



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:16 pm BST

PDB ID : 4UQZ
Title : Coevolution of the ATPase ClpV, the TssB-TssC Sheath and the Accessory HsiE Protein Distinguishes Two Type VI Secretion Classes
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Deposited on : 2014-06-25
Resolution : 1.60 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

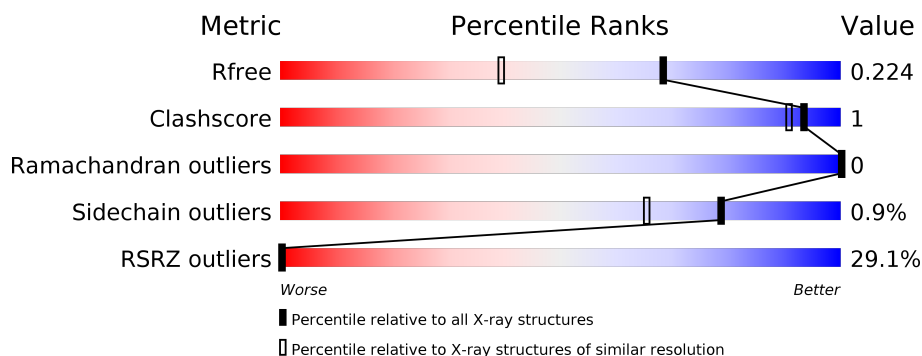
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 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 $\leq 5\%$. 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	261	
2	B	172	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2509 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 HSIE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	3	0
			1997	1265	350	378	4			

- Molecule 2 is a protein called HSIB1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	0	0	0
			194	124	36	34			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

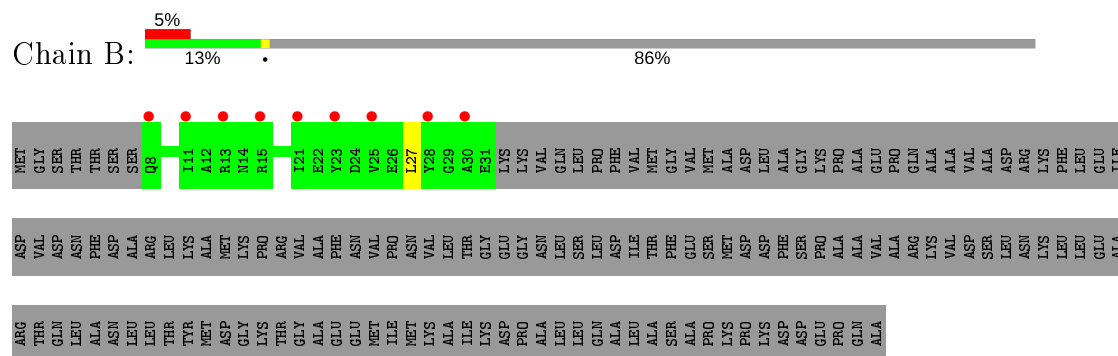


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	288	Total 288	O 288	0	0
4	B	26	Total 26	O 26	0	0

- Molecule 1: HSIE1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.11Å 67.32Å 94.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.21 – 1.60 41.21 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (41.21-1.60) 94.5 (41.21-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 1.60Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.221 0.191 , 0.224	Depositor DCC
R_{free} test set	2102 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.0	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	0.96	EDS
Total number of atoms	2509	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.57	0/2036	0.73	2/2777 (0.1%)
2	B	0.54	0/197	0.63	0/265
All	All	0.56	0/2233	0.73	2/3042 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	235	ARG	NE-CZ-NH1	-5.07	117.76	120.30

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	1997	0	1994	6	0
2	B	194	0	188	1	0
3	A	4	0	3	1	0
4	A	288	0	0	2	0
4	B	26	0	0	0	0
All	All	2509	0	2185	6	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 1.

All (6) 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:272:GLY:O	4:A:2268:HOH:O	2.09	0.68
1:A:142:HIS:ND1	3:A:301:ACT:H3	2.26	0.51
1:A:33:GLU:OE2	1:A:36:ARG:NH1	2.46	0.48
1:A:32:GLU:HG2	2:B:27:LEU:HD12	1.97	0.46
1:A:137:LEU:HD12	1:A:149:LEU:HD12	2.03	0.41
1:A:100[A]:THR:OG1	4:A:2093:HOH:O	2.21	0.41

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	259/261 (99%)	258 (100%)	1 (0%)	0	100	100
2	B	22/172 (13%)	22 (100%)	0	0	100	100
All	All	281/433 (65%)	280 (100%)	1 (0%)	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	203/202 (100%)	201 (99%)	2 (1%)	76	61
2	B	18/140 (13%)	18 (100%)	0	100	100
All	All	221/342 (65%)	219 (99%)	2 (1%)	78	65

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	PHE
1	A	202	LEU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	A	301	-	1,3,3	1.81	0	0,3,3	0.00	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	ACT	1	0

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	258/261 (98%)	1.62	73 (28%)  	13, 22, 41, 59	0
2	B	24/172 (13%)	1.93	9 (37%)  	20, 32, 43, 56	0
All	All	282/433 (65%)	1.64	82 (29%)  	13, 22, 42, 59	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	THR	9.5
1	A	89	ALA	6.7
1	A	31	ALA	5.5
2	B	21	ILE	5.4
1	A	30	ILE	5.2
1	A	271	ALA	5.0
1	A	35	LEU	4.7
1	A	260	LEU	4.1
1	A	214	VAL	4.1
1	A	286	PRO	4.0
1	A	257	ASP	3.9
1	A	106	ALA	3.7
1	A	116	LEU	3.6
1	A	266	LEU	3.5
2	B	30	ALA	3.4
1	A	143	GLY	3.3
1	A	216	LEU	3.3
2	B	8	GLN	3.2
1	A	88	ASP	3.2
1	A	107	LEU	3.2
1	A	185	VAL	3.2
1	A	194	LEU	3.1
1	A	109	ARG	3.0
1	A	54	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	121	LEU	3.0
1	A	187	VAL	3.0
1	A	268	VAL	3.0
1	A	119	VAL	2.9
2	B	25	VAL	2.9
1	A	171	TRP	2.9
1	A	87	LEU	2.9
1	A	137	LEU	2.9
2	B	11	ILE	2.9
1	A	39	ARG	2.9
1	A	166	GLU	2.8
1	A	277	PHE	2.8
1	A	104	CYS	2.7
1	A	183	LEU	2.7
1	A	101	ALA	2.7
1	A	46	ALA	2.6
1	A	231	LEU	2.6
1	A	213	LEU	2.5
1	A	232	LEU	2.5
1	A	120	ILE	2.5
1	A	91	ALA	2.5
1	A	139	ALA	2.5
1	A	215	TRP	2.5
2	B	13	ARG	2.4
1	A	55	PRO	2.4
1	A	140	GLU	2.4
1	A	234	ALA	2.4
1	A	186	ILE	2.4
2	B	23	TYR	2.4
1	A	93	PRO	2.3
1	A	193	TRP	2.3
1	A	60	LEU	2.3
1	A	144	GLU	2.3
1	A	246	ALA	2.3
1	A	92	LEU	2.3
1	A	279	LEU	2.3
1	A	240	VAL	2.3
1	A	256	LEU	2.3
1	A	228	THR	2.2
1	A	115	ARG	2.2
1	A	40	LEU	2.2
1	A	233	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	113	ALA	2.1
1	A	169	PHE	2.1
1	A	50	GLN	2.1
1	A	192	ALA	2.1
1	A	136[A]	SER	2.1
1	A	52	ARG	2.1
1	A	236	TYR	2.1
1	A	206	ALA	2.1
1	A	90	SER	2.0
1	A	195	PRO	2.0
1	A	281	GLU	2.0
2	B	15	ARG	2.0
1	A	63	PHE	2.0
1	A	34	LEU	2.0
1	A	62	ILE	2.0
2	B	28	TYR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	A	301	4/4	0.59	0.16	35,37,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.