



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3OW7 / pdb_00003ow7
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli.
Authors : Su, C.-C.
Deposited on : 2010-09-17
Resolution : 3.78 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

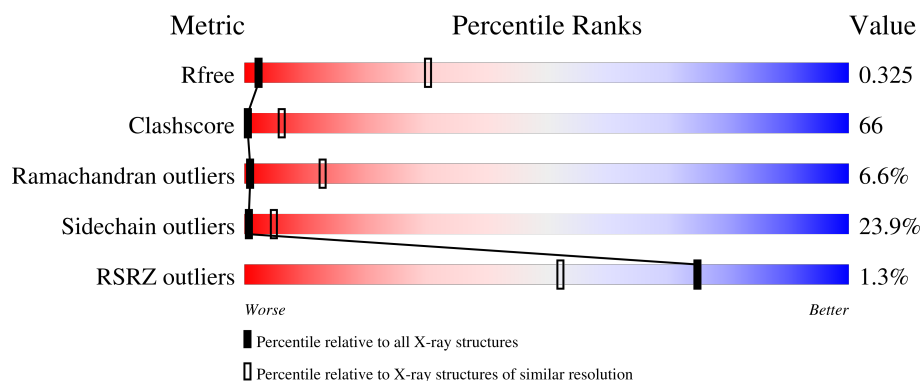
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.78 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	1085 (3.94-3.62)
Clashscore	190562	1029 (3.92-3.64)
Ramachandran outliers	187476	1064 (3.94-3.62)
Sidechain outliers	187428	1059 (3.94-3.62)
RSRZ outliers	180081	1084 (3.94-3.62)

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	413	
1	B	413	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4545 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	296	Total	C	N	O	S	0	0	0
			2267	1444	391	427	5			
1	B	297	Total	C	N	O	S	0	0	0
			2274	1448	392	429	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	expression tag	UNP P77239
A	409	HIS	-	expression tag	UNP P77239
A	410	HIS	-	expression tag	UNP P77239
A	411	HIS	-	expression tag	UNP P77239
A	412	HIS	-	expression tag	UNP P77239
A	413	HIS	-	expression tag	UNP P77239
B	408	HIS	-	expression tag	UNP P77239
B	409	HIS	-	expression tag	UNP P77239
B	410	HIS	-	expression tag	UNP P77239
B	411	HIS	-	expression tag	UNP P77239
B	412	HIS	-	expression tag	UNP P77239
B	413	HIS	-	expression tag	UNP P77239

- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

SER	K324	G189	E262	K324	G189
GLY	L325	M190	S253	L325	M190
ALA	L326	P191	I254	L326	P191
LEU	I327	E192	A255	I327	E192
GLU	P328	A193	W256	P328	A193
ARG	S329	D194	L257	S329	D194
MET	Q330	I195	W258	Q330	I195
ARG	A331	R196	K259	A331	R196
SER	L332	R197	D260	L332	R197
GLU	I333	L198	T265	I333	L198
SER	D334	I199	T265	D334	I199
ALA	T335			ALA	T335
THR	G336	Q202	A270	THR	G336
HIS	S337	K203	R271	HIS	S337
ALA	E338	I204	P272	ALA	E338
HIS	Q339	Q205	D273	HIS	Q339
HIS	R340	T206	K274	HIS	R340
HIS	V341	R207	T275	HIS	V341
HIS	I342	F208	L276	HIS	I342
HIS	T343	T209	T277	HIS	T343
HIS	V344	L210	I278	HIS	V344
HIS	D345	K211	K279	HIS	D345
	A346	A212	K280		A346
	D347	P213	W281		D347
	G348	I214	T282		G348
	R349	D215	L283		R349
	F350	G216			F350
	V351	V217	V287		V351
	P352	I218	D288		P352
	K353	T219			K353
	R354	A220	T291		R354
	V355	F221	R292		V355
	A356	D222	T293		A356
	V357	L223	L294		V357
	F358	R224			F358
	Q359	A225	L297		Q359
		G226	L298		
	T365	M227	E299		T365
	A366	N228	V300		A366
	L367	I229	D301		L367
	R368	A230	N302		R368
	S369	K231	A303		S369
	G370	D232	D304		G370
	L371	N233	E305		L371
		V234	A306		
	V377	V235	L307		V377
	V378	A236	K308		V378
	S379	K237	P309		S379
	S380	I238	G310		S380
	G381	Q239	N311		G381
	L382	G240	K312		L382
	F383	M241	A313		F383
	L384	D242	L317		L384
	I385	P243	N318		I385
	ASP	V244	SER		ASP
	SER	W245	T319		SER
	GLU	V246	A320		GLU
	ALA		S321		ALA
	ASN	I250	E322		ASN
	ILE	P251	P323		ILE

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.24Å 111.01Å 258.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.63 – 3.78 36.63 – 3.78	Depositor EDS
% Data completeness (in resolution range)	82.8 (36.63-3.78) 95.1 (36.63-3.78)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.324 0.288 , 0.325	Depositor DCC
R_{free} test set	588 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	148.8	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 223.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å ²)	227.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.62% 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: CU1

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	0.51	0/2306	1.02	10/3142 (0.3%)
1	B	0.48	1/2313 (0.0%)	1.01	16/3152 (0.5%)
All	All	0.50	1/4619 (0.0%)	1.01	26/6294 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	ASP	C-N	-5.70	1.25	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	LYS	N-CA-C	11.09	126.71	111.74
1	A	252	GLU	N-CA-C	9.16	121.26	111.28
1	A	251	PRO	N-CA-C	-7.71	98.13	111.32
1	B	110	PHE	CA-C-N	7.47	127.75	119.90
1	B	110	PHE	C-N-CA	7.47	127.75	119.90

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	2267	0	2336	347	0
1	B	2274	0	2342	278	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
All	All	4545	0	4678	612	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 66.

The worst 5 of 612 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:250:ILE:CG2	1:A:255:ALA:HB2	1.57	1.34
1:A:256:TRP:CH2	1:A:257:LEU:HD22	1.64	1.32
1:A:251:PRO:HG2	1:A:254:ILE:CG2	1.66	1.23
1:A:256:TRP:CZ3	1:A:257:LEU:HD22	1.75	1.20
1:A:257:LEU:O	1:A:259:LYS:HD3	1.42	1.19

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	294/413 (71%)	227 (77%)	44 (15%)	23 (8%)	1	11
1	B	295/413 (71%)	240 (81%)	39 (13%)	16 (5%)	1	16
All	All	589/826 (71%)	467 (79%)	83 (14%)	39 (7%)	1	13

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL

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Mol	Chain	Res	Type
1	A	151	LEU
1	A	204	ILE
1	A	214	ILE
1	A	236	ALA

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	242/338 (72%)	184 (76%)	58 (24%)	1	5
1	B	243/338 (72%)	185 (76%)	58 (24%)	1	5
All	All	485/676 (72%)	369 (76%)	116 (24%)	1	5

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	ILE
1	B	345	ASP
1	B	144	VAL
1	B	340	ARG
1	B	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	359	GLN
1	B	145	GLN
1	B	362	GLN
1	B	318	ASN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 4 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	296/413 (71%)	-0.01	5 (1%)	69 46	133, 211, 301, 394	0
1	B	297/413 (71%)	-0.09	3 (1%)	79 57	135, 224, 341, 582	0
All	All	593/826 (71%)	-0.05	8 (1%)	75 52	133, 218, 329, 582	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	ARG	2.7
1	A	213	PRO	2.5
1	A	156	PRO	2.3
1	A	149	PRO	2.3
1	B	235	VAL	2.3

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	CU1	A	415	1/1	0.58	0.23	247,247,247,247	0
2	CU1	B	415	1/1	0.64	0.23	547,547,547,547	0
2	CU1	A	414	1/1	0.93	0.21	452,452,452,452	0
2	CU1	B	414	1/1	0.94	0.11	296,296,296,296	0

6.5 Other polymers [i](#)

There are no such residues in this entry.