



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2022 – 03:16 pm GMT

PDB ID : 8AKO
Title : Structure of EspB-EspK complex: the non-identical twin of the PE-PPE-EspG secretion mechanism.
Authors : Gijsbers, A.; Eymery, M.; Menart, I.; Vinciauskaite, V.; Gao, Y.; Siliqi, D.; Peters, P.; Mccarthy, A.; Ravelli, R.B.G.
Deposited on : 2022-07-30
Resolution : 2.29 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 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 : 2.31.3
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) : 2.31.3

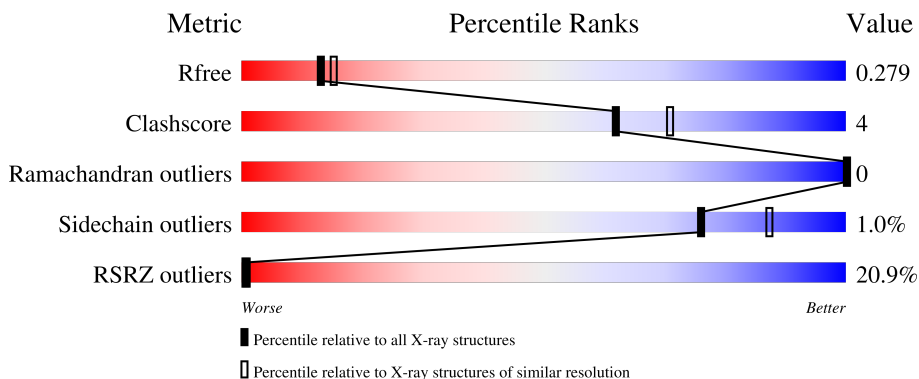
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	300	 8% 80% 6% • 13%
2	B	246	 34% 89% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3930 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 ESX-1 secretion-associated protein EspB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	261	2032	1269	361	395	7	0	0	0

- Molecule 2 is a protein called ESX-1 secretion-associated protein EspK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	246	1860	1173	325	354	8	0	0	0

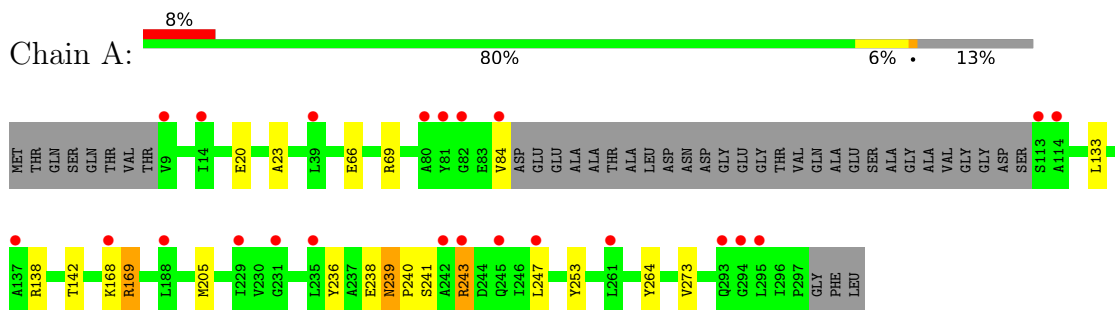
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	8	Total	O	0	0
			8	8		

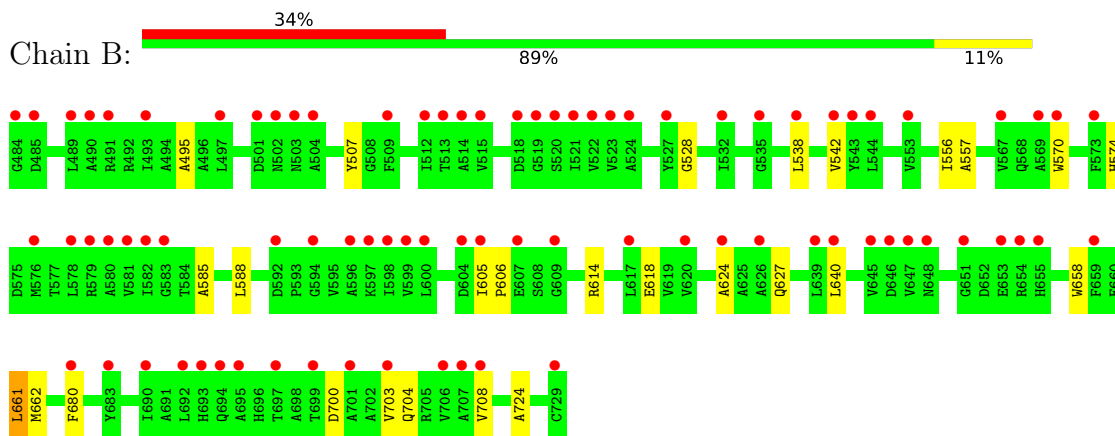
3 Residue-property plots [i](#)

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: ESX-1 secretion-associated protein EspB



- Molecule 2: ESX-1 secretion-associated protein EspK



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	101.58Å 101.58Å 377.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.82 – 2.29 85.67 – 2.29	Depositor EDS
% Data completeness (in resolution range)	53.2 (85.82-2.29) 53.2 (85.67-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.235 , 0.279 0.235 , 0.279	Depositor DCC
R_{free} test set	1444 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3930	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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	0.42	0/2077	0.76	0/2830
2	B	0.32	0/1903	0.68	1/2606 (0.0%)
All	All	0.38	0/3980	0.72	1/5436 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	661	LEU	CB-CG-CD1	-5.39	101.84	111.00

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	2032	0	1979	17	0
2	B	1860	0	1816	18	0
3	A	30	0	0	3	0
3	B	8	0	0	0	0
All	All	3930	0	3795	34	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 (34) 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:B:658:TRP:O	2:B:661:LEU:HB3	1.90	0.70
2:B:570:TRP:O	2:B:574:HIS:HB2	1.92	0.70
1:A:23:ALA:O	1:A:169:ARG:NH2	2.33	0.61
2:B:624:ALA:HA	2:B:627:GLN:HE21	1.67	0.60
1:A:20:GLU:HB3	3:A:406:HOH:O	2.01	0.59
1:A:247:LEU:HD23	2:B:507:TYR:HB2	1.87	0.56
2:B:658:TRP:O	2:B:662:MET:HG3	2.07	0.54
1:A:240:PRO:O	1:A:243:ARG:HG2	2.07	0.54
1:A:239:ASN:N	1:A:239:ASN:OD1	2.43	0.52
1:A:84:VAL:O	1:A:84:VAL:HG12	2.10	0.51
1:A:239:ASN:C	1:A:241:SER:H	2.14	0.50
1:A:133:LEU:HD21	1:A:253:TYR:HB3	1.94	0.49
1:A:168:LYS:HE2	3:A:407:HOH:O	2.12	0.49
1:A:205:MET:HG2	1:A:273:VAL:HG21	1.95	0.48
1:A:238:GLU:O	1:A:240:PRO:HD3	2.12	0.48
2:B:557:ALA:HB2	2:B:724:ALA:HB1	1.94	0.48
1:A:238:GLU:HA	1:A:238:GLU:OE1	2.15	0.47
1:A:236:TYR:CE1	1:A:243:ARG:HB2	2.50	0.46
2:B:542:VAL:O	2:B:614:ARG:NH2	2.48	0.46
1:A:169:ARG:HG2	3:A:404:HOH:O	2.14	0.45
2:B:538:LEU:HD22	2:B:542:VAL:HG11	1.98	0.45
1:A:239:ASN:C	1:A:241:SER:N	2.70	0.45
2:B:528:GLY:HA3	2:B:680:PHE:CD2	2.51	0.45
2:B:700:ASP:O	2:B:704:GLN:HG3	2.17	0.44
2:B:495:ALA:HB1	2:B:606:PRO:HD2	1.99	0.44
2:B:495:ALA:HA	2:B:605:ILE:HG22	1.99	0.43
2:B:585:ALA:HA	2:B:588:LEU:HB2	1.99	0.43
2:B:640:LEU:HD13	2:B:708:VAL:HG22	2.00	0.42
2:B:700:ASP:HB3	2:B:703:VAL:HB	2.01	0.42
2:B:556:ILE:HD13	2:B:556:ILE:HA	1.96	0.42
1:A:66:GLU:OE2	1:A:69:ARG:NH1	2.52	0.41
1:A:138:ARG:O	1:A:142:THR:OG1	2.32	0.41
2:B:662:MET:HB3	2:B:662:MET:HE2	1.96	0.41
2:B:614:ARG:HB3	2:B:618:GLU:HB2	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	257/300 (86%)	248 (96%)	9 (4%)	0	100	100
2	B	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
All	All	501/546 (92%)	485 (97%)	16 (3%)	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	210/237 (89%)	206 (98%)	4 (2%)	57	73
2	B	187/187 (100%)	187 (100%)	0	100	100
All	All	397/424 (94%)	393 (99%)	4 (1%)	76	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	239	ASN
1	A	243	ARG
1	A	264	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
2	B	627	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 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

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	261/300 (87%)	1.11	23 (8%) 10 13	30, 55, 116, 153	0
2	B	246/246 (100%)	1.69	83 (33%) 0 0	48, 108, 168, 192	0
All	All	507/546 (92%)	1.39	106 (20%) 1 1	30, 75, 156, 192	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	ALA	6.4
2	B	578	LEU	6.3
1	A	113	SER	5.8
1	A	294	GLY	5.8
2	B	647	VAL	5.8
2	B	605	ILE	5.6
2	B	581	VAL	5.5
1	A	80	ALA	5.4
2	B	503	ASN	5.3
2	B	596	ALA	5.0
2	B	703	VAL	4.9
2	B	521	ILE	4.8
2	B	582	ILE	4.8
2	B	708	VAL	4.7
1	A	247	LEU	4.7
2	B	573	PHE	4.7
2	B	497	LEU	4.5
2	B	600	LEU	4.5
2	B	518	ASP	4.3
2	B	489	LEU	4.3
1	A	235	LEU	4.2
1	A	114	ALA	4.2
2	B	707	ALA	4.2
2	B	524	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	693	HIS	4.1
2	B	645	VAL	3.9
1	A	81	TYR	3.9
2	B	695	ALA	3.8
2	B	514	ALA	3.7
2	B	493	ILE	3.7
2	B	576	MET	3.7
2	B	502	ASN	3.6
2	B	617	LEU	3.6
2	B	538	LEU	3.5
2	B	583	GLY	3.4
1	A	245	GLN	3.4
2	B	567	VAL	3.3
1	A	243	ARG	3.3
2	B	570	TRP	3.3
2	B	515	VAL	3.3
2	B	535	GLY	3.2
2	B	651	GLY	3.2
2	B	543	TYR	3.2
2	B	523	VAL	3.1
2	B	690	ILE	3.1
1	A	84	VAL	3.0
2	B	569	ALA	3.0
2	B	532	ILE	3.0
2	B	598	ILE	2.9
2	B	580	ALA	2.9
2	B	592	ASP	2.9
2	B	659	PHE	2.9
1	A	295	LEU	2.9
2	B	594	GLY	2.8
2	B	648	ASN	2.8
2	B	640	LEU	2.8
2	B	609	GLY	2.8
2	B	542	VAL	2.8
2	B	484	GLY	2.8
2	B	626	ALA	2.8
2	B	512	ILE	2.8
2	B	701	ALA	2.7
2	B	544	LEU	2.7
2	B	485	ASP	2.7
2	B	519	GLY	2.7
2	B	692	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	504	ALA	2.6
2	B	699	THR	2.5
2	B	509	PHE	2.5
2	B	522	VAL	2.5
2	B	553	VAL	2.5
2	B	620	VAL	2.5
2	B	607	GLU	2.5
2	B	697	THR	2.5
2	B	654	ARG	2.4
1	A	9	VAL	2.4
1	A	293	GLN	2.4
2	B	646	ASP	2.4
1	A	229	ILE	2.4
2	B	604	ASP	2.4
2	B	624	ALA	2.4
2	B	520	SER	2.4
2	B	491	ARG	2.3
2	B	579	ARG	2.3
1	A	82	GLY	2.3
1	A	188	LEU	2.3
2	B	729	CYS	2.3
1	A	261	LEU	2.3
2	B	639	LEU	2.3
2	B	683	TYR	2.3
1	A	231	GLY	2.2
2	B	513	THR	2.2
2	B	653	GLU	2.2
2	B	680	PHE	2.2
1	A	168	LYS	2.2
2	B	694	GLN	2.2
2	B	599	VAL	2.1
2	B	490	ALA	2.1
1	A	39	LEU	2.1
2	B	501	ASP	2.1
1	A	14	ILE	2.1
2	B	527	TYR	2.1
2	B	706	VAL	2.1
2	B	597	LYS	2.1
2	B	655	HIS	2.0
1	A	137	ALA	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.