



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:28 PM UTC

PDB ID : 8XJE / pdb_00008xje
Title : Crystal structure of the YqeY protein from Campylobacter jejuni
Authors : Kim, S.Y.; Yoon, S.I.
Deposited on : 2023-12-21
Resolution : 2.10 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

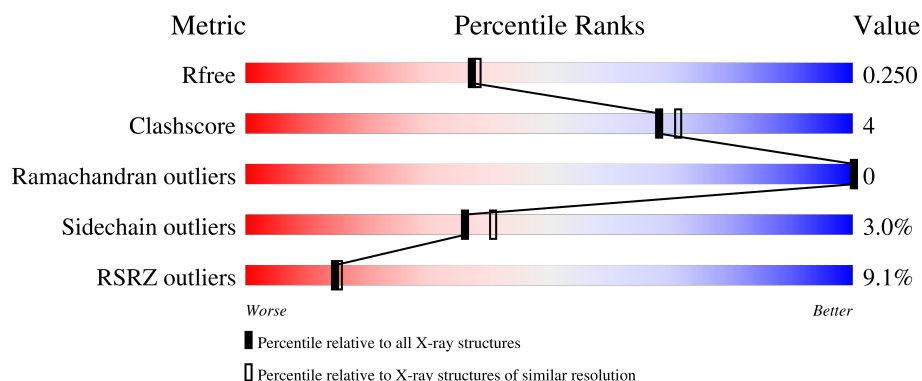
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	153	14% 86% 9% 5%
1	B	153	14% 88% 9% ...
1	C	153	7% 81% 12% 7%
1	D	153	12% 82% 6% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4476 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 YqeY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1151	730	195	223	3			
1	B	149	Total	C	N	O	S	0	0	0
			1140	721	197	219	3			
1	C	142	Total	C	N	O	S	0	0	0
			1099	696	187	213	3			
1	D	135	Total	C	N	O	S	0	0	0
			996	625	174	196	1			

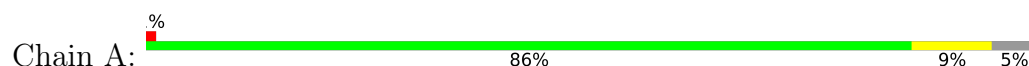
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	38	Total	O	0	0
			38	38		
2	C	19	Total	O	0	0
			19	19		
2	D	11	Total	O	0	0
			11	11		

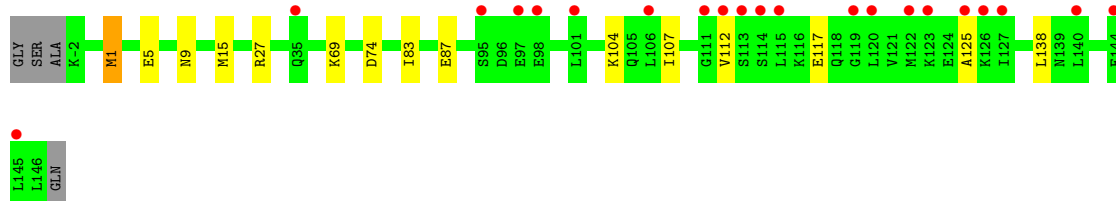
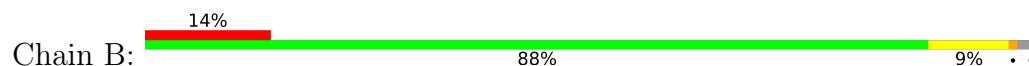
3 Residue-property plots [i](#)

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.

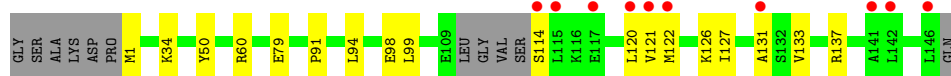
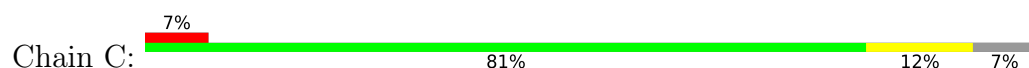
• Molecule 1: YqeY



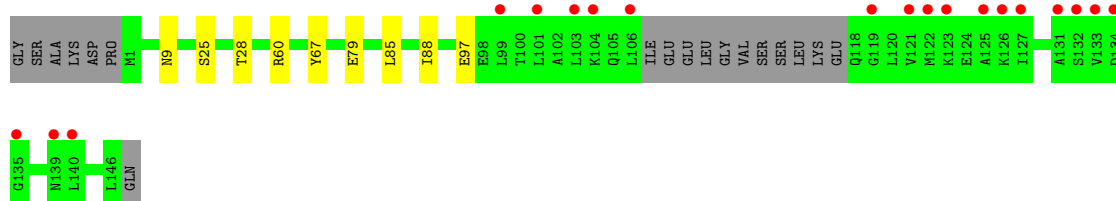
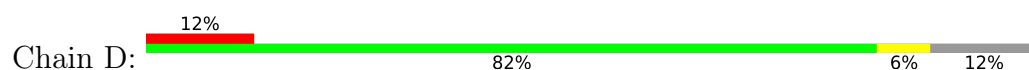
• Molecule 1: YqeY



• Molecule 1: YqeY



• Molecule 1: YqeY



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.20Å 153.71Å 54.02Å 90.00° 91.74° 90.00°	Depositor
Resolution (Å)	29.91 – 2.10 29.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.91-2.10) 97.6 (29.91-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.211 , 0.251 0.211 , 0.250	Depositor DCC
R_{free} test set	1674 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.096 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4476	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 22.16 % 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 6.0342e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.36	0/1157	0.53	0/1549
1	B	0.35	0/1147	0.55	0/1542
1	C	0.29	0/1104	0.48	0/1482
1	D	0.29	0/1001	0.46	0/1352
All	All	0.32	0/4409	0.51	0/5925

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	1151	0	1186	9	0
1	B	1140	0	1143	8	0
1	C	1099	0	1104	9	0
1	D	996	0	921	6	0
2	A	22	0	0	1	0
2	B	38	0	0	0	0
2	C	19	0	0	0	0
2	D	11	0	0	0	0
All	All	4476	0	4354	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 4.

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:D:67:TYR:HE2	1:D:79:GLU:HG3	1.65	0.61
1:A:107:ILE:HG23	1:A:112:VAL:HG23	1.83	0.60
1:B:83:ILE:O	1:B:87:GLU:HG3	2.02	0.59
1:A:27:ARG:NH1	2:A:202:HOH:O	2.23	0.57
1:C:94:LEU:O	1:C:137:ARG:NH2	2.31	0.56
1:C:50:TYR:CD1	1:C:91:PRO:HD3	2.44	0.53
1:A:67:TYR:HE2	1:A:79:GLU:HG3	1.75	0.51
1:C:60:ARG:HG2	1:C:79:GLU:OE1	2.12	0.50
1:A:34:LYS:HB3	1:B:69:LYS:HD2	1.94	0.49
1:D:85:LEU:O	1:D:88:ILE:HG12	2.13	0.48
1:B:107:ILE:HG23	1:B:112:VAL:O	2.14	0.48
1:C:99:LEU:HD13	1:C:133:VAL:HG21	1.95	0.48
1:B:1:MET:HG2	1:B:5:GLU:HB2	1.96	0.47
1:A:60:ARG:HG2	1:A:79:GLU:OE1	2.14	0.47
1:C:94:LEU:HD22	1:C:98:GLU:HB3	1.98	0.46
1:A:67:TYR:CE2	1:A:79:GLU:HG3	2.51	0.46
1:D:9:ASN:HD22	1:D:9:ASN:N	2.14	0.45
1:C:122:MET:O	1:C:126:LYS:HG3	2.16	0.45
1:D:60:ARG:HG2	1:D:79:GLU:OE1	2.16	0.45
1:B:15:MET:HE3	1:B:27:ARG:NH2	2.33	0.44
1:A:3:LEU:O	1:A:3:LEU:HD23	2.17	0.43
1:D:25:SER:O	1:D:28:THR:HB	2.20	0.42
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.84	0.42
1:B:74:ASP:OD1	1:B:74:ASP:N	2.53	0.42
1:C:50:TYR:CE1	1:C:91:PRO:HD3	2.56	0.41
1:B:125:ALA:HB3	1:B:138:LEU:HD21	2.02	0.41
1:B:1:MET:HE1	1:B:9:ASN:HB2	2.04	0.40
1:C:34:LYS:HE3	1:C:34:LYS:HB3	1.89	0.40
1:C:50:TYR:HB3	1:C:131:ALA:CB	2.51	0.40
1:D:85:LEU:HD23	1:D:85:LEU:HA	1.91	0.40
1:A:74:ASP:N	1:A:74:ASP:OD1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	144/153 (94%)	141 (98%)	3 (2%)	0	100	100
1	B	147/153 (96%)	145 (99%)	2 (1%)	0	100	100
1	C	138/153 (90%)	136 (99%)	2 (1%)	0	100	100
1	D	131/153 (86%)	130 (99%)	1 (1%)	0	100	100
All	All	560/612 (92%)	552 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	120/136 (88%)	116 (97%)	4 (3%)	33	37
1	B	114/136 (84%)	111 (97%)	3 (3%)	40	46
1	C	111/136 (82%)	106 (96%)	5 (4%)	24	25
1	D	88/136 (65%)	87 (99%)	1 (1%)	65	74
All	All	433/544 (80%)	420 (97%)	13 (3%)	36	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ILE
1	A	93	GLN

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Mol	Chain	Res	Type
1	A	109	GLU
1	A	123	LYS
1	B	1	MET
1	B	104	LYS
1	B	117	GLU
1	C	1	MET
1	C	114	SER
1	C	120	LEU
1	C	121	VAL
1	C	127	ILE
1	D	97	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	30	ASN
1	A	93	GLN
1	B	6	GLN
1	B	71	ASN
1	C	6	GLN
1	C	9	ASN
1	C	139	ASN
1	D	6	GLN
1	D	9	ASN

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

There are no ligands in this entry.

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, 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	146/153 (95%)	0.32	2 (1%) 73 75	21, 37, 60, 86	0
1	B	149/153 (97%)	0.62	21 (14%) 6 6	22, 37, 77, 88	0
1	C	142/153 (92%)	0.58	10 (7%) 22 24	29, 44, 70, 80	0
1	D	135/153 (88%)	0.93	19 (14%) 6 6	25, 48, 87, 104	0
All	All	572/612 (93%)	0.61	52 (9%) 15 15	21, 41, 78, 104	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	LEU	5.3
1	D	121	VAL	5.2
1	A	113	SER	5.0
1	D	127	ILE	4.9
1	B	122	MET	4.6
1	D	122	MET	4.6
1	B	112	VAL	4.5
1	B	97	GLU	4.2
1	D	104	LYS	4.2
1	D	123	LYS	4.1
1	D	126	LYS	4.0
1	B	113	SER	3.8
1	D	119	GLY	3.6
1	B	127	ILE	3.6
1	D	125	ALA	3.3
1	D	106	LEU	3.3
1	D	133	VAL	3.1
1	B	114	SER	3.0
1	B	101	LEU	2.9
1	D	134	ASP	2.9
1	C	114	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	126	LYS	2.8
1	B	125	ALA	2.7
1	D	131	ALA	2.7
1	B	140	LEU	2.6
1	B	98	GLU	2.6
1	B	111	GLY	2.6
1	D	139	ASN	2.6
1	B	145	LEU	2.5
1	C	115	LEU	2.5
1	B	120	LEU	2.4
1	B	115	LEU	2.4
1	C	120	LEU	2.4
1	B	119	GLY	2.4
1	B	144	GLU	2.3
1	C	121	VAL	2.3
1	C	117	GLU	2.2
1	B	123	LYS	2.2
1	C	142	LEU	2.2
1	B	95	SER	2.2
1	C	131	ALA	2.2
1	C	141	ALA	2.2
1	D	101	LEU	2.2
1	A	62	ASP	2.2
1	C	146	LEU	2.2
1	D	99	LEU	2.2
1	C	122	MET	2.1
1	B	35	GLN	2.1
1	D	135	GLY	2.1
1	D	140	LEU	2.1
1	D	132	SER	2.1
1	B	106	LEU	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.