



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 6, 2024 – 08:36 am GMT

PDB ID : 8CPK
Title : Crystal structure of EtpA secretion domain from Enterotoxigenic Escherichia coli
Authors : Ntui, C.M.; Schubert, W.D.; Fleckenstein, J.M.
Deposited on : 2023-03-02
Resolution : 1.76 Å(reported)

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

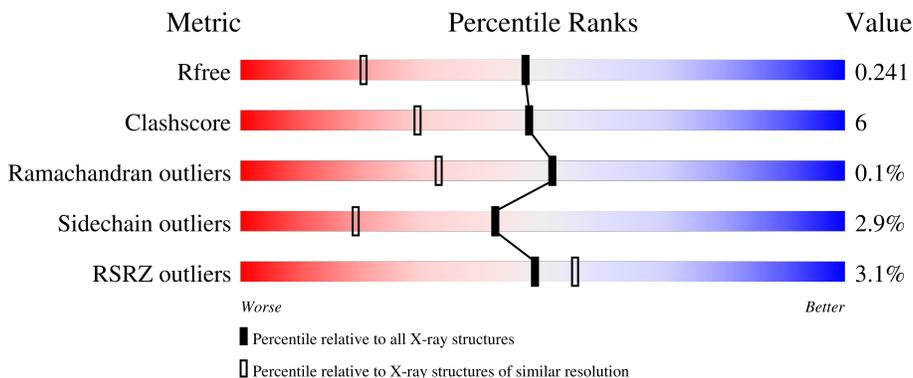
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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)
RSRZ outliers	127900	2298 (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 of 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	384	 2% (poor fit), 88% (0-1 outliers), 11% (2-3+ outliers)
1	B	384	 2% (poor fit), 89% (0-1 outliers), 10% (2-3+ outliers)
1	C	384	 4% (poor fit), 84% (0-1 outliers), 15% (2-3+ outliers)
1	D	384	 4% (poor fit), 87% (0-1 outliers), 12% (2-3+ outliers)

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23857 atoms, of which 11605 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 EtpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	384	5799	1766	2906	535	579	13	0	30	0
1	B	383	5763	1756	2884	538	574	11	0	28	0
1	C	383	5711	1741	2853	533	572	12	0	25	0
1	D	383	5882	1793	2962	538	576	13	0	37	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q29XT7
A	-2	SER	-	expression tag	UNP Q29XT7
A	-1	GLY	-	expression tag	UNP Q29XT7
A	0	SER	-	expression tag	UNP Q29XT7
A	348	GLY	SER	engineered mutation	UNP Q29XT7
A	380	ALA	-	expression tag	UNP Q29XT7
B	-3	ALA	-	expression tag	UNP Q29XT7
B	-2	SER	-	expression tag	UNP Q29XT7
B	-1	GLY	-	expression tag	UNP Q29XT7
B	0	SER	-	expression tag	UNP Q29XT7
B	348	GLY	SER	engineered mutation	UNP Q29XT7
B	380	ALA	-	expression tag	UNP Q29XT7
C	-3	ALA	-	expression tag	UNP Q29XT7
C	-2	SER	-	expression tag	UNP Q29XT7
C	-1	GLY	-	expression tag	UNP Q29XT7
C	0	SER	-	expression tag	UNP Q29XT7
C	348	GLY	SER	engineered mutation	UNP Q29XT7
C	380	ALA	-	expression tag	UNP Q29XT7
D	-3	ALA	-	expression tag	UNP Q29XT7
D	-2	SER	-	expression tag	UNP Q29XT7
D	-1	GLY	-	expression tag	UNP Q29XT7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q29XT7
D	348	GLY	SER	engineered mutation	UNP Q29XT7
D	380	ALA	-	expression tag	UNP Q29XT7

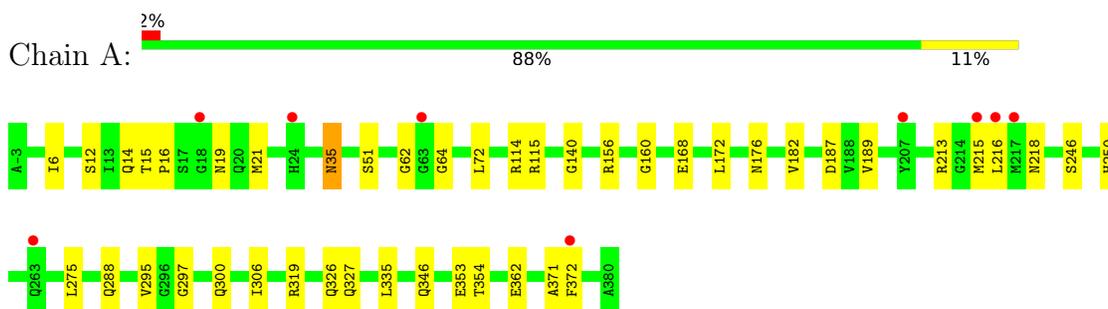
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	199	Total 199	O 199	0	0
2	B	173	Total 173	O 173	0	0
2	C	153	Total 153	O 153	0	0
2	D	177	Total 177	O 177	0	0

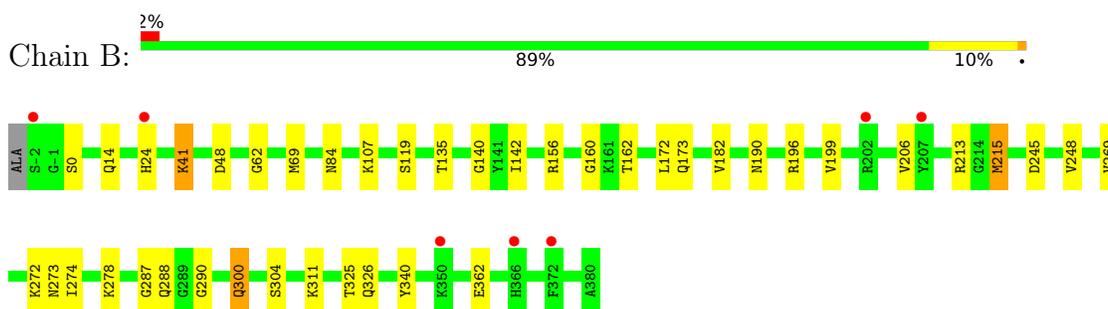
3 Residue-property plots [i](#)

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.

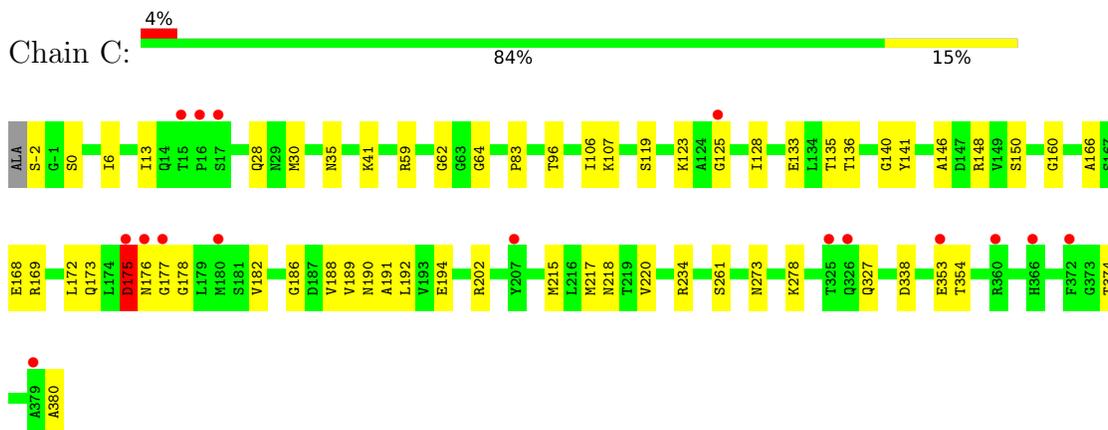
- Molecule 1: EtpA



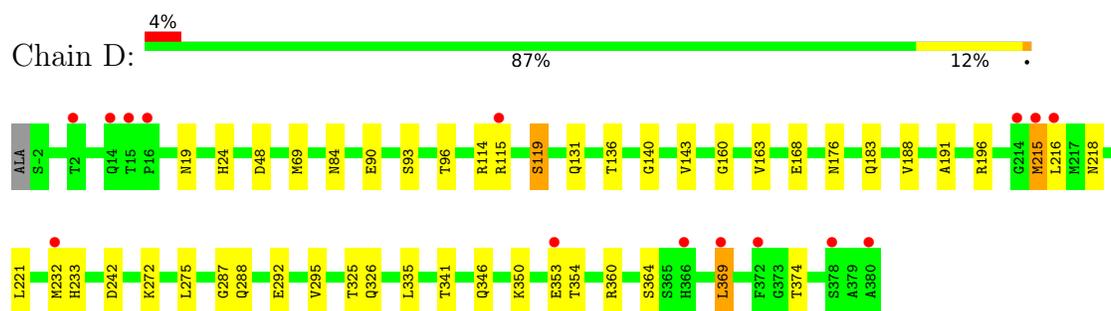
- Molecule 1: EtpA



- Molecule 1: EtpA



- Molecule 1: EtpA



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.71Å 64.19Å 123.96Å 91.61° 90.89° 90.02°	Depositor
Resolution (Å)	61.95 – 1.76 64.16 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.8 (61.95-1.76) 97.0 (64.16-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.76Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.240 0.200 , 0.241	Depositor DCC
R_{free} test set	5504 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-l 0.108 for -h,k,-l 0.000 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23857	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.52% 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](#)

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	0.46	0/3015	0.63	0/4061
1	B	0.47	0/2995	0.63	0/4035
1	C	0.45	0/2956	0.65	1/3983 (0.0%)
1	D	0.47	0/3062	0.62	0/4125
All	All	0.46	0/12028	0.63	1/16204 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	ASP	CB-CG-OD1	9.88	127.19	118.30

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	2893	2906	2896	34	2
1	B	2879	2884	2886	38	0
1	C	2858	2853	2848	39	2
1	D	2920	2962	2953	30	0
2	A	199	0	0	17	6
2	B	173	0	0	19	1
2	C	153	0	0	15	3
2	D	177	0	0	15	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12252	11605	11583	141	9

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 6.

The worst 5 of 141 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:D:69[B]:MET:SD	2:D:556:HOH:O	2.09	1.09
1:A:168[B]:GLU:OE2	2:A:401:HOH:O	1.84	0.94
1:D:242:ASP:O	2:D:401:HOH:O	1.88	0.90
1:C:125:GLY:N	2:C:401:HOH:O	1.81	0.88
1:D:119:SER:OG	2:D:402:HOH:O	1.93	0.87

The worst 5 of 9 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)
2:A:599:HOH:O	2:C:553:HOH:O[1_545]	1.84	0.36
2:A:537:HOH:O	2:C:547:HOH:O[1_655]	1.93	0.27
2:A:597:HOH:O	2:C:553:HOH:O[1_545]	1.96	0.24
2:A:547:HOH:O	2:B:524:HOH:O[1_654]	1.99	0.21
2:D:516:HOH:O	2:D:568:HOH:O[1_455]	2.02	0.18

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	412/384 (107%)	400 (97%)	12 (3%)	0	100 100
1	B	409/384 (106%)	397 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	406/384 (106%)	392 (97%)	12 (3%)	2 (0%)	29	12
1	D	419/384 (109%)	402 (96%)	15 (4%)	2 (0%)	29	12
All	All	1646/1536 (107%)	1591 (97%)	51 (3%)	4 (0%)	51	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	176[A]	ASN
1	C	176[B]	ASN
1	D	216[A]	LEU
1	D	216[B]	LEU

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	313/283 (111%)	307 (98%)	6 (2%)	57	37
1	B	310/283 (110%)	297 (96%)	13 (4%)	30	9
1	C	306/283 (108%)	294 (96%)	12 (4%)	32	11
1	D	319/283 (113%)	299 (94%)	20 (6%)	18	3
All	All	1248/1132 (110%)	1197 (96%)	51 (4%)	42	10

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	261[A]	SER
1	D	119	SER
1	D	369[A]	LEU
1	C	261[B]	SER
1	D	93	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	344	HIS
1	D	84	ASN
1	D	327	GLN
1	C	19	ASN
1	A	250	HIS

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 [i](#)

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	384/384 (100%)	0.32	9 (2%) 60 67	17, 28, 44, 61	0
1	B	383/384 (99%)	0.30	7 (1%) 68 76	18, 29, 47, 60	0
1	C	383/384 (99%)	0.42	16 (4%) 36 42	19, 32, 51, 70	0
1	D	383/384 (99%)	0.41	15 (3%) 39 45	18, 29, 47, 67	0
All	All	1533/1536 (99%)	0.36	47 (3%) 49 55	17, 29, 48, 70	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	177[A]	GLY	7.5
1	D	216[A]	LEU	5.0
1	A	216	LEU	4.8
1	C	15	THR	4.7
1	D	215[A]	MET	4.5

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.