

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID : 3DWA

> Title : Crystal structure of the B-subunit of the AB5 toxin from E. coli

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2.08 Å(reported) Resolution

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

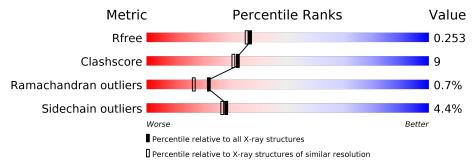
Validation Pipeline (wwPDB-VP) 2.11

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 2.08 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)

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	126	78%	14%	• 6%
1	В	126	72%	19%	• 7%
1	С	126	75%	17%	• 5%
1	D	126	74%	18%	• 7%
1	Е	126	75%	16%	•• 8%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4966 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 Subtilase cytotoxin, subunit B.

Mol	Chain	Residues	${f Atoms}$					ZeroOcc	AltConf	Trace	
1	A	118	Total	С	N	О	S	Se	0	0	0
1	Λ	110	911	580	148	177	4	2	0	0	
1	В	117	Total	С	N	О	S	Se	0	0	0
1	Ъ	111	905	577	147	175	4	2	U	0	U
1	С	120	Total	С	N	О	S	Se	0	0	0
1		120	928	591	150	181	4	2	U	0	
1	D	D 117	Total C N	О	S	Se	0	0	0		
1	D	111	905	577	147	175	4	2	U	U	U
1	Е	116	Total	С	N	О	S	Se	0	0	0
1	נו	110	897	573	145	173	4	2	U	U	U

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
A	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
A	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
A	125	HIS	_	EXPRESSION TAG	UNP Q3ZTX8
A	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
В	119	LEU	=	EXPRESSION TAG	UNP Q3ZTX8
В	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
В	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
В	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
В	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
В	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
В	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
В	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
С	119	LEU	=	EXPRESSION TAG	UNP Q3ZTX8
С	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
С	121	HIS	=	EXPRESSION TAG	UNP Q3ZTX8

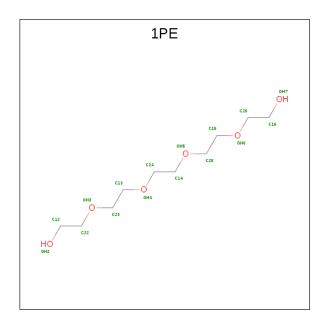
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Chain	Residue	Modelled	Actual	Comment	Reference
С	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
С	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
С	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
С	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
С	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
D	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
D	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
D	125	HIS	_	EXPRESSION TAG	UNP Q3ZTX8
D	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
Е	119	LEU	-	EXPRESSION TAG	UNP Q3ZTX8
Е	120	GLU	-	EXPRESSION TAG	UNP Q3ZTX8
Е	121	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
Е	122	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
Е	123	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
Е	124	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
Е	125	HIS	-	EXPRESSION TAG	UNP Q3ZTX8
Е	126	HIS	-	EXPRESSION TAG	UNP Q3ZTX8

 \bullet Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $\mathrm{C_{10}H_{22}O_6}).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 16	C 10	O 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total C O 16 10 6	0	0
2	С	1	Total C O 16 10 6	0	0
2	D	1	Total C O 16 10 6	0	0
2	E	1	Total C O 16 10 6	0	0

• Molecule 3 is water.

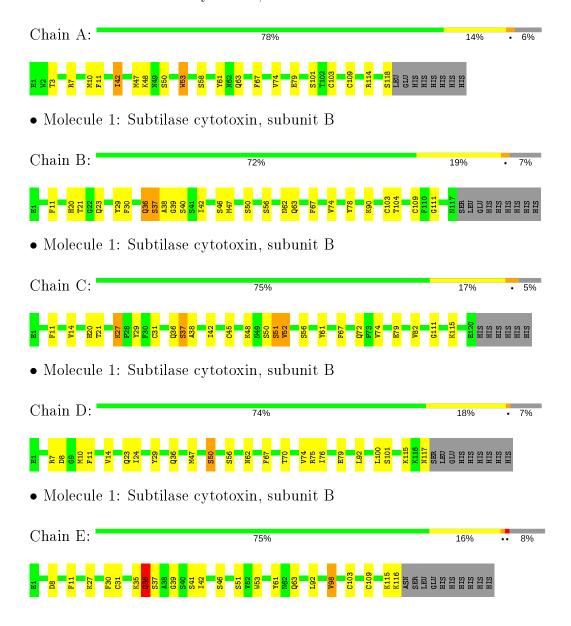
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	В	65	Total O 65 65	0	0
3	С	82	Total O 82 82	0	0
3	D	57	Total O 57 57	0	0
3	E	69	Total O 69 69	0	0



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: Subtilase cytotoxin, subunit B





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	97.63Å 97.63Å 165.36Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.80 - 2.08	Depositor
Resolution (A)	48.82 - 2.09	EDS
% Data completeness	87.0 (48.80-2.08)	Depositor
(in resolution range)	87.2 (48.82-2.09)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.04 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.189 , 0.236	Depositor
R, R_{free}	0.261 , 0.253	DCC
R_{free} test set	2343 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 48.9	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4966	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 1PE

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).

Mal	Chain	Boı	nd lengths	Bo	nd angles
Mol Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.91	0/935	0.77	0/1268
1	В	0.95	0/929	0.81	0/1260
1	С	0.85	1/952~(0.1%)	0.82	2/1291 (0.2%)
1	D	0.91	$1/929 \ (0.1\%)$	0.74	0/1260
1	E	0.95	1/921 (0.1%)	0.84	1/1249 (0.1%)
All	All	0.92	3/4666 (0.1%)	0.80	3/6328 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	С	72	GLN	CB-CG	-7.54	1.32	1.52
1	E	31	CYS	CB-SG	-5.91	1.72	1.81
1	D	29	TYR	CD2-CE2	5.05	1.47	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	38	ALA	N-CA-C	-8.62	87.71	111.00
1	С	72	GLN	CB-CA-C	-5.64	99.12	110.40
1	Ε	98	VAL	CG1-CB-CG2	5.56	119.79	110.90

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	С	37	SER	Peptide

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	911	0	863	15	0
1	В	905	0	858	20	0
1	С	928	0	882	15	0
1	D	905	0	860	15	0
1	Ε	897	0	854	18	0
2	A	16	0	22	1	0
2	В	16	0	22	1	0
2	С	16	0	22	1	0
2	D	16	0	22	1	0
2	E	16	0	22	1	0
3	A	67	0	0	1	0
3	В	65	0	0	2	0
3	С	82	0	0	1	0
3	D	57	0	0	0	0
3	Ε	69	0	0	3	0
All	All	4966	0	4427	77	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 9.

The worst 5 of 77 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:11:PHE:CE2	1:B:42:ILE:HD13	1.67	1.28
1:B:62:ASN:HB3	3:E:193:HOH:O	1.50	1.11
1:A:53:TRP:HZ3	1:A:79:GLU:OE1	1.50	0.95
1:B:11:PHE:HE2	1:B:42:ILE:HD13	1.11	0.89
1:A:53:TRP:CZ3	1:A:79:GLU:OE1	2.28	0.86

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	Perce	$_{ m ntiles}$
1	A	$116/126 \ (92\%)$	109 (94%)	7 (6%)	0	100	100
1	В	115/126~(91%)	111 (96%)	4 (4%)	0	100	100
1	С	118/126~(94%)	112 (95%)	3 (2%)	3 (2%)	5	2
1	D	115/126~(91%)	110 (96%)	5 (4%)	0	100	100
1	E	114/126~(90%)	110 (96%)	3 (3%)	1 (1%)	17	12
All	All	$578/630 \ (92\%)$	552 (96%)	22 (4%)	4 (1%)	22	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	51	SER
1	E	36	GLN
1	С	50	SER
1	С	37	SER

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	Rotameric Outliers	
1	A	100/106 (94%)	96 (96%)	4 (4%)	31 31
1	В	99/106 (93%)	92 (93%)	7 (7%)	14 11
1	С	102/106 (96%)	99 (97%)	3 (3%)	42 44
1	D	99/106 (93%)	95 (96%)	4 (4%)	31 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	98/106 (92%)	94 (96%)	4 (4%)	30 30
All	All	498/530 (94%)	476 (96%)	22 (4%)	28 27

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	90	LYS
1	С	27	LYS
1	Ε	51	SER
1	В	104	THR
1	С	21	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	20	HIS
1	С	63	GLN
1	D	72	GLN
1	В	72	GLN
1	Е	36	GLN

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)

5 ligands are 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	Chain	Chain	Chain	Res	Link	Во	Bond lengths			Bond angles		
MIOI	Mol Type Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2					
2	1PE	В	127	-	15,15,15	0.54	0	14,14,14	0.37	0				
2	1PE	Е	127	_	15,15,15	0.59	0	14,14,14	0.35	0				
2	1PE	D	127	_	15,15,15	0.58	0	14,14,14	0.39	0				
2	1PE	A	127	_	15,15,15	0.52	0	14,14,14	0.31	0				
2	1PE	С	127	-	15,15,15	0.58	0	14,14,14	0.28	0				

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1PE	В	127	_	-	9/13/13/13	-
2	1PE	Е	127	_	-	6/13/13/13	-
2	1PE	D	127	-	-	5/13/13/13	-
2	1PE	A	127	-	-	7/13/13/13	-
2	1PE	С	127	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	127	1PE	OH5-C14-C24-OH4
2	D	127	1PE	OH5-C14-C24-OH4
2	A	127	1PE	OH6-C15-C25-OH5
2	D	127	1PE	OH6-C15-C25-OH5
2	С	127	1PE	OH5-C14-C24-OH4

There are no ring outliers.

5 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	127	1PE	1	0
2	E	127	1PE	1	0
2	D	127	1PE	1	0
2	A	127	1PE	1	0
2	С	127	1PE	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

