



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2022 – 04:07 pm BST

PDB ID : 7QIH
Title : Complex of the Yersinia enterocolitica Type III secretion proteins YscX and YscY
Authors : Gilzer, D.; Niemann, H.H.
Deposited on : 2021-12-15
Resolution : 1.92 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
Xtrriage (Phenix) : 1.13
EDS : 2.28.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2977 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 Chaperone protein YscY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	111	921	574	176	166	5	0	4	0
1	C	110	891	555	172	160	4	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P0C2N2
A	-6	GLY	-	expression tag	UNP P0C2N2
A	-5	HIS	-	expression tag	UNP P0C2N2
A	-4	HIS	-	expression tag	UNP P0C2N2
A	-3	HIS	-	expression tag	UNP P0C2N2
A	-2	HIS	-	expression tag	UNP P0C2N2
A	-1	HIS	-	expression tag	UNP P0C2N2
A	0	HIS	-	expression tag	UNP P0C2N2
A	1	GLY	-	expression tag	UNP P0C2N2
C	-7	MET	-	initiating methionine	UNP P0C2N2
C	-6	GLY	-	expression tag	UNP P0C2N2
C	-5	HIS	-	expression tag	UNP P0C2N2
C	-4	HIS	-	expression tag	UNP P0C2N2
C	-3	HIS	-	expression tag	UNP P0C2N2
C	-2	HIS	-	expression tag	UNP P0C2N2
C	-1	HIS	-	expression tag	UNP P0C2N2
C	0	HIS	-	expression tag	UNP P0C2N2
C	1	GLY	-	expression tag	UNP P0C2N2

- Molecule 2 is a protein called Yop proteins translocation protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	71	573	357	104	111	1	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	65	Total	C	N	O	S	0	0	0
			522	326	91	104	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	46	GLY	-	expression tag	UNP P0C2N4
B	47	ALA	-	expression tag	UNP P0C2N4
B	48	MET	-	expression tag	UNP P0C2N4
B	49	GLY	-	expression tag	UNP P0C2N4
D	46	GLY	-	expression tag	UNP P0C2N4
D	47	ALA	-	expression tag	UNP P0C2N4
D	48	MET	-	expression tag	UNP P0C2N4
D	49	GLY	-	expression tag	UNP P0C2N4

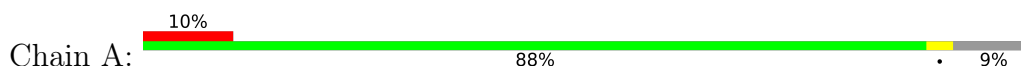
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	1
			32	32		
3	B	9	Total	O	0	0
			9	9		
3	C	24	Total	O	0	1
			25	25		
3	D	4	Total	O	0	0
			4	4		

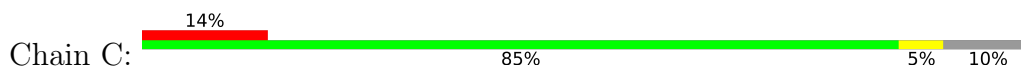
3 Residue-property plots [i](#)

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.

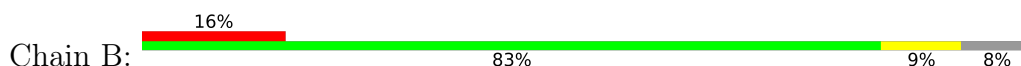
- Molecule 1: Chaperone protein YscY



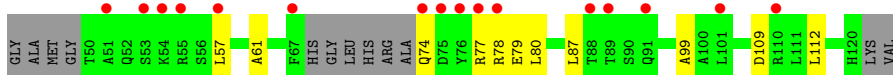
- Molecule 1: Chaperone protein YscY



- Molecule 2: Yop proteins translocation protein X



- Molecule 2: Yop proteins translocation protein X



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	41.55Å 140.83Å 59.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.62 – 1.92 45.62 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.62-1.92) 99.7 (45.62-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.92Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.221 , 0.262 0.221 , 0.259	Depositor DCC
R_{free} test set	1386 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtrriage
Anisotropy	0.480	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2977	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.17 % 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 5.2048e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.24	0/950	0.46	0/1286
1	C	0.23	0/907	0.44	0/1227
2	B	0.23	0/585	0.44	0/791
2	D	0.22	0/528	0.44	0/713
All	All	0.23	0/2970	0.45	0/4017

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	921	0	913	3	0
1	C	891	0	883	6	0
2	B	573	0	567	5	0
2	D	522	0	515	9	0
3	A	32	0	0	0	0
3	B	9	0	0	0	0
3	C	25	0	0	1	0
3	D	4	0	0	1	0
All	All	2977	0	2878	15	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 3.

All (15) 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)
2:D:78:ARG:NH2	3:D:201:HOH:O	2.33	0.60
1:C:86:ARG:HG3	2:D:57:LEU:HD11	1.85	0.57
1:A:52:VAL:HG21	2:B:61:ALA:HB2	1.89	0.53
1:C:12:PHE:HZ	2:D:80:LEU:HD12	1.75	0.52
1:C:50:ARG:NH1	3:C:202:HOH:O	2.43	0.51
1:C:52:VAL:HG21	2:D:61:ALA:HB2	1.93	0.50
1:C:8:ARG:NH2	2:D:79:GLU:OE2	2.45	0.50
1:A:44:LEU:HD11	1:A:73[B]:HIS:CE1	2.48	0.48
2:D:87:LEU:HB2	2:D:99:ALA:HB2	1.95	0.47
2:B:109:ASP:OD2	1:C:25:HIS:ND1	2.47	0.47
2:B:50:THR:HG22	2:B:52:GLN:H	1.81	0.46
2:B:87:LEU:HB2	2:B:99:ALA:HB2	1.99	0.44
2:B:101:LEU:HD13	2:D:112:LEU:HD11	2.00	0.43
1:A:25:HIS:ND1	2:D:109:ASP:OD2	2.50	0.41
2:D:74:GLN:HB3	2:D:77:ARG:HB3	2.02	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	113/122 (93%)	110 (97%)	3 (3%)	0	100	100
1	C	108/122 (88%)	105 (97%)	3 (3%)	0	100	100
2	B	70/77 (91%)	69 (99%)	1 (1%)	0	100	100
2	D	61/77 (79%)	60 (98%)	1 (2%)	0	100	100
All	All	352/398 (88%)	344 (98%)	8 (2%)	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	98/103 (95%)	98 (100%)	0	100	100
1	C	93/103 (90%)	93 (100%)	0	100	100
2	B	63/65 (97%)	63 (100%)	0	100	100
2	D	58/65 (89%)	58 (100%)	0	100	100
All	All	312/336 (93%)	312 (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. There are no such sidechains identified.

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 monosaccharides 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	111/122 (90%)	1.13	12 (10%) 5 7	30, 43, 79, 91	0
1	C	110/122 (90%)	1.24	17 (15%) 2 2	35, 52, 80, 104	0
2	B	71/77 (92%)	1.34	12 (16%) 1 1	42, 60, 77, 89	0
2	D	65/77 (84%)	1.64	16 (24%) 0 0	49, 64, 109, 118	0
All	All	357/398 (89%)	1.30	57 (15%) 1 2	30, 55, 87, 118	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	LEU	7.6
2	D	67	PHE	7.3
1	A	23	CYS	5.8
2	B	70	LEU	5.8
1	A	56	ASN	5.7
2	D	76	TYR	5.7
2	D	78	ARG	5.2
2	D	88	THR	5.0
1	C	95	ASP	4.8
2	B	58	TRP	4.7
2	B	118	LEU	4.6
2	D	51	ALA	4.4
1	A	57	ASN	4.3
1	C	2	ASN	4.0
1	C	57	ASN	3.8
1	A	58	ASN	3.8
1	C	19	LEU	3.7
1	C	99	HIS	3.5
1	C	83	CYS	3.5
2	B	116	LEU	3.4
2	D	53	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	94	LEU	3.3
2	B	119	LEU	3.3
2	B	110	ARG	3.2
1	A	8	ARG	3.2
1	C	111	ASN	3.1
1	C	14	LEU	3.0
1	C	96	LYS	3.0
2	D	75	ASP	3.0
1	A	93	ASP	2.9
2	B	120	HIS	2.9
1	C	109	ASP	2.9
1	A	92	GLY	2.8
2	D	89	THR	2.8
2	D	110	ARG	2.8
1	C	41	PRO	2.7
2	D	91	GLN	2.7
1	C	32	LEU	2.6
1	A	49[A]	CYS	2.6
1	C	71	ILE	2.6
2	D	74	GLN	2.5
2	B	84	GLN	2.5
1	A	99	HIS	2.4
2	D	54	LYS	2.3
2	B	52	GLN	2.3
1	C	3	ILE	2.3
2	D	101	LEU	2.3
2	D	55	ARG	2.2
2	D	77	ARG	2.2
1	A	24	GLY	2.2
2	B	51	ALA	2.2
1	C	15	LEU	2.2
2	D	57	LEU	2.1
1	C	103	HIS	2.1
1	A	89	GLN	2.1
2	B	113	GLN	2.0
2	B	73	ALA	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.