Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:41 pm BST

PDB ID	:	1TQ5
Title	:	Crystal Structure of YhhW from Escherichia coli
Authors	:	Adams, M.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2004-06-16
Resolution	:	1.76 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 following versions of software and data (see references ⓘ) were used in the production of this report:

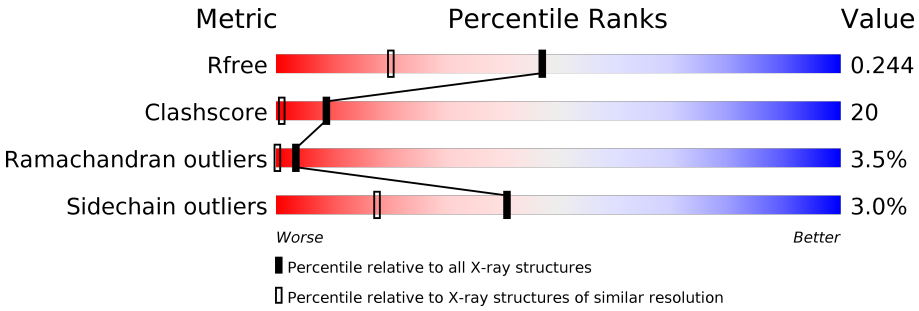
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 on 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%

Mol	Chain	Length	Quality of chain
1	A	242	66% 28%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2018 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 Protein yhhW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	Se	0	0	0
			1870	1176	334	353	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P46852
A	35	MSE	MET	MODIFIED RESIDUE	UNP P46852
A	62	MSE	MET	MODIFIED RESIDUE	UNP P46852
A	79	MSE	MET	MODIFIED RESIDUE	UNP P46852
A	93	MSE	MET	MODIFIED RESIDUE	UNP P46852
A	120	MSE	MET	MODIFIED RESIDUE	UNP P46852
A	160	MSE	MET	MODIFIED RESIDUE	UNP P46852
A	232	SER	-	CLONING ARTIFACT	UNP P46852
A	233	GLY	-	CLONING ARTIFACT	UNP P46852
A	234	ARG	-	CLONING ARTIFACT	UNP P46852
A	235	VAL	-	CLONING ARTIFACT	UNP P46852
A	236	GLU	-	CLONING ARTIFACT	UNP P46852
A	237	HIS	-	EXPRESSION TAG	UNP P46852
A	238	HIS	-	EXPRESSION TAG	UNP P46852
A	239	HIS	-	EXPRESSION TAG	UNP P46852
A	240	HIS	-	EXPRESSION TAG	UNP P46852
A	241	HIS	-	EXPRESSION TAG	UNP P46852
A	242	HIS	-	EXPRESSION TAG	UNP P46852

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Cd	0	0
			6	6		

- Molecule 3 is water.

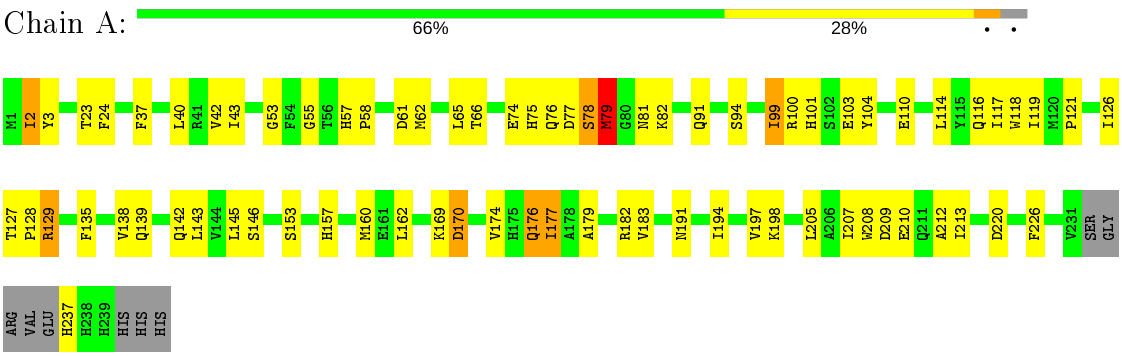
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Protein yhhW

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	62.77Å 62.77Å 98.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.23 – 1.76 47.54 – 1.76	Depositor EDS
% Data completeness (in resolution range)	92.9 (54.23-1.76) 92.8 (47.54-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.197 , 0.250 0.243 , 0.244	Depositor DCC
R_{free} test set	1074 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.040 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2018	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.60% 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: CD

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	0.42	0/1913	0.60	0/2582

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	1870	0	1765	74	1
2	A	6	0	0	0	0
3	A	142	0	0	4	0
All	All	2018	0	1765	74	1

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 20.

All (74) 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:24:PHE:HE2	1:A:43:ILE:HD13	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HD13	1:A:100:ARG:H	1.46	0.80
1:A:2:ILE:HD12	1:A:197:VAL:HG21	1.64	0.78
1:A:24:PHE:CE2	1:A:43:ILE:HD13	2.22	0.74
1:A:76:GLN:HG2	1:A:82:LYS:HD2	1.69	0.74
1:A:177:ILE:HD13	1:A:183:VAL:HG21	1.70	0.73
1:A:42:VAL:C	1:A:43:ILE:HD12	2.10	0.72
1:A:40:LEU:HD11	1:A:43:ILE:HD11	1.71	0.71
1:A:42:VAL:O	1:A:43:ILE:HD12	1.90	0.71
1:A:43:ILE:HG13	1:A:117:ILE:HD12	1.73	0.71
1:A:66:THR:HB	1:A:91:GLN:HG2	1.75	0.68
1:A:76:GLN:NE2	1:A:104:TYR:HE2	1.93	0.66
1:A:78:SER:HB3	1:A:99:ILE:HD13	1.78	0.65
1:A:94:SER:HB3	1:A:126:ILE:HD11	1.80	0.63
1:A:177:ILE:CD1	1:A:183:VAL:HG21	2.29	0.61
1:A:74:GLU:HG2	1:A:104:TYR:CE2	2.36	0.61
1:A:99:ILE:HD13	1:A:100:ARG:N	2.15	0.61
1:A:2:ILE:HD11	1:A:205:LEU:HD22	1.83	0.61
1:A:77:ASP:O	1:A:79:MSE:N	2.33	0.60
1:A:77:ASP:CG	1:A:81:ASN:HB2	2.22	0.60
1:A:194:ILE:HD12	1:A:205:LEU:HD12	1.83	0.60
1:A:66:THR:HG23	1:A:116:GLN:HE21	1.67	0.59
1:A:114:LEU:HD12	1:A:114:LEU:C	2.24	0.58
1:A:176:GLN:O	1:A:177:ILE:HB	2.04	0.57
1:A:110:GLU:HG2	3:A:1064:HOH:O	2.06	0.56
1:A:62:MSE:HA	1:A:121:PRO:HD3	1.87	0.56
1:A:2:ILE:HD13	1:A:3:TYR:N	2.21	0.55
1:A:76:GLN:HE21	1:A:104:TYR:HE2	1.55	0.55
1:A:2:ILE:HD13	1:A:2:ILE:C	2.27	0.55
1:A:143:LEU:HD21	1:A:146:SER:OG	2.07	0.54
1:A:77:ASP:OD2	1:A:81:ASN:HB2	2.09	0.53
1:A:40:LEU:CD1	1:A:43:ILE:HD11	2.38	0.52
1:A:77:ASP:OD1	1:A:81:ASN:HB2	2.10	0.52
1:A:176:GLN:O	1:A:177:ILE:CB	2.58	0.52
1:A:66:THR:HG23	1:A:116:GLN:NE2	2.24	0.51
1:A:42:VAL:HB	1:A:118:TRP:HB2	1.92	0.51
1:A:191:ASN:HB3	3:A:1065:HOH:O	2.11	0.50
1:A:177:ILE:HD13	1:A:183:VAL:CG2	2.40	0.49
1:A:2:ILE:HG12	1:A:207:ILE:HG12	1.94	0.49
1:A:114:LEU:O	1:A:114:LEU:HD12	2.12	0.49
1:A:210:GLU:HG3	1:A:212:ALA:H	1.78	0.49
1:A:177:ILE:HD12	1:A:213:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HB3	1:A:142:GLN:NE2	2.28	0.48
1:A:119:ILE:HD13	1:A:160:MSE:HE3	1.94	0.48
1:A:114:LEU:CD1	1:A:116:GLN:HG2	2.44	0.48
1:A:37:PHE:CZ	1:A:182:ARG:HB3	2.49	0.48
1:A:55:GLY:O	1:A:57:HIS:CD2	2.66	0.47
1:A:65:LEU:HD12	1:A:91:GLN:O	2.16	0.46
1:A:40:LEU:CG	1:A:43:ILE:HD11	2.45	0.46
1:A:94:SER:HB2	1:A:129:ARG:HG3	1.98	0.46
1:A:65:LEU:HD22	1:A:145:LEU:HD11	1.97	0.45
1:A:126:ILE:HD13	1:A:157:HIS:CD2	2.50	0.45
1:A:74:GLU:HG2	1:A:104:TYR:CZ	2.52	0.45
1:A:114:LEU:HD13	1:A:116:GLN:HG2	1.99	0.43
1:A:2:ILE:HG23	1:A:2:ILE:O	2.17	0.43
1:A:160:MSE:SE	1:A:160:MSE:C	3.06	0.43
1:A:174:VAL:HA	1:A:213:ILE:O	2.20	0.42
1:A:23:THR:HB	1:A:43:ILE:HB	1.99	0.42
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.85	0.42
1:A:78:SER:HB2	1:A:100:ARG:HB2	2.01	0.42
1:A:53:GLY:HA3	1:A:104:TYR:HA	2.02	0.42
1:A:169:LYS:HG2	1:A:170:ASP:OD1	2.19	0.42
1:A:43:ILE:HG13	1:A:117:ILE:CD1	2.47	0.42
1:A:75:HIS:HD2	1:A:103:GLU:OE2	2.02	0.42
1:A:127:THR:HA	1:A:128:PRO:HD3	1.94	0.41
1:A:162:LEU:HD13	1:A:226:PHE:CD1	2.54	0.41
1:A:143:LEU:HG	1:A:153:SER:HB3	2.03	0.41
1:A:198:LYS:HG3	3:A:1065:HOH:O	2.20	0.41
1:A:208:TRP:O	1:A:209:ASP:HB2	2.21	0.41
1:A:58:PRO:HA	1:A:99:ILE:O	2.21	0.41
1:A:237:HIS:CD2	1:A:237:HIS:N	2.87	0.41
1:A:76:GLN:HG2	1:A:82:LYS:CD	2.46	0.41
1:A:78:SER:HB3	1:A:99:ILE:CD1	2.50	0.40
1:A:57:HIS:HD2	3:A:1105:HOH:O	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:OD2	1:A:220:ASP:OD2[6_764]	2.00	0.20

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	230/242 (95%)	209 (91%)	13 (6%)	8 (4%)	3 0

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	78	SER
1	A	138	VAL
1	A	139	GLN
1	A	177	ILE
1	A	61	ASP
1	A	79	MSE
1	A	179	ALA

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	198/201 (98%)	192 (97%)	6 (3%)	41 18

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	79	MSE
1	A	99	ILE

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Mol	Chain	Res	Type
1	A	101	HIS
1	A	129	ARG
1	A	170	ASP

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

Mol	Chain	Res	Type
1	A	12	HIS
1	A	33	ASN
1	A	52	GLN
1	A	75	HIS
1	A	76	GLN
1	A	81	ASN
1	A	84	GLN
1	A	116	GLN
1	A	175	HIS
1	A	239	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.