



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:47 AM UTC

PDB ID : 5WYL / pdb_00005wyl
Title : Crystal structure of Chaetomium thermophilum Utp10 N-terminal domain in complex with Utp17 C-terminal helices
Authors : Chen, R.; Zhu, X.; Ye, K.
Deposited on : 2017-01-13
Resolution : 2.64 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

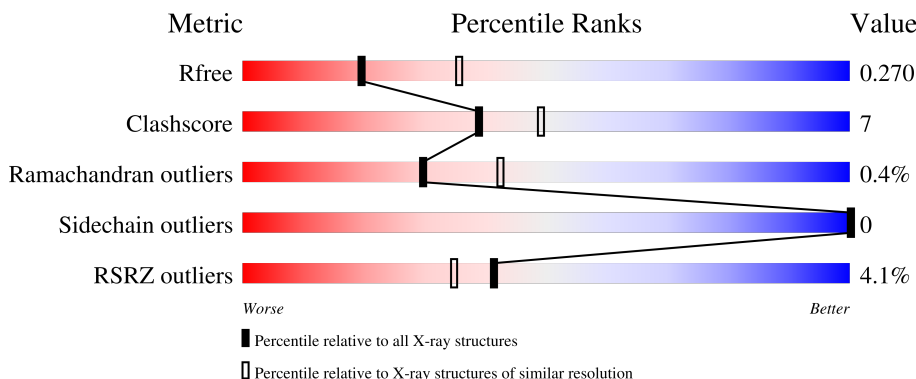
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	471	4% 75% 13% 13%
1	C	471	3% 74% 15% 11%
2	B	54	6% 67% 6% 28%
2	D	54	2% 67% 9% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7086 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3184	2041	550	579	14			
1	C	418	Total	C	N	O	S	0	0	0
			3242	2069	572	587	14			

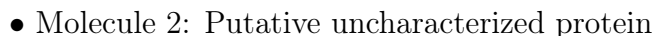
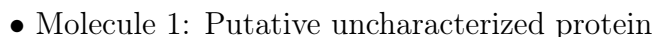
- Molecule 2 is a protein called Putative uncharacterized protein.

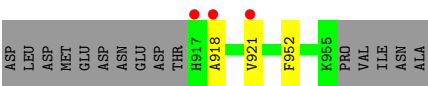
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	S	0	0	0
			294	196	45	52	1			
2	D	41	Total	C	N	O	S	0	0	0
			311	205	49	56	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	1	Total	O	0	0
			1	1		
3	C	18	Total	O	0	0
			18	18		
3	D	6	Total	O	0	0
			6	6		

- Molecule 1: Putative uncharacterized protein





● Molecule 2: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.31Å 98.31Å 235.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.01 – 2.64 39.01 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.01-2.64) 99.8 (39.01-2.64)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.40 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11rc1_2513: ???)	Depositor
R, R_{free}	0.212 , 0.267 0.214 , 0.270	Depositor DCC
R_{free} test set	2000 reflections (5.72%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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	0.41	0/3240	0.61	0/4394
1	C	0.40	0/3300	0.61	0/4477
2	B	0.34	0/303	0.55	0/416
2	D	0.45	0/320	0.59	0/439
All	All	0.40	0/7163	0.60	0/9726

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	3184	0	3269	42	0
1	C	3242	0	3331	50	0
2	B	294	0	287	4	0
2	D	311	0	303	4	0
3	A	30	0	0	4	0
3	B	1	0	0	0	0
3	C	18	0	0	2	0
3	D	6	0	0	0	0
All	All	7086	0	7190	96	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 7.

All (96) 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:C:83:ARG:NH2	1:C:95:ASP:OD1	2.11	0.84
1:A:83:ARG:NH2	1:A:95:ASP:OD1	2.12	0.81
1:A:336:PRO:O	3:A:501:HOH:O	2.04	0.74
1:C:415:ASN:O	1:C:419:GLN:HG2	1.89	0.72
1:A:319:ARG:O	1:A:353:LYS:NZ	2.24	0.71
1:C:87:THR:HG22	1:C:88:ALA:H	1.55	0.70
1:A:450:GLU:O	1:A:454:LEU:HD22	1.91	0.70
1:A:163:GLU:OE1	3:A:502:HOH:O	2.10	0.69
1:C:413:ASP:HA	1:C:416:ILE:HG22	1.76	0.67
1:C:333:ILE:HD12	1:C:377:VAL:HG11	1.77	0.67
1:C:87:THR:HB	1:C:90:GLU:H	1.62	0.64
1:A:232:MET:HE3	1:A:232:MET:HA	1.80	0.63
1:C:116:LYS:NZ	3:C:502:HOH:O	2.32	0.62
1:C:163:GLU:H	1:C:163:GLU:CD	2.07	0.61
1:C:410:VAL:O	1:C:413:ASP:HB2	1.99	0.61
1:A:86:MET:HE1	1:A:94:LEU:HD22	1.81	0.61
1:C:333:ILE:CD1	1:C:377:VAL:HG11	2.32	0.59
1:C:36:GLU:HG3	1:C:37:PRO:HD2	1.84	0.58
1:C:87:THR:HG22	1:C:88:ALA:N	2.19	0.58
1:C:442:ILE:HA	1:C:445:VAL:HG12	1.85	0.57
1:C:389:GLU:O	1:C:393:LYS:HG3	2.04	0.57
1:C:129:GLU:HG2	1:C:156:PRO:HG3	1.87	0.56
1:C:253:PRO:O	1:C:257:GLU:HG2	2.05	0.56
1:C:190:PRO:O	3:C:501:HOH:O	2.17	0.56
1:A:390:LYS:O	1:A:394:VAL:HG12	2.06	0.55
1:C:372:ILE:HG23	1:C:375:LEU:HD12	1.87	0.55
1:A:249:GLN:NE2	3:A:507:HOH:O	2.40	0.55
1:C:445:VAL:O	1:C:446:ASP:HB2	2.08	0.54
1:A:227:GLY:O	1:A:231:LYS:HG2	2.08	0.54
1:C:132:THR:HG23	1:C:155:LEU:HD22	1.90	0.53
1:A:281:LYS:O	1:A:283:SER:N	2.42	0.53
1:C:157:VAL:HG22	1:C:165:ARG:HH12	1.74	0.53
1:C:279:ALA:HB2	1:C:315:LEU:HD23	1.90	0.52
1:C:425:VAL:O	1:C:429:GLN:HG3	2.09	0.52
1:A:356:ASN:HD22	1:A:391:GLN:HB3	1.75	0.52
1:C:413:ASP:CA	1:C:416:ILE:HG22	2.40	0.52
1:C:290:THR:HA	1:C:293:MET:HE2	1.93	0.50
1:C:435:GLY:O	1:C:439:ARG:HG2	2.13	0.49
1:A:293:MET:HB3	1:A:328:VAL:HG11	1.95	0.49
1:A:281:LYS:NZ	2:B:921:VAL:HG12	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ILE:HG13	1:C:406:ILE:O	2.12	0.49
1:C:333:ILE:O	1:C:333:ILE:HG13	2.13	0.48
1:A:50:SER:O	1:A:54:GLU:HG2	2.13	0.48
1:A:383:LEU:HD21	1:A:427:LEU:HD23	1.94	0.48
1:C:165:ARG:NH2	1:C:168:ASP:OD2	2.46	0.48
1:A:310:VAL:HG12	1:A:345:ILE:HG12	1.95	0.48
1:C:293:MET:HB3	1:C:328:VAL:HG11	1.95	0.48
1:A:284:LEU:HD13	1:A:288:ILE:HG23	1.96	0.48
1:C:371:ASP:CG	1:C:373:ARG:HG2	2.41	0.46
1:A:442:ILE:HG21	1:A:449:ILE:HD11	1.97	0.46
1:C:166:PHE:HB3	1:C:185:GLN:CD	2.40	0.46
1:A:324:LEU:HD11	1:A:354:LEU:HD12	1.98	0.45
1:A:205:ARG:NH1	1:A:257:GLU:OE1	2.46	0.45
1:C:270:ALA:O	1:C:273:MET:HB2	2.16	0.45
1:A:277:ILE:HG23	2:B:952:PHE:CE2	2.51	0.45
1:A:350:GLN:NE2	3:A:505:HOH:O	2.50	0.45
1:A:451:GLU:O	1:A:455:LYS:HB3	2.16	0.45
1:C:284:LEU:HD22	1:C:288:ILE:HG21	1.99	0.45
1:C:324:LEU:HG	1:C:357:GLY:HA3	1.99	0.45
1:C:413:ASP:O	1:C:416:ILE:HG22	2.17	0.44
1:A:267:ILE:HD12	1:A:267:ILE:HA	1.91	0.44
1:C:372:ILE:HD11	1:C:416:ILE:HG13	1.99	0.44
1:C:350:GLN:HG3	2:D:954:THR:O	2.18	0.44
1:A:324:LEU:HG	1:A:357:GLY:HA3	1.99	0.44
1:A:356:ASN:ND2	1:A:391:GLN:HB3	2.33	0.44
1:A:290:THR:O	1:A:294:GLU:HG3	2.18	0.44
1:C:362:PHE:HB3	1:C:374:THR:HB	2.00	0.43
1:A:83:ARG:HA	1:A:86:MET:HE3	2.01	0.43
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.85	0.43
1:A:86:MET:HB2	1:A:91:ASN:ND2	2.34	0.43
1:C:382:LEU:HD23	1:C:382:LEU:HA	1.86	0.43
1:A:192:LEU:O	1:A:196:ILE:HG13	2.19	0.43
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.79	0.43
2:B:921:VAL:HG11	2:B:952:PHE:CZ	2.53	0.43
1:C:324:LEU:HD11	1:C:354:LEU:HD12	2.00	0.42
1:C:356:ASN:O	1:C:359:VAL:HG12	2.19	0.42
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.86	0.42
2:D:938:MET:HE3	2:D:939:PRO:HD2	2.02	0.42
1:A:381:LEU:O	1:A:384:SER:OG	2.33	0.42
1:C:278:LEU:HB3	1:C:284:LEU:HD11	2.01	0.42
1:A:31:LYS:HB3	1:A:154:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:O	1:A:313:THR:HG23	2.20	0.41
1:A:59:LEU:HA	1:A:62:LEU:HD12	2.01	0.41
1:A:290:THR:HA	1:A:293:MET:HE2	2.02	0.41
1:A:189:ARG:HD3	1:A:189:ARG:HA	1.80	0.41
1:C:255:LEU:O	1:C:259:MET:HG3	2.20	0.41
1:A:288:ILE:HD12	1:A:288:ILE:HA	1.88	0.41
2:D:919:VAL:CG1	2:D:954:THR:HG22	2.51	0.41
1:C:261:MET:HE2	1:C:261:MET:HB3	1.66	0.41
1:A:284:LEU:HB3	1:A:288:ILE:CG2	2.51	0.41
1:C:353:LYS:HB2	1:C:353:LYS:HE3	1.78	0.41
1:C:439:ARG:HG2	1:C:439:ARG:H	1.68	0.41
1:C:346:SER:HA	1:C:349:HIS:O	2.22	0.40
1:A:177:PRO:HA	1:A:178:PRO:HD2	1.98	0.40
1:A:281:LYS:HZ3	2:B:921:VAL:HG12	1.86	0.40
2:D:955:LYS:HE3	2:D:955:LYS:HB2	1.91	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	405/471 (86%)	395 (98%)	9 (2%)	1 (0%)	43	58
1	C	416/471 (88%)	403 (97%)	11 (3%)	2 (0%)	24	36
2	B	37/54 (68%)	36 (97%)	0	1 (3%)	4	4
2	D	39/54 (72%)	38 (97%)	1 (3%)	0	100	100
All	All	897/1050 (85%)	872 (97%)	21 (2%)	4 (0%)	30	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	GLY
2	B	918	ALA
1	C	87	THR
1	C	408	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	343/397 (86%)	343 (100%)	0	100	100
1	C	349/397 (88%)	349 (100%)	0	100	100
2	B	30/45 (67%)	30 (100%)	0	100	100
2	D	32/45 (71%)	32 (100%)	0	100	100
All	All	754/884 (85%)	754 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	131	ASN
1	A	250	GLN
1	A	356	ASN
1	C	298	HIS
1	C	349	HIS
1	C	350	GLN
1	C	415	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	411/471 (87%)	0.30	21 (5%) 33 27	40, 59, 93, 108	0
1	C	418/471 (88%)	0.12	12 (2%) 53 48	37, 59, 94, 128	0
2	B	39/54 (72%)	0.72	3 (7%) 19 16	54, 71, 90, 109	0
2	D	41/54 (75%)	0.01	1 (2%) 59 55	41, 51, 73, 97	0
All	All	909/1050 (86%)	0.22	37 (4%) 41 35	37, 59, 94, 128	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	412	ALA	4.1
1	A	283	SER	4.0
1	C	414	GLY	3.7
1	A	27	ALA	3.6
1	C	425	VAL	3.2
1	C	410	VAL	3.2
1	A	229	ILE	3.1
1	A	456	LEU	2.9
1	A	449	ILE	2.9
1	A	406	ILE	2.9
1	A	248	LEU	2.6
1	C	411	ASP	2.6
2	B	918	ALA	2.6
1	A	402	ALA	2.6
2	B	917	HIS	2.5
1	C	428	SER	2.5
1	A	446	ASP	2.5
1	A	448	ASN	2.4
1	A	454	LEU	2.4
1	A	458	ALA	2.4
1	A	284	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	347	LYS	2.3
1	A	417	ARG	2.3
1	C	88	ALA	2.3
2	D	955	LYS	2.3
1	C	427	LEU	2.2
1	A	256	SER	2.2
1	A	407	ASP	2.2
1	A	288	ILE	2.2
1	A	457	GLY	2.1
1	C	406	ILE	2.1
2	B	921	VAL	2.1
1	C	29	HIS	2.1
1	A	396	TYR	2.1
1	A	445	VAL	2.1
1	A	233	ARG	2.0
1	C	372	ILE	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.