	1:B:90:GLU:O	2.18	0.43
1:A:274:LEU:HB2	1:A:312:LEU:HD11	1.99	0.43
1:A:149:LYS:HD2	1:A:149:LYS:HA	1.78	0.43
1:B:227:GLU:OE2	2:B:404:HOH:O	2.21	0.43
1:B:276:ARG:O	1:B:277:SER:HB3	2.18	0.43
1:C:144:GLU:O	1:C:148:LYS:HG3	2.19	0.43
1:C:89:ALA:O	1:C:92:GLN:HG2	2.18	0.42
1:D:304:ALA:N	2:D:415:HOH:O	2.52	0.42
1:D:117:GLY:HA2	1:D:121:CYS:SG	2.59	0.42
1:C:148:LYS:O	1:C:152:GLN:HG3	2.18	0.42
1:C:215:THR:HG23	1:C:260:ALA:HB3	2.01	0.42
1:D:268:PRO:HB3	1:D:292:SER:HB3	2.02	0.42
1:C:170:PHE:HB3	1:C:210:PHE:HB2	2.01	0.42
1:C:173:ILE:O	1:C:177:GLN:HG2	2.20	0.42
1:A:288:HIS:HE1	2:A:403:HOH:O	2.02	0.42
1:B:253:SER:HB3	1:B:257:HIS:HB2	2.02	0.41
1:B:108:GLN:NE2	2:B:416:HOH:O	2.52	0.41
1:A:192:GLU:CD	1:A:192:GLU:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:PRO:HA	1:A:291:PHE:O	2.21	0.41
1:D:268:PRO:HA	1:D:291:PHE:O	2.20	0.41
1:A:156:THR:HG21	2:A:444:HOH:O	2.21	0.41
1:A:245:SER:HB2	2:A:418:HOH:O	2.20	0.41
1:C:97:ILE:HD11	1:C:276:ARG:CG	2.50	0.41
1:B:234:THR:HG22	1:B:235:ASN:N	2.36	0.40
1:D:189:ILE:HG13	1:D:193:GLU:HB3	2.03	0.40
1:C:113:ARG:HB3	1:C:320:ILE:HB	2.03	0.40
1:A:86:THR:HG22	2:A:441:HOH:O	2.22	0.40
1:D:98:LEU:HD22	1:D:274:LEU:HD22	2.02	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:A:407:HOH:O	2:D:492:HOH:O[4_445]	2.00	0.20

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	236/251 (94%)	233 (99%)	3 (1%)	0	100	100
1	B	235/251 (94%)	225 (96%)	7 (3%)	3 (1%)	9	9
1	C	234/251 (93%)	225 (96%)	9 (4%)	0	100	100
1	D	237/251 (94%)	231 (98%)	6 (2%)	0	100	100
All	All	942/1004 (94%)	914 (97%)	25 (3%)	3 (0%)	36	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	SER
1	B	139	ASP
1	B	185	HIS

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	216/220 (98%)	211 (98%)	5 (2%)	44	60
1	B	216/220 (98%)	210 (97%)	6 (3%)	38	53
1	C	215/220 (98%)	210 (98%)	5 (2%)	44	60
1	D	215/220 (98%)	209 (97%)	6 (3%)	38	53
All	All	862/880 (98%)	840 (97%)	22 (3%)	40	56

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	181	VAL
1	A	214	VAL
1	A	267	VAL
1	A	283	ASN
1	B	95	SER
1	B	181	VAL
1	B	187	SER
1	B	231	SER
1	B	233	LEU
1	B	274	LEU
1	C	75	LEU
1	C	84	LEU
1	C	166	THR
1	C	181	VAL
1	C	267	VAL
1	D	166	THR
1	D	181	VAL
1	D	189	ILE

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Mol	Chain	Res	Type
1	D	267	VAL
1	D	274	LEU
1	D	286	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	133	HIS
1	A	152	GLN
1	A	240	GLN
1	A	255	HIS
1	A	287	ASN
1	B	183	GLN
1	B	235	ASN
1	B	287	ASN
1	C	133	HIS
1	D	287	ASN
1	D	289	HIS
1	D	296	ASN

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, 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	242/251 (96%)	-0.05	6 (2%) 58 60	22, 34, 55, 92	0
1	B	241/251 (96%)	0.30	14 (5%) 29 30	27, 41, 64, 100	0
1	C	240/251 (95%)	0.26	11 (4%) 37 38	29, 41, 63, 95	0
1	D	243/251 (96%)	0.29	14 (5%) 29 30	25, 39, 64, 96	0
All	All	966/1004 (96%)	0.20	45 (4%) 36 37	22, 39, 63, 100	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	304	ALA	6.4
1	D	301	ALA	6.2
1	C	304	ALA	6.0
1	A	304	ALA	5.7
1	D	284	ILE	5.4
1	B	304	ALA	5.1
1	A	300	GLY	4.7
1	D	302	ALA	4.5
1	D	277	SER	4.3
1	C	165	PHE	4.1
1	D	75	LEU	4.0
1	A	75	LEU	3.9
1	D	275	ASP	3.6
1	D	300	GLY	3.4
1	B	75	LEU	3.4
1	C	277	SER	3.4
1	A	277	SER	3.4
1	C	75	LEU	3.3
1	B	305	GLU	3.2
1	B	276	ARG	3.1
1	D	92	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	234	THR	3.1
1	C	184	GLY	3.0
1	B	283	ASN	3.0
1	B	299	ASP	3.0
1	B	277	SER	2.9
1	B	232	GLY	2.9
1	D	299	ASP	2.9
1	B	184	GLY	2.8
1	B	186	GLU	2.8
1	C	151	GLU	2.5
1	A	299	ASP	2.5
1	B	284	ILE	2.4
1	C	297	SER	2.3
1	D	285	SER	2.3
1	A	283	ASN	2.3
1	D	276	ARG	2.3
1	D	274	LEU	2.2
1	B	296	ASN	2.2
1	C	185	HIS	2.2
1	C	295	ALA	2.1
1	D	296	ASN	2.1
1	C	213	PHE	2.1
1	C	164	GLU	2.0
1	B	298	SER	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.