



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 11:00 AM EST

PDB ID : 7MZV
Title : Structure of yeast pseudouridine synthase 7 (PUS7)
Authors : Purchal, M.; Koutmos, M.
Deposited on : 2021-05-24
Resolution : 3.20 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

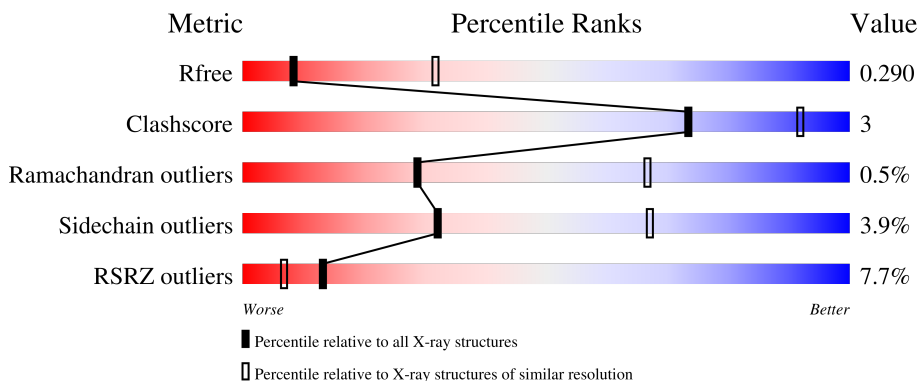
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	676	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1003	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9428 atoms, of which 4722 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 Multisubstrate pseudouridine synthase 7.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	583	9401	2943	4722	824	895	2	15	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

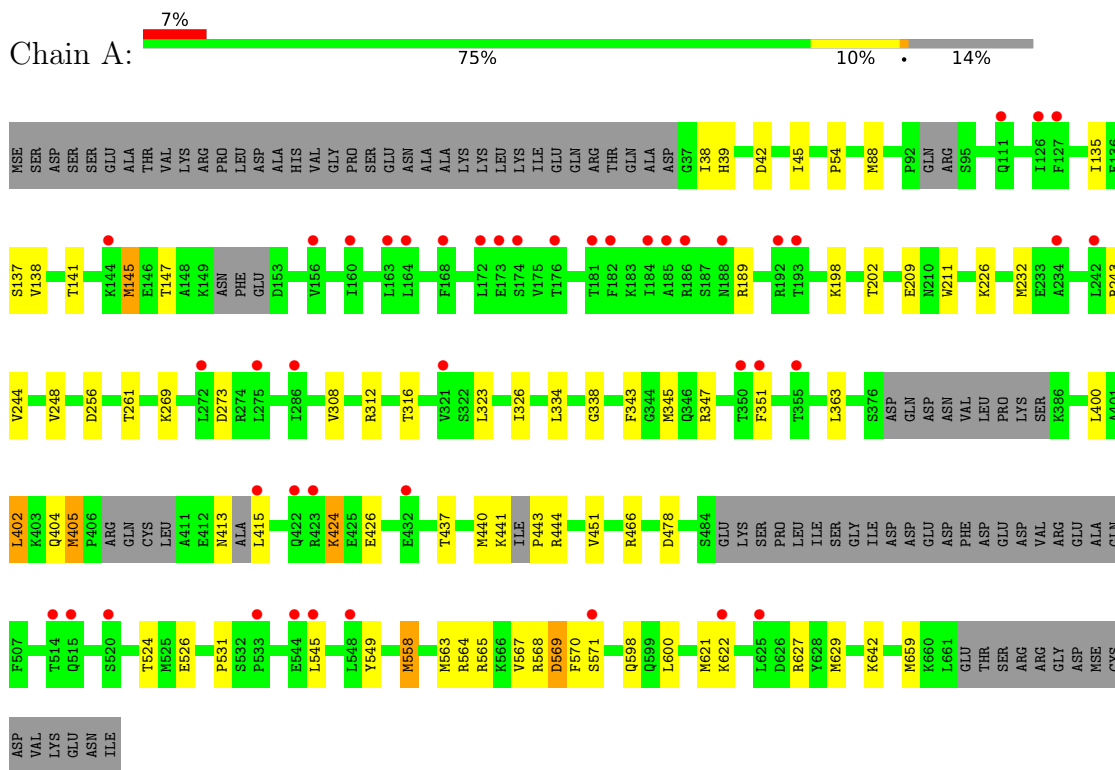
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		

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: Multisubstrate pseudouridine synthase 7



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.89Å 171.80Å 105.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 3.20 46.27 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.32-3.20) 99.9 (46.27-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.230 , 0.287 0.238 , 0.290	Depositor DCC
R_{free} test set	881 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtrriage
Anisotropy	0.226	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 86.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9428	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.64	0/4732	0.77	8/6335 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	MSE	CG-SE-CE	7.26	114.87	98.90
1	A	558	MSE	CG-SE-CE	6.45	113.09	98.90
1	A	405	MSE	CG-SE-CE	5.72	111.49	98.90
1	A	145	MSE	CG-SE-CE	5.64	111.30	98.90
1	A	440	MSE	CG-SE-CE	5.62	111.25	98.90
1	A	659	MSE	CG-SE-CE	5.39	110.75	98.90
1	A	629	MSE	CG-SE-CE	5.39	110.75	98.90
1	A	621	MSE	CG-SE-CE	5.25	110.45	98.90

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	4679	4722	4722	31	0
2	A	15	0	0	0	0
3	A	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4706	4722	4722	31	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 3.

All (31) 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:524:THR:HG23	1:A:526:GLU:HG2	1.90	0.54
1:A:567:VAL:HG12	1:A:568:ARG:H	1.75	0.52
1:A:226:LYS:HE2	1:A:261:THR:OG1	2.11	0.50
1:A:424:LYS:HE2	1:A:424:LYS:H	1.76	0.50
1:A:413:ASN:O	1:A:415:LEU:N	2.45	0.49
1:A:135:ILE:O	1:A:138:VAL:HG22	2.13	0.48
1:A:211:TRP:CH2	1:A:273:ASP:HB3	2.50	0.47
1:A:138:VAL:O	1:A:141:THR:O	2.33	0.47
1:A:137:SER:O	1:A:141:THR:OG1	2.26	0.47
1:A:38:ILE:HG13	1:A:42:ASP:HB2	1.97	0.46
1:A:202:THR:OG1	1:A:209:GLU:O	2.19	0.45
1:A:441:LYS:O	1:A:443:PRO:N	2.50	0.45
1:A:244:VAL:HG11	1:A:248:VAL:HG21	1.99	0.45
1:A:312:ARG:NH2	1:A:600:LEU:HG	2.32	0.45
1:A:308:VAL:HG22	1:A:642:LYS:HG3	1.99	0.45
1:A:564:ARG:O	1:A:565:ARG:NH1	2.49	0.44
1:A:45:ILE:HD13	1:A:345:MSE:HE1	2.00	0.43
1:A:54:PRO:HB2	1:A:326:ILE:HG12	1.99	0.43
1:A:466:ARG:HD3	1:A:545:LEU:HD21	2.01	0.42
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.85	0.42
1:A:343:PHE:CD1	1:A:347:ARG:HD3	2.54	0.41
1:A:569:ASP:C	1:A:571:SER:H	2.22	0.41
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.84	0.41
1:A:568:ARG:C	1:A:570:PHE:H	2.24	0.41
1:A:244:VAL:CG1	1:A:248:VAL:HG11	2.51	0.41
1:A:312:ARG:NH2	1:A:598:GLN:O	2.54	0.41
1:A:334:LEU:O	1:A:338:GLY:HA2	2.21	0.41
1:A:363:LEU:HG	1:A:451:VAL:HG12	2.03	0.41
1:A:531:PRO:HD2	1:A:549:TYR:OH	2.21	0.41
1:A:316:THR:HG22	1:A:323:LEU:HD13	2.01	0.40
1:A:88:MSE:HE1	1:A:273:ASP: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	567/676 (84%)	493 (87%)	71 (12%)	3 (0%)	29 67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	351	PHE
1	A	404	GLN
1	A	569	ASP

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	516/582 (89%)	496 (96%)	20 (4%)	32 67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	145	MSE
1	A	147	THR
1	A	189	ARG
1	A	198	LYS
1	A	232	MSE
1	A	243	ARG
1	A	256	ASP

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Mol	Chain	Res	Type
1	A	269	LYS
1	A	400	LEU
1	A	402	LEU
1	A	405	MSE
1	A	424	LYS
1	A	426	GLU
1	A	437	THR
1	A	444	ARG
1	A	478	ASP
1	A	558	MSE
1	A	622	LYS
1	A	627	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1001	-	4,4,4	0.40	0	6,6,6	0.07	0
2	SO4	A	1003	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	1002	-	4,4,4	0.38	0	6,6,6	0.05	0

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 [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	568/676 (84%)	0.80	44 (7%) 13 7	77, 121, 195, 227	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	ILE	7.8
1	A	163	LEU	6.3
1	A	188	ASN	6.3
1	A	182	PHE	6.2
1	A	168	PHE	5.3
1	A	127	PHE	5.2
1	A	351	PHE	5.2
1	A	174	SER	4.6
1	A	173	GLU	4.3
1	A	176	THR	4.3
1	A	185	ALA	4.2
1	A	172	LEU	4.1
1	A	422	GLN	3.6
1	A	164	LEU	3.3
1	A	275	LEU	3.0
1	A	126	ILE	2.8
1	A	144	LYS	2.8
1	A	415	LEU	2.8
1	A	544	GLU	2.7
1	A	181	THR	2.7
1	A	111	GLN	2.6
1	A	184	ILE	2.6
1	A	193	THR	2.5
1	A	286	ILE	2.4
1	A	514	THR	2.4
1	A	234	ALA	2.4
1	A	545	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	350	THR	2.4
1	A	186	ARG	2.4
1	A	192	ARG	2.4
1	A	432	GLU	2.3
1	A	321	VAL	2.3
1	A	622	LYS	2.3
1	A	533	PRO	2.2
1	A	515	GLN	2.2
1	A	625	LEU	2.2
1	A	355	THR	2.2
1	A	242	LEU	2.2
1	A	571	SER	2.2
1	A	156	VAL	2.1
1	A	548	LEU	2.1
1	A	272	LEU	2.1
1	A	520	SER	2.1
1	A	423	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	1003	5/5	0.60	0.42	194,202,212,216	0
2	SO4	A	1002	5/5	0.64	0.35	167,174,179,181	0
2	SO4	A	1001	5/5	0.88	0.32	100,104,108,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.