



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3H94 / pdb_00003h94
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli
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Deposited on : 2009-04-30
Resolution : 3.84 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

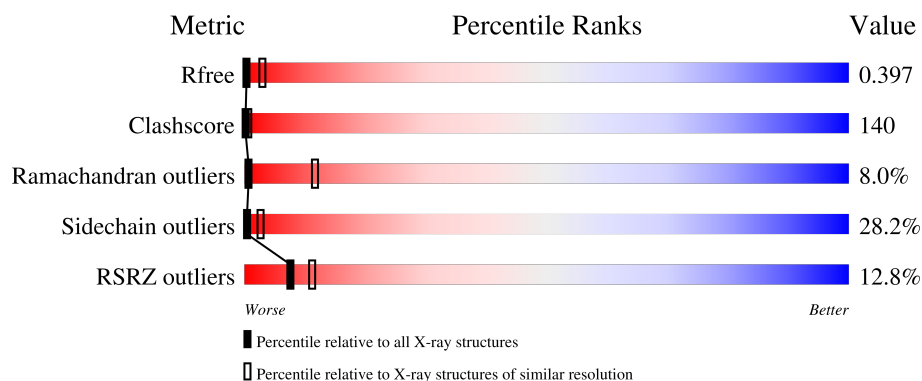
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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}	180053	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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	407	9% 10% 33% 25% 5% 27%
1	B	407	10% 11% 32% 23% 7% 27%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AG	A	408	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4550 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 Cation efflux system protein cusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

- Molecule 2 is SILVER ION (CCD ID: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ag	0	0
			1	1		
2	B	1	Total	Ag	0	0
			1	1		

- Molecule 1: Cation efflux system protein cusB



A366	L367	R368	S369	G370	L371	A372	E373	G374	E375	K376	V377	V378	S379	S380	G381	L382	F383	L384	I385	ASP	SER	GLU	ALA	ASN	ILE	SER	GLY	ALA	LEU	GLU	ARG	MET	ARG	SER	GLU	SER	ALA	THR	HIS	ALA	HIS																		
V244	W245	V246	T247	G248	A249	L250	P251	E252	S253	L254	A255	W256	L257	V258	K259	D260	A261	T265	L266	T267	V268	P269	A270	R271	P272	D273	K274	T275	L276	T277	I278	R279	K280	W281	T282	L283	L284	P285	G286	V287	D288	A289	A290	T291	R292	T293	L294	Q295	L296	R297	L298	E299	V300	D301	N302	A303	D304	E305	
A306	L307	K308	P309	G310	M311	N312	A313	W314	L315	Q316	L317	N318	T319	A320	S321	E322	P323	M324	L325	L326	I327	P328	S329	Q330	A331	L332	I333	D334	T335	G336	S337	E338	Q339	R340	V341	I342	T343	V344	D345	A346	D347	G348	R349	F350	V351	P352	K353	R354	V355	A356	V357	F358	Q359	A360	S361	Q362	G363	V364	T365
R184	L185	R186	L187	A188	G189	W190	P191	E192	A193	D194	I195	R196	L197	L198	I199	A200	T201	Q202	K203	T204	Q205	T206	R207	F208	T209	L210	K211	A212	P213	L214	D215	G216	W217	L218	T219	A220	F221	D222	L223	R224	A225	Q226	W227	N228	I229	A230	K231	D232	W233	V234	W235	A236	K237	T238	Q239	G240	K241	D242	P243
I123	V124	Q125	A126	R127	A128	A129	G130	F131	I132	D133	K134	V135	I136	P137	L138	T139	V140	G141	D142	F143	V144	Q145	K146	G147	I148	P149	L150	L151	D152	L153	T154	I155	P156	D157	W158	V159	E160	A161	Q162	S163	E164	Y165	L166	L167	L168	T171	G172	G173	T174	A175	T176	Q177	T178	E179	G180	I181	L182	E183	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	85.00Å 114.42Å 259.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 3.84 47.20 – 3.84	Depositor EDS
% Data completeness (in resolution range)	87.3 (47.20-3.84) 99.6 (47.20-3.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.300 0.397 , 0.397	Depositor DCC
R_{free} test set	675 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	153.0	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 251.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4550	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% 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: AG

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	1.27	19/2313 (0.8%)	1.91	86/3152 (2.7%)
1	B	1.24	24/2313 (1.0%)	1.96	96/3152 (3.0%)
All	All	1.26	43/4626 (0.9%)	1.94	182/6304 (2.9%)

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	VAL	C-N	15.75	1.52	1.33
1	A	97	ALA	C-O	-15.51	1.04	1.23
1	A	89	THR	C-N	12.86	1.51	1.33
1	A	149	PRO	C-N	12.33	1.50	1.33
1	A	377	VAL	C-O	-10.85	1.10	1.23

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	VAL	O-C-N	19.56	147.02	122.57
1	B	119	TYR	N-CA-CB	-18.91	80.77	110.46
1	A	274	LYS	N-CA-C	-18.16	91.48	111.28
1	A	235	VAL	N-CA-C	-16.87	96.13	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	VAL	N-CA-C	16.81	128.01	110.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	PRO	Mainchain
1	B	323	PRO	Mainchain
1	B	341	VAL	Peptide

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	2274	0	2342	670	0
1	B	2274	0	2343	658	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4550	0	4685	1295	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 140.

The worst 5 of 1295 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:B:283:LEU:CD2	1:B:294:LEU:HD12	1.43	1.49
1:B:147:GLY:CA	1:B:212:ALA:HB3	1.45	1.45
1:B:370:GLY:C	1:B:371:LEU:HD23	1.44	1.42
1:A:92:LEU:HD13	1:A:93:GLY:N	1.32	1.41
1:B:187:LEU:HD12	1:B:188:ALA:N	1.38	1.39

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	295/407 (72%)	242 (82%)	27 (9%)	26 (9%)	0	10
1	B	295/407 (72%)	248 (84%)	26 (9%)	21 (7%)	1	13
All	All	590/814 (72%)	490 (83%)	53 (9%)	47 (8%)	1	12

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	140	VAL
1	A	149	PRO
1	A	236	ALA
1	A	258	VAL

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	243/332 (73%)	179 (74%)	64 (26%)	0	3
1	B	243/332 (73%)	170 (70%)	73 (30%)	0	2
All	All	486/664 (73%)	349 (72%)	137 (28%)	0	3

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	301	ASP

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Mol	Chain	Res	Type
1	B	326	LEU
1	B	365	THR
1	A	332	LEU
1	A	327	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	GLN
1	B	339	GLN
1	B	359	GLN
1	A	339	GLN
1	A	359	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	297/407 (72%)	0.82	36 (12%)	8 12	20, 161, 275, 353	0
1	B	297/407 (72%)	0.88	40 (13%)	7 10	20, 167, 274, 377	0
All	All	594/814 (72%)	0.85	76 (12%)	7 11	20, 164, 275, 377	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	MET	4.7
1	A	342	ILE	4.7
1	B	156	PRO	4.6
1	A	300	VAL	4.4
1	B	254	ILE	4.3

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	AG	A	408	1/1	0.73	0.53	30,30,30,30	0
2	AG	B	408	1/1	0.88	0.51	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.