Full wwPDB X-ray Structure Validation Report ⓘ

Jul 17, 2024 – 08:09 PM JST

PDB ID	:	8WIA
Title	:	Crystal structure of E. coli ThrS catalytic domain mutant G463S
Authors	:	Qiao, H.; Wang, Z.; Wang, J.; Fang, P.
Deposited on	:	2023-09-24
Resolution	:	1.96 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:

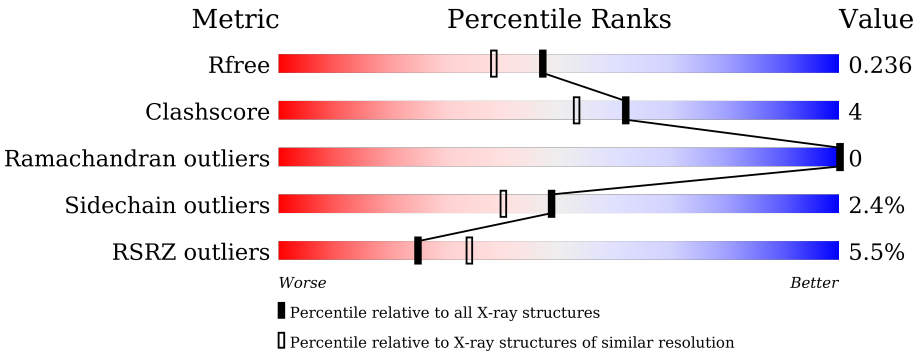
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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% 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	410	6% 87% 11% .
1	B	410	5% 82% 14% . .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7126 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 Threonine–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	1	0
			3285	2077	574	610	24			
1	B	399	Total	C	N	O	S	0	1	0
			3265	2061	577	604	23			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	initiating methionine	UNP A0A8S7FUD7
A	463	SER	GLY	engineered mutation	UNP A0A8S7FUD7
A	643	LEU	-	expression tag	UNP A0A8S7FUD7
A	644	GLU	-	expression tag	UNP A0A8S7FUD7
A	645	HIS	-	expression tag	UNP A0A8S7FUD7
A	646	HIS	-	expression tag	UNP A0A8S7FUD7
A	647	HIS	-	expression tag	UNP A0A8S7FUD7
A	648	HIS	-	expression tag	UNP A0A8S7FUD7
A	649	HIS	-	expression tag	UNP A0A8S7FUD7
A	650	HIS	-	expression tag	UNP A0A8S7FUD7
B	241	MET	-	initiating methionine	UNP A0A8S7FUD7
B	463	SER	GLY	engineered mutation	UNP A0A8S7FUD7
B	643	LEU	-	expression tag	UNP A0A8S7FUD7
B	644	GLU	-	expression tag	UNP A0A8S7FUD7
B	645	HIS	-	expression tag	UNP A0A8S7FUD7
B	646	HIS	-	expression tag	UNP A0A8S7FUD7
B	647	HIS	-	expression tag	UNP A0A8S7FUD7
B	648	HIS	-	expression tag	UNP A0A8S7FUD7
B	649	HIS	-	expression tag	UNP A0A8S7FUD7
B	650	HIS	-	expression tag	UNP A0A8S7FUD7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is water.

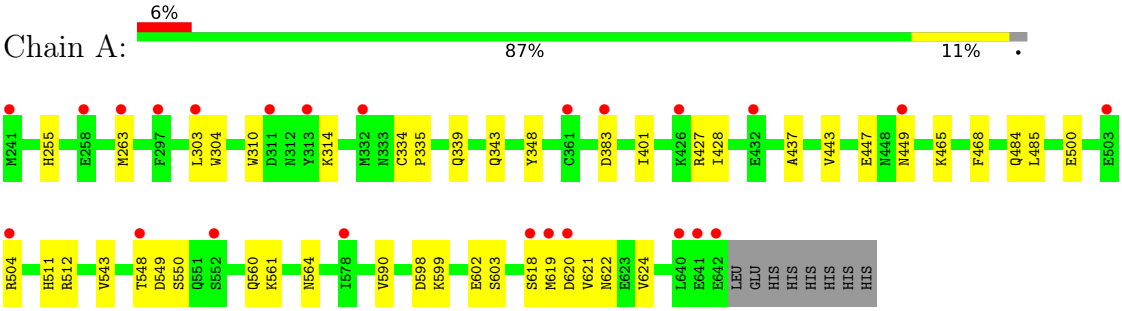
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	273	Total O 273 273	0	0
3	B	301	Total O 301 301	0	0

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.

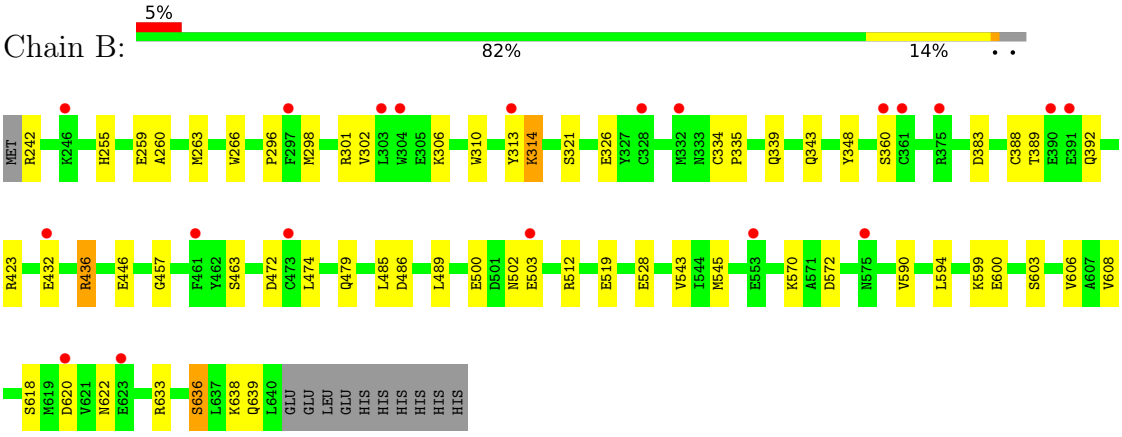
• Molecule 1: Threonine–tRNA ligase

Chain A:



• Molecule 1: Threonine–tRNA ligase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.96Å 107.41Å 112.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.18 – 1.96 77.78 – 1.96	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.18-1.96) 97.2 (77.78-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.212 , 0.237 0.212 , 0.236	Depositor DCC
R_{free} test set	3848 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7126	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ZN

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	0.25	0/3357	0.50	0/4521
1	B	0.24	0/3336	0.50	0/4492
All	All	0.25	0/6693	0.50	0/9013

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	3285	0	3204	24	0
1	B	3265	0	3195	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	273	0	0	1	0
3	B	301	0	0	6	0
All	All	7126	0	6399	57	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 (57) 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:633:ARG:HD3	3:B:981:HOH:O	1.60	1.01
1:B:360:SER:HB2	3:B:1042:HOH:O	1.94	0.65
1:B:639:GLN:CB	3:B:1026:HOH:O	2.44	0.65
1:A:484:GLN:HB2	1:A:511:HIS:HB2	1.82	0.61
1:B:348:TYR:CZ	1:B:500:GLU:HG3	2.36	0.60
1:A:465:LYS:HB3	1:A:484:GLN:HG2	1.84	0.59
1:A:619:MET:HE2	1:A:624:VAL:HG22	1.86	0.58
1:A:561:LYS:NZ	1:A:622:ASN:OD1	2.37	0.58
1:B:389:THR:H	1:B:392:GLN:NE2	2.03	0.56
1:A:263:MET:HB3	1:B:296:PRO:HB3	1.87	0.55
1:A:620:ASP:OD1	1:A:621:VAL:N	2.40	0.55
1:A:599:LYS:O	1:A:603:SER:OG	2.20	0.54
1:B:301:ARG:NH1	1:B:326:GLU:OE1	2.42	0.52
1:A:310:TRP:O	1:A:314:LYS:HB3	2.10	0.52
1:A:543:VAL:HG23	1:A:590:VAL:HG11	1.91	0.52
1:B:334:CYS:HB2	1:B:335:PRO:HD3	1.91	0.51
1:A:334:CYS:HB2	1:A:335:PRO:HD3	1.92	0.50
1:B:335:PRO:O	1:B:339:GLN:HG2	2.11	0.50
1:B:594:LEU:HD22	1:B:608:VAL:HG22	1.93	0.49
1:B:389:THR:H	1:B:392:GLN:HE21	1.59	0.48
1:A:348:TYR:CZ	1:A:500:GLU:HG3	2.49	0.48
1:B:446:GLU:OE2	3:B:802:HOH:O	2.20	0.48
1:A:255:HIS:ND1	1:B:343:GLN:HG3	2.29	0.47
1:B:310:TRP:O	1:B:314:LYS:HB2	2.14	0.47
1:B:570:LYS:HB3	1:B:570:LYS:HE2	1.64	0.47
1:B:594:LEU:HB3	1:B:606:VAL:HG21	1.96	0.47
1:B:313:TYR:OH	3:B:801:HOH:O	2.20	0.47
1:A:504:ARG:NH1	3:A:810:HOH:O	2.48	0.46
1:B:543:VAL:HG23	1:B:590:VAL:HG11	1.97	0.46
1:A:335:PRO:O	1:A:339:GLN:HG2	2.15	0.46
1:B:636:SER:OG	1:B:638:LYS:O	2.34	0.46
1:A:427:ARG:HG2	1:A:428:ILE:N	2.31	0.46
1:A:437:ALA:HA	1:A:485:LEU:HD23	1.97	0.45
1:B:472:ASP:HB2	1:B:528:GLU:OE1	2.16	0.45
1:A:560:GLN:HE21	1:A:564:ASN:ND2	2.15	0.45
1:B:242:ARG:N	3:B:813:HOH:O	2.49	0.45
1:B:242:ARG:HD2	1:B:474:LEU:HD11	1.99	0.45
1:B:620:ASP:OD1	1:B:622:ASN:N	2.49	0.44
1:B:301:ARG:HD2	1:B:310:TRP:CZ2	2.53	0.44
1:A:401:ILE:HD12	1:A:468:PHE:HZ	1.83	0.43
1:A:304:TRP:CZ3	1:A:335:PRO:HG2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:LYS:NZ	1:B:600:GLU:OE2	2.31	0.43
1:B:348:TYR:CE2	1:B:500:GLU:HG3	2.54	0.43
1:B:266:TRP:HZ2	1:B:519:GLU:HG3	1.84	0.43
1:B:432:GLU:O	1:B:436[B]:ARG:HG3	2.19	0.43
1:A:548:THR:OG1	1:A:549:ASP:N	2.52	0.43
1:B:302:VAL:O	1:B:306:LYS:HG3	2.20	0.42
1:B:463:SER:HB2	1:B:485:LEU:O	2.19	0.42
1:B:545:MET:HG2	1:B:572:ASP:HB3	2.01	0.42
1:B:260:ALA:HB1	1:B:263:MET:HE3	2.01	0.42
1:A:598:ASP:O	1:A:602:GLU:HG3	2.20	0.41
1:B:486:ASP:OD2	1:B:489:LEU:HB2	2.20	0.41
1:A:343:GLN:HG3	1:B:255:HIS:CG	2.55	0.41
1:A:443:VAL:O	1:A:447:GLU:HG3	2.20	0.41
1:B:423:ARG:O	1:B:457:GLY:HA2	2.21	0.41
1:A:303:LEU:HD13	1:B:259:GLU:HG2	2.02	0.40
1:B:388:CYS:HB2	1:B:392:GLN:HE21	1.86	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	401/410 (98%)	399 (100%)	2 (0%)	0	100	100
1	B	398/410 (97%)	397 (100%)	1 (0%)	0	100	100
All	All	799/820 (97%)	796 (100%)	3 (0%)	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	356/366 (97%)	351 (99%)	5 (1%)	67 62
1	B	354/366 (97%)	341 (96%)	13 (4%)	34 22
All	All	710/732 (97%)	692 (98%)	18 (2%)	49 38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	ASP
1	A	449	ASN
1	A	512	ARG
1	A	550	SER
1	A	618	SER
1	B	298	MET
1	B	314	LYS
1	B	321	SER
1	B	383	ASP
1	B	436[A]	ARG
1	B	436[B]	ARG
1	B	479	GLN
1	B	502	ASN
1	B	503	GLU
1	B	512	ARG
1	B	603	SER
1	B	618	SER
1	B	636	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	449	ASN
1	A	564	ASN
1	B	392	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	479	GLN
1	B	630	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - 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

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, 95^{th} 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	402/410 (98%)	0.55	24 (5%)	21	30	28, 36, 50, 75	287 (71%)
1	B	399/410 (97%)	0.52	20 (5%)	28	39	29, 35, 44, 80	282 (70%)
All	All	801/820 (97%)	0.53	44 (5%)	25	34	28, 36, 48, 80	569 (71%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	TYR	7.6
1	B	297	PHE	4.6
1	B	332	MET	4.3
1	A	620	ASP	4.2
1	B	313	TYR	3.8
1	B	328	CYS	3.6
1	B	361	CYS	3.6
1	A	332	MET	3.4
1	A	241	MET	3.2
1	A	642	GLU	3.1
1	B	553	GLU	3.0
1	A	383	ASP	2.9
1	A	619	MET	2.8
1	B	390	GLU	2.8
1	A	297[A]	PHE	2.8
1	A	303	LEU	2.7
1	A	449	ASN	2.7
1	B	503	GLU	2.6
1	A	361	CYS	2.6
1	A	258	GLU	2.5
1	A	578	ILE	2.5
1	A	641	GLU	2.5
1	B	575	ASN	2.4
1	B	620	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	473	CYS	2.3
1	A	640	LEU	2.3
1	B	303	LEU	2.3
1	A	503	GLU	2.2
1	B	304	TRP	2.2
1	B	432	GLU	2.2
1	A	311	ASP	2.2
1	B	375	ARG	2.2
1	A	618	SER	2.1
1	B	360	SER	2.1
1	A	263	MET	2.1
1	A	504	ARG	2.1
1	B	461	PHE	2.1
1	A	432	GLU	2.0
1	A	552	SER	2.0
1	B	623	GLU	2.0
1	B	391	GLU	2.0
1	A	426	LYS	2.0
1	B	246	LYS	2.0
1	A	548	THR	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, 95^{th} 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	ZN	A	701	1/1	0.77	0.20	38,38,38,38	1
2	ZN	B	701	1/1	0.85	0.15	37,37,37,37	1

6.5 Other polymers (i)

There are no such residues in this entry.