



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 AM UTC

PDB ID : 7XS0 / pdb_00007xs0
Title : Trimer structure of HtrA from Helicobacter pylori bound with a tripeptide
Authors : Cui, L.; Liu, W.
Deposited on : 2022-05-12
Resolution : 2.59 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

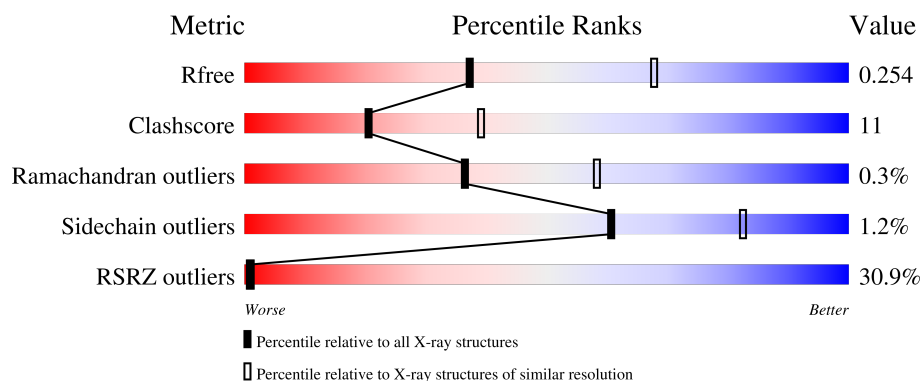
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	441	26% 66% 17% • 15%
2	B	3	67% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2939 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 Periplasmic serine endoprotease DegP-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2858	1785	501	569	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP O25663
A	-7	GLY	-	expression tag	UNP O25663
A	-6	HIS	-	expression tag	UNP O25663
A	-5	HIS	-	expression tag	UNP O25663
A	-4	HIS	-	expression tag	UNP O25663
A	-3	HIS	-	expression tag	UNP O25663
A	-2	HIS	-	expression tag	UNP O25663
A	-1	HIS	-	expression tag	UNP O25663

- Molecule 2 is a protein called UNK-UNK-UNK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			16	9	3	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	139.51Å 139.51Å 191.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.21 – 2.59 41.21 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.21-2.59) 97.4 (41.21-2.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.231 , 0.258 0.231 , 0.254	Depositor DCC
R_{free} test set	1125 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 79.4	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	0.91	EDS
Total number of atoms	2939	wwPDB-VP
Average B, all atoms (Å ²)	60.0	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	0.23	0/2886	0.51	0/3889

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ALA	Peptide
1	A	352	ARG	Peptide
1	A	353	ASP	Peptide
1	A	405	ASP	Peptide
1	A	96	GLU	Peptide

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	2858	0	2907	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	5	1	0
3	A	64	0	0	7	0
3	B	1	0	0	0	0
All	All	2939	0	2912	65	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 11.

All (65) 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:407:VAL:HG11	1:A:431:ILE:HD13	1.57	0.86
1:A:97:ARG:NH2	1:A:134:GLU:OE2	2.10	0.83
1:A:454:LYS:O	3:A:501:HOH:O	1.94	0.83
1:A:260:ASP:OD2	3:A:502:HOH:O	2.05	0.74
1:A:398:LYS:HB2	1:A:404:SER:HA	1.70	0.73
1:A:292:ASP:OD2	3:A:503:HOH:O	2.11	0.68
1:A:97:ARG:O	1:A:97:ARG:HG3	1.94	0.68
1:A:434:LYS:HD2	1:A:439:GLU:HA	1.76	0.67
1:A:96:GLU:HA	1:A:98:ALA:N	2.10	0.67
1:A:408:GLN:OE1	1:A:441:LYS:NZ	2.22	0.66
1:A:133:LYS:O	3:A:504:HOH:O	2.13	0.66
1:A:275:TYR:OH	1:A:303:GLU:OE1	2.13	0.66
1:A:201:ILE:HG12	1:A:332:GLU:HG2	1.80	0.64
1:A:420:PRO:O	1:A:423:GLN:NE2	2.31	0.64
1:A:345:ARG:HD2	1:A:360:THR:HG22	1.84	0.58
1:A:418:ASN:N	1:A:422:GLU:OE1	2.36	0.58
1:A:145:GLU:OE2	1:A:334:ARG:NH2	2.37	0.58
1:A:115:ASN:HD22	1:A:144:SER:HA	1.69	0.57
1:A:93:GLU:O	3:A:505:HOH:O	2.17	0.57
1:A:267:LYS:O	1:A:269:GLY:N	2.38	0.56
1:A:434:LYS:HB3	1:A:461:LEU:HB3	1.86	0.56
1:A:287:LEU:HA	1:A:293:ASN:H	1.72	0.55
1:A:60:THR:O	1:A:97:ARG:HD2	2.08	0.54
1:A:464:ASP:O	1:A:468:GLY:HA2	2.06	0.54
1:A:376:SER:HA	1:A:443:VAL:HG11	1.90	0.53
1:A:57:ASN:OD1	1:A:58:ILE:N	2.41	0.53
1:A:201:ILE:HD13	1:A:335:ASN:HB2	1.90	0.53
1:A:395:GLN:O	1:A:399:ARG:HG2	2.09	0.52
1:A:135:TYR:CE2	1:A:155:LYS:HD2	2.44	0.52
1:A:453:TYR:HA	1:A:456:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD13	1:A:409:GLY:O	2.09	0.52
1:A:352:ARG:O	1:A:353:ASP:HB2	2.11	0.51
1:A:135:TYR:HE2	1:A:155:LYS:HD2	1.75	0.51
1:A:466:ASN:C	1:A:468:GLY:H	2.19	0.50
1:A:354:LYS:O	1:A:354:LYS:HD3	2.12	0.50
1:A:61:GLU:H	1:A:123:LYS:HE3	1.77	0.50
1:A:176:PHE:CD1	1:A:176:PHE:N	2.80	0.50
1:A:155:LYS:HD3	1:A:158:LEU:HD21	1.93	0.49
1:A:292:ASP:CG	3:A:503:HOH:O	2.56	0.48
1:A:114:ASN:HB2	1:A:117:VAL:HG23	1.95	0.48
1:A:94:ARG:HD2	1:A:94:ARG:O	2.12	0.47
1:A:399:ARG:HA	1:A:399:ARG:HD3	1.73	0.47
1:A:211:GLN:HA	1:A:250:GLY:O	2.15	0.47
1:A:275:TYR:CZ	1:A:277:GLY:HA2	2.52	0.45
1:A:345:ARG:HH11	1:A:360:THR:HG22	1.81	0.44
1:A:135:TYR:CD1	1:A:135:TYR:N	2.85	0.44
1:A:458:LYS:HB3	1:A:474:VAL:HG22	1.99	0.44
1:A:135:TYR:N	1:A:135:TYR:HD1	2.14	0.44
1:A:175:VAL:C	1:A:176:PHE:CD1	2.96	0.44
1:A:267:LYS:C	1:A:269:GLY:H	2.26	0.43
1:A:96:GLU:HA	1:A:97:ARG:C	2.44	0.43
1:A:254:PRO:O	1:A:258:VAL:HG23	2.19	0.43
1:A:405:ASP:HA	1:A:406:ASP:HA	1.86	0.43
1:A:280:LEU:H	2:B:1:UNK:HA	1.84	0.43
1:A:430:ASN:HD22	1:A:464:ASP:HA	1.84	0.42
1:A:458:LYS:HB3	1:A:474:VAL:CG2	2.50	0.42
1:A:458:LYS:HD3	1:A:460:PHE:HE1	1.85	0.42
1:A:116:HIS:HA	1:A:119:ASP:HB2	2.02	0.42
1:A:189:THR:HG21	1:A:215:SER:HB3	2.02	0.41
1:A:92:LYS:N	1:A:93:GLU:HA	2.36	0.41
1:A:249:ILE:O	3:A:506:HOH:O	2.21	0.41
1:A:392:ASP:OD1	1:A:443:VAL:N	2.49	0.41
1:A:57:ASN:OD1	1:A:57:ASN:C	2.64	0.40
1:A:464:ASP:H	1:A:468:GLY:HA2	1.85	0.40
1:A:176:PHE:N	1:A:176:PHE:HD1	2.20	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	362/441 (82%)	344 (95%)	17 (5%)	1 (0%)	36	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	GLU

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	320/372 (86%)	316 (99%)	4 (1%)	61	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	135	TYR
1	A	176	PHE
1	A	201	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	423	GLN
1	A	466	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	376/441 (85%)	1.31	116 (30%) ⓘ ⓘ	16, 49, 116, 148	0
2	B	0/3	-	-	-	-
All	All	376/444 (84%)	1.31	116 (30%) ⓘ ⓘ	16, 49, 116, 148	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	ILE	7.5
1	A	353	ASP	7.4
1	A	404	SER	6.6
1	A	239	ILE	6.4
1	A	377	ALA	6.4
1	A	387	GLY	6.1
1	A	374	THR	5.9
1	A	453	TYR	5.9
1	A	123	LYS	5.4
1	A	379	ASN	5.3
1	A	465	LEU	5.3
1	A	-4	HIS	5.2
1	A	423	GLN	5.2
1	A	455	GLY	5.1
1	A	421	ALA	5.1
1	A	429	GLY	4.8
1	A	354	LYS	4.6
1	A	287	LEU	4.5
1	A	285	GLY	4.5
1	A	249	ILE	4.5
1	A	456	LYS	4.4
1	A	365	GLU	4.4
1	A	424	ALA	4.4
1	A	407	VAL	4.3
1	A	454	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	378	GLN	4.2
1	A	355	LYS	4.2
1	A	94	ARG	4.2
1	A	294	LYS	4.2
1	A	376	SER	4.2
1	A	416	ASN	4.2
1	A	400	SER	4.1
1	A	467	GLN	4.0
1	A	466	ASN	4.0
1	A	122	ASP	4.0
1	A	452	LYS	4.0
1	A	61	GLU	4.0
1	A	200	GLY	4.0
1	A	293	ASN	3.9
1	A	92	LYS	3.9
1	A	474	VAL	3.8
1	A	95	MET	3.8
1	A	435	ILE	3.8
1	A	415	VAL	3.8
1	A	412	VAL	3.8
1	A	97	ARG	3.8
1	A	414	GLN	3.8
1	A	286	ASP	3.5
1	A	411	LEU	3.4
1	A	251	PHE	3.4
1	A	460	PHE	3.4
1	A	405	ASP	3.4
1	A	432	ILE	3.3
1	A	398	LYS	3.3
1	A	-5	HIS	3.2
1	A	469	TYR	3.2
1	A	393	LEU	3.2
1	A	268	THR	3.2
1	A	396	GLU	3.1
1	A	457	PRO	3.1
1	A	157	ASN	3.1
1	A	410	VAL	3.1
1	A	417	GLU	3.1
1	A	292	ASP	3.1
1	A	427	ARG	3.0
1	A	406	ASP	3.0
1	A	388	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	426	PHE	2.9
1	A	463	LEU	2.9
1	A	399	ARG	2.9
1	A	428	GLN	2.9
1	A	132	ASN	2.8
1	A	430	ASN	2.8
1	A	447	ASN	2.8
1	A	361	LEU	2.8
1	A	462	VAL	2.8
1	A	413	SER	2.8
1	A	418	ASN	2.8
1	A	364	ALA	2.7
1	A	390	VAL	2.7
1	A	450	LEU	2.7
1	A	473	LEU	2.7
1	A	391	GLU	2.7
1	A	284	SER	2.7
1	A	345	ARG	2.7
1	A	419	SER	2.7
1	A	264	GLN	2.7
1	A	446	PHE	2.6
1	A	119	ASP	2.6
1	A	471	ILE	2.6
1	A	120	GLY	2.6
1	A	468	GLY	2.6
1	A	451	GLU	2.6
1	A	60	THR	2.5
1	A	154	THR	2.5
1	A	420	PRO	2.5
1	A	449	ALA	2.5
1	A	96	GLU	2.5
1	A	131	SER	2.4
1	A	441	LYS	2.4
1	A	283	LEU	2.3
1	A	121	ALA	2.3
1	A	408	GLN	2.2
1	A	267	LYS	2.2
1	A	363	LEU	2.2
1	A	448	HIS	2.2
1	A	145	GLU	2.2
1	A	93	GLU	2.1
1	A	436	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	156	ASP	2.1
1	A	464	ASP	2.1
1	A	389	GLN	2.1
1	A	395	GLN	2.1
1	A	162	LYS	2.1
1	A	-2	HIS	2.0
1	A	302	VAL	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.