Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 01:07 AM EDT

PDB ID	:	7RUO / pdb_00007ruo
Title	:	Crystal structure of human UTP15
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Deposited on	:	2021-08-17
Resolution	:	1.80 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:

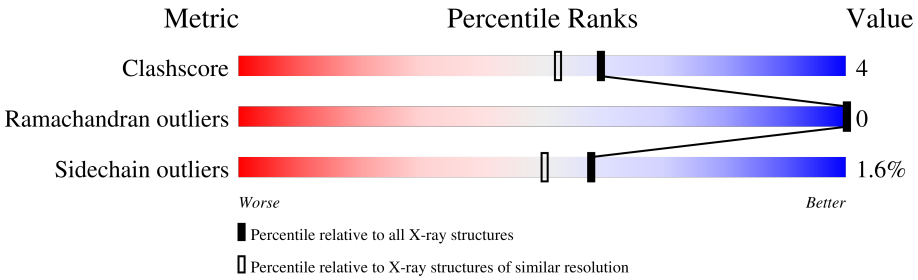
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	388	72% 5% • 22%
1	B	388	70% 7% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5020 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 U3 small nucleolar RNA-associated protein 15 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	4	0
			2364	1504	407	445	8			
1	B	300	Total	C	N	O	S	0	5	0
			2359	1503	401	447	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q8TED0
A	-16	HIS	-	expression tag	UNP Q8TED0
A	-15	HIS	-	expression tag	UNP Q8TED0
A	-14	HIS	-	expression tag	UNP Q8TED0
A	-13	HIS	-	expression tag	UNP Q8TED0
A	-12	HIS	-	expression tag	UNP Q8TED0
A	-11	HIS	-	expression tag	UNP Q8TED0
A	-10	SER	-	expression tag	UNP Q8TED0
A	-9	SER	-	expression tag	UNP Q8TED0
A	-8	GLY	-	expression tag	UNP Q8TED0
A	-7	ARG	-	expression tag	UNP Q8TED0
A	-6	GLU	-	expression tag	UNP Q8TED0
A	-5	ASN	-	expression tag	UNP Q8TED0
A	-4	LEU	-	expression tag	UNP Q8TED0
A	-3	TYR	-	expression tag	UNP Q8TED0
A	-2	PHE	-	expression tag	UNP Q8TED0
A	-1	GLN	-	expression tag	UNP Q8TED0
A	0	GLY	-	expression tag	UNP Q8TED0
B	-17	MET	-	initiating methionine	UNP Q8TED0
B	-16	HIS	-	expression tag	UNP Q8TED0
B	-15	HIS	-	expression tag	UNP Q8TED0
B	-14	HIS	-	expression tag	UNP Q8TED0
B	-13	HIS	-	expression tag	UNP Q8TED0
B	-12	HIS	-	expression tag	UNP Q8TED0
B	-11	HIS	-	expression tag	UNP Q8TED0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	SER	-	expression tag	UNP Q8TED0
B	-9	SER	-	expression tag	UNP Q8TED0
B	-8	GLY	-	expression tag	UNP Q8TED0
B	-7	ARG	-	expression tag	UNP Q8TED0
B	-6	GLU	-	expression tag	UNP Q8TED0
B	-5	ASN	-	expression tag	UNP Q8TED0
B	-4	LEU	-	expression tag	UNP Q8TED0
B	-3	TYR	-	expression tag	UNP Q8TED0
B	-2	PHE	-	expression tag	UNP Q8TED0
B	-1	GLN	-	expression tag	UNP Q8TED0
B	0	GLY	-	expression tag	UNP Q8TED0

- Molecule 2 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total X 3 3	0	0
2	B	2	Total X 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	142	Total O 143 143	0	1
3	B	148	Total O 149 149	0	1

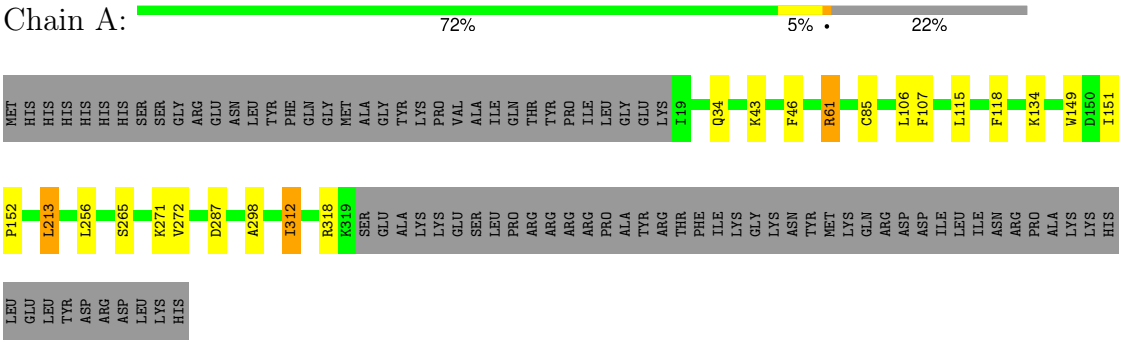
3 Residue-property plots (i)

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. 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.

Note EDS failed to run properly.

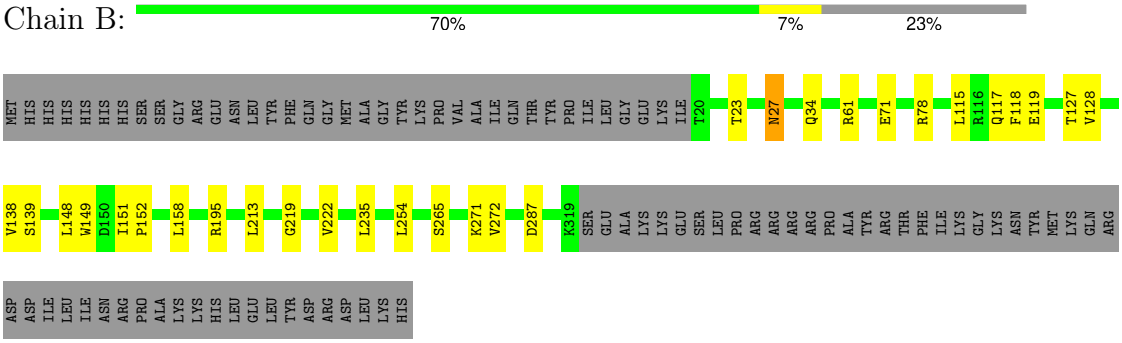
• Molecule 1: U3 small nucleolar RNA-associated protein 15 homolog

Chain A:



• Molecule 1: U3 small nucleolar RNA-associated protein 15 homolog

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.33Å 59.09Å 61.87Å 90.11° 66.82° 62.87°	Depositor
Resolution (Å)	42.69 – 1.80	Depositor
% Data completeness (in resolution range)	93.6 (42.69-1.80)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.231 , 0.263	Depositor
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.323	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5020	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 22.17 % 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 6.0223e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: UNX

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	0.71	0/2419	0.82	0/3283
1	B	0.68	0/2414	0.84	0/3277
All	All	0.69	0/4833	0.83	0/6560

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	2364	0	2312	19	0
1	B	2359	0	2298	20	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	143	0	0	2	0
3	B	149	0	0	5	0
All	All	5020	0	4610	39	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 4.

All (39) 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:61[B]:ARG:NH1	3:A:1101:HOH:O	2.12	0.81
1:B:195:ARG:NH1	3:B:501:HOH:O	2.18	0.76
1:A:151[A]:ILE:HB	1:A:152:PRO:HD3	1.69	0.74
1:B:78:ARG:HG2	1:B:115:LEU:HD11	1.70	0.73
1:B:271:LYS:HE3	1:B:287:ASP:OD2	1.93	0.69
1:A:271:LYS:HE2	3:B:638:HOH:O	1.98	0.62
1:B:117:GLN:CD	3:B:607[B]:HOH:O	2.41	0.60
1:B:23:THR:O	1:B:27:ASN:HB2	2.02	0.59
1:A:61[B]:ARG:HG2	1:A:61[B]:ARG:HH11	1.69	0.57
1:B:222[A]:VAL:HG13	1:B:254:LEU:HD13	1.88	0.56
1:B:148:LEU:HD23	1:B:158:LEU:HD13	1.88	0.55
1:B:78:ARG:NH1	1:B:117:GLN:OE1	2.40	0.55
1:A:106:LEU:HD11	1:A:151[A]:ILE:HD12	1.90	0.52
1:B:271:LYS:HE2	3:B:518:HOH:O	2.10	0.51
1:B:271:LYS:CE	3:B:518:HOH:O	2.58	0.51
1:B:151:ILE:HB	1:B:152:PRO:HD3	1.92	0.51
1:A:34:GLN:HG3	1:A:312:ILE:CD1	2.41	0.50
1:A:213[B]:LEU:HD11	1:A:256:LEU:HG	1.93	0.49
1:A:271:LYS:HE3	1:A:287:ASP:OD2	2.13	0.48
1:B:219:GLY:HA2	1:B:235:LEU:HG	1.97	0.47
1:B:118:PHE:HB3	1:B:149:TRP:CZ3	2.51	0.46
1:B:213:LEU:HB2	1:B:222[A]:VAL:CG1	2.46	0.45
1:A:34:GLN:HG3	1:A:312:ILE:HD13	1.98	0.45
1:A:34:GLN:OE1	1:A:34:GLN:N	2.49	0.45
1:B:213:LEU:CB	1:B:222[A]:VAL:HG12	2.46	0.45
1:A:151[B]:ILE:HB	1:A:152:PRO:HD3	2.00	0.43
1:B:128:VAL:HA	1:B:138:VAL:O	2.18	0.43
1:B:265:SER:O	1:B:272:VAL:HA	2.18	0.43
1:A:61[B]:ARG:NH1	1:A:61[B]:ARG:HG2	2.33	0.42
1:A:134:LYS:NZ	3:A:1111:HOH:O	2.52	0.42
1:B:213:LEU:HB3	1:B:222[A]:VAL:HG12	2.02	0.41
1:A:61[B]:ARG:N	1:A:61[B]:ARG:HD3	2.36	0.41
1:B:117:GLN:CD	1:B:119[B]:GLU:OE2	2.59	0.41
1:A:107:PHE:CD2	1:A:115:LEU:HD23	2.56	0.41
1:A:118:PHE:HB3	1:A:149:TRP:CZ3	2.56	0.41
1:A:265:SER:O	1:A:272:VAL:HA	2.21	0.41
1:B:127:THR:O	1:B:139:SER:HA	2.21	0.41
1:A:46:PHE:CE1	1:A:298:ALA:HB2	2.56	0.41
1:A:43:LYS:HD3	1:A:85:CYS:HA	2.03	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	303/388 (78%)	293 (97%)	10 (3%)	0	100	100
1	B	303/388 (78%)	290 (96%)	13 (4%)	0	100	100
All	All	606/776 (78%)	583 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	258/339 (76%)	252 (98%)	6 (2%)	45	34
1	B	257/339 (76%)	253 (98%)	4 (2%)	58	50
All	All	515/678 (76%)	505 (98%)	10 (2%)	58	43

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61[A]	ARG
1	A	61[B]	ARG
1	A	213[A]	LEU
1	A	213[B]	LEU
1	A	312	ILE
1	A	318	ARG
1	B	27	ASN
1	B	34	GLN

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Mol	Chain	Res	Type
1	B	61	ARG
1	B	71	GLU

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

Mol	Chain	Res	Type
1	B	70	GLN

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

Of 5 ligands modelled in this entry, 5 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.