Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2020 – 11:02 PM GMT

PDB ID	:	6TPI
Title	:	EnvC bound to the FtsX periplasmic domain
Authors	:	Crow, A.
Deposited on	:	2019-12-13
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 following versions of software and data (see references ①) were used in the production of this report:

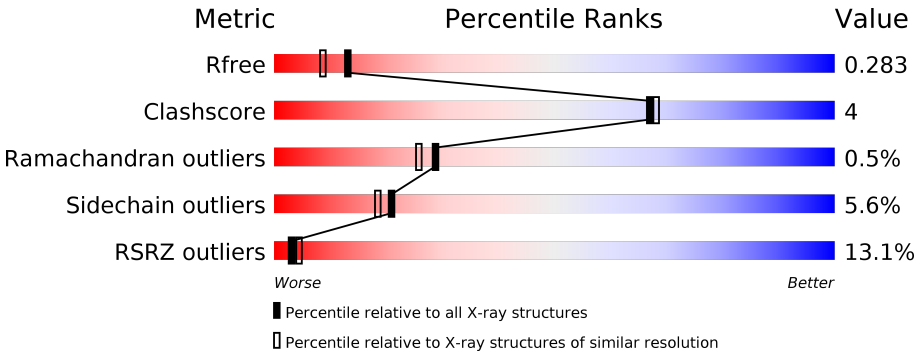
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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% 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	386	6% 89% 9%
2	B	110	% 87% 8%
2	C	110	46% 65% 20% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4767 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 Murein hydrolase activator EnvC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	4	0
			3012	1840	586	581	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	initiating methionine	UNP P37690

- Molecule 2 is a protein called Cell division protein FtsX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			776	482	132	160	2			
2	C	97	Total	C	N	O	S	0	0	0
			750	469	128	151	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	108	MET	-	initiating methionine	UNP P0AC30
B	109	GLY	-	expression tag	UNP P0AC30
B	210	LEU	-	expression tag	UNP P0AC30
B	211	GLU	-	expression tag	UNP P0AC30
B	212	HIS	-	expression tag	UNP P0AC30
B	213	HIS	-	expression tag	UNP P0AC30
B	214	HIS	-	expression tag	UNP P0AC30
B	215	HIS	-	expression tag	UNP P0AC30
B	216	HIS	-	expression tag	UNP P0AC30
B	217	HIS	-	expression tag	UNP P0AC30
C	108	MET	-	initiating methionine	UNP P0AC30
C	109	GLY	-	expression tag	UNP P0AC30
C	210	LEU	-	expression tag	UNP P0AC30

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	211	GLU	-	expression tag	UNP P0AC30
C	212	HIS	-	expression tag	UNP P0AC30
C	213	HIS	-	expression tag	UNP P0AC30
C	214	HIS	-	expression tag	UNP P0AC30
C	215	HIS	-	expression tag	UNP P0AC30
C	216	HIS	-	expression tag	UNP P0AC30
C	217	HIS	-	expression tag	UNP P0AC30

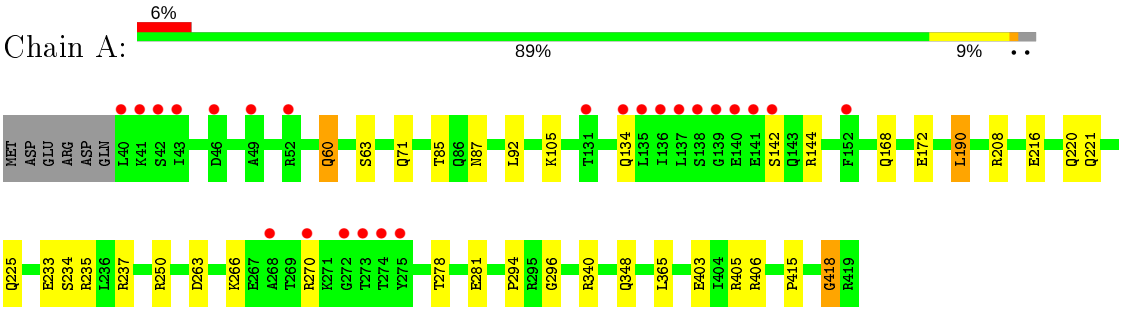
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	173	Total O 173 173	0	0
3	B	53	Total O 53 53	0	0
3	C	3	Total O 3 3	0	0

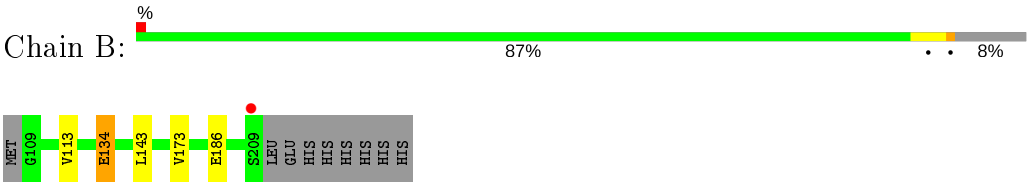
3 Residue-property plots (i)

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.

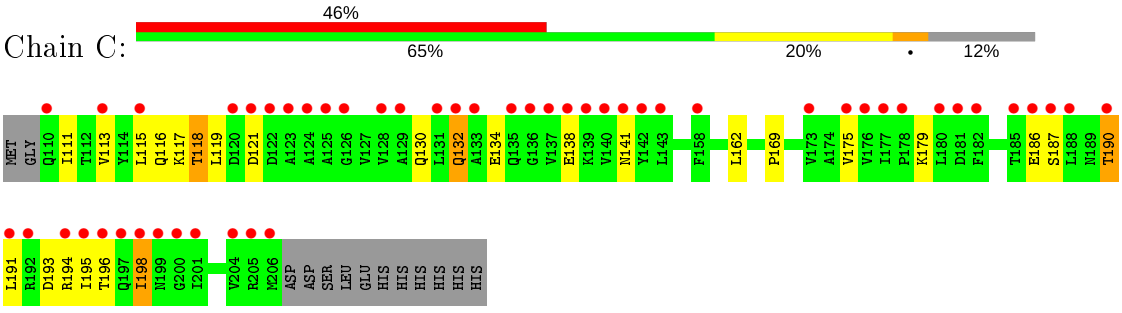
- Molecule 1: Murein hydrolase activator EnvC



- Molecule 2: Cell division protein FtsX



- Molecule 2: Cell division protein FtsX



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.03Å 100.47Å 107.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.82 – 2.10 55.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.82-2.10) 100.0 (55.76-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.275 0.225 , 0.283	Depositor DCC
R_{free} test set	2102 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4767	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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

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	0.69	0/3043	0.85	0/4079
2	B	0.68	0/785	0.80	0/1064
2	C	0.69	0/759	0.78	0/1029
All	All	0.69	0/4587	0.83	0/6172

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	3012	0	3042	19	0
2	B	776	0	755	3	0
2	C	750	0	739	13	0
3	A	173	0	0	3	0
3	B	53	0	0	0	0
3	C	3	0	0	0	0
All	All	4767	0	4536	35	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 (35) 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:C:132:GLN:HA	2:C:132:GLN:HE21	1.38	0.89
1:A:233[B]:GLU:OE1	1:A:237[B]:ARG:NH1	2.26	0.68
1:A:418:GLY:HA2	3:A:538:HOH:O	1.95	0.66
1:A:60:GLN:HE21	1:A:60:GLN:HA	1.67	0.59
1:A:233[A]:GLU:O	1:A:237[A]:ARG:HG3	2.05	0.56
2:C:162:LEU:HD22	2:C:169:PRO:HG2	1.87	0.56
1:A:365:LEU:HD23	1:A:365:LEU:C	2.29	0.53
1:A:85:THR:HG23	1:A:190:LEU:CD2	2.40	0.52
1:A:365:LEU:HB3	1:A:403:GLU:HB2	1.92	0.51
1:A:296:GLY:O	1:A:418:GLY:HA3	2.11	0.50
2:C:138:GLU:HG2	2:C:179:LYS:HA	1.93	0.50
2:B:143:LEU:HB2	2:B:173:VAL:HG13	1.93	0.50
1:A:237[B]:ARG:NH2	3:A:515:HOH:O	2.45	0.50
2:C:195:ILE:O	2:C:198:ILE:HG23	2.11	0.50
1:A:278:THR:OG1	1:A:281:GLU:HG3	2.12	0.49
1:A:85:THR:HG23	1:A:190:LEU:HD22	1.92	0.49
2:C:162:LEU:HD22	2:C:169:PRO:CG	2.42	0.49
2:C:187:SER:O	2:C:190:THR:HG22	2.15	0.46
1:A:250:ARG:CZ	1:A:340:ARG:HD2	2.46	0.45
2:C:191:LEU:HA	2:C:194:ARG:HD2	1.98	0.45
2:C:111:ILE:HD11	2:C:191:LEU:HD12	1.98	0.44
2:C:130:GLN:CD	2:C:198:ILE:HD12	2.37	0.44
1:A:168:GLN:HE21	1:A:172:GLU:HG3	1.82	0.44
2:C:141:ASN:HB3	2:C:175:VAL:HG12	1.99	0.44
1:A:71:GLN:OE1	1:A:208:ARG:HA	2.19	0.42
1:A:220:GLN:O	1:A:225:GLN:NE2	2.36	0.42
1:A:235:ARG:HH21	1:A:348:GLN:HB3	1.83	0.41
2:B:186:GLU:OE1	2:B:186:GLU:HA	2.20	0.41
2:C:175:VAL:HG13	2:C:175:VAL:O	2.20	0.41
1:A:294:PRO:HB2	1:A:415:PRO:HB2	2.03	0.41
1:A:263:ASP:O	1:A:266:LYS:N	2.41	0.41
2:C:115:LEU:HD12	2:C:115:LEU:N	2.36	0.41
1:A:405:ARG:NH2	3:A:520:HOH:O	2.47	0.40
2:C:116:GLN:HB3	2:C:118:THR:HG22	2.03	0.40
2:B:134:GLU:OE1	2:B:134:GLU:HA	2.21	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	382/386 (99%)	369 (97%)	10 (3%)	3 (1%)	19 15
2	B	99/110 (90%)	97 (98%)	2 (2%)	0	100 100
2	C	95/110 (86%)	93 (98%)	2 (2%)	0	100 100
All	All	576/606 (95%)	559 (97%)	14 (2%)	3 (0%)	29 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	142	SER
1	A	418	GLY

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	305/307 (99%)	293 (96%)	12 (4%)	32 33
2	B	83/92 (90%)	81 (98%)	2 (2%)	49 53
2	C	80/92 (87%)	68 (85%)	12 (15%)	3 1
All	All	468/491 (95%)	442 (94%)	26 (6%)	21 18

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	63	SER
1	A	87	ASN
1	A	92	LEU
1	A	105	LYS
1	A	144	ARG
1	A	190	LEU
1	A	216	GLU
1	A	221	GLN
1	A	234	SER
1	A	270	ARG
1	A	406	ARG
2	B	113	VAL
2	B	134	GLU
2	C	113	VAL
2	C	117	LYS
2	C	118	THR
2	C	119	LEU
2	C	121	ASP
2	C	132	GLN
2	C	134	GLU
2	C	186	GLU
2	C	190	THR
2	C	193	ASP
2	C	196	THR
2	C	198	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	143	GLN
1	A	168	GLN
1	A	198	GLN
1	A	315	GLN
2	B	154	ASN
2	C	110	GLN
2	C	132	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

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, 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	380/386 (98%)	0.23	24 (6%) 20 24	27, 45, 103, 142	0
2	B	101/110 (91%)	-0.30	1 (0%) 82 85	35, 48, 72, 103	0
2	C	97/110 (88%)	2.61	51 (52%) 0 0	55, 124, 166, 194	0
All	All	578/606 (95%)	0.54	76 (13%) 3 4	27, 50, 141, 194	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	139	LYS	9.1
2	C	181	ASP	9.0
2	C	182	PHE	8.9
2	C	129	ALA	8.7
2	C	137	VAL	7.9
2	C	197	GLN	7.8
2	C	180	LEU	7.5
1	A	139	GLY	6.8
2	C	177	ILE	6.7
2	C	128	VAL	6.7
2	C	135	GLN	6.6
2	C	186	GLU	6.6
2	C	198	ILE	6.4
1	A	138	SER	6.3
2	C	200	GLY	6.2
2	C	133	ALA	5.9
1	A	134	GLN	5.8
2	C	191	LEU	5.7
1	A	137	LEU	5.7
2	C	142	TYR	5.5
1	A	40	LEU	5.5
2	C	195	ILE	5.3
2	C	175	VAL	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	194	ARG	5.0
2	C	126	GLY	4.9
1	A	140	GLU	4.9
2	C	140	VAL	4.7
2	C	131	LEU	4.7
1	A	272	GLY	4.6
2	C	122	ASP	4.6
2	C	132	GLN	4.6
1	A	141	GLU	4.5
1	A	42	SER	4.4
1	A	142	SER	4.4
2	C	188	LEU	4.3
1	A	136	ILE	4.3
2	C	143	LEU	4.1
1	A	41	LYS	4.0
2	C	199	ASN	3.9
2	C	178	PRO	3.8
1	A	268	ALA	3.7
1	A	274	THR	3.7
2	C	201	ILE	3.6
2	C	113	VAL	3.6
2	C	176	VAL	3.6
1	A	135	LEU	3.6
2	C	120	ASP	3.6
1	A	131	THR	3.6
2	C	115	LEU	3.4
2	C	187	SER	3.4
2	C	205	ARG	3.4
2	C	141	ASN	3.4
2	C	206	MET	3.3
2	C	125	ALA	3.3
2	C	110	GLN	3.1
2	C	173	VAL	3.1
2	C	124	ALA	3.0
1	A	49	ALA	3.0
2	C	196	THR	2.9
2	B	209	SER	2.9
1	A	43	ILE	2.9
2	C	190	THR	2.8
2	C	123	ALA	2.5
1	A	46	ASP	2.5
2	C	192	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	275	TYR	2.4
2	C	204	VAL	2.3
2	C	121	ASP	2.2
2	C	185	THR	2.2
1	A	273	THR	2.2
2	C	136	GLY	2.2
2	C	138	GLU	2.2
2	C	158	PHE	2.1
1	A	52	ARG	2.1
1	A	270	ARG	2.1
1	A	152	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.