



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:50 PM GMT

PDB ID : 3OOC
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli
Authors : Su, C.-C.; Yang, F.; Long, F.; Reyon, D.; Routh, M.D.; Kuo, D.W.; Mokhtari, A.K.; Van Ornam, J.D.; Rabe, K.L.; Hoy, J.A.; Lee, Y.J.; Rajashankar, K.R.; Yu, E.W.
Deposited on : 2010-08-30
Resolution : 3.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

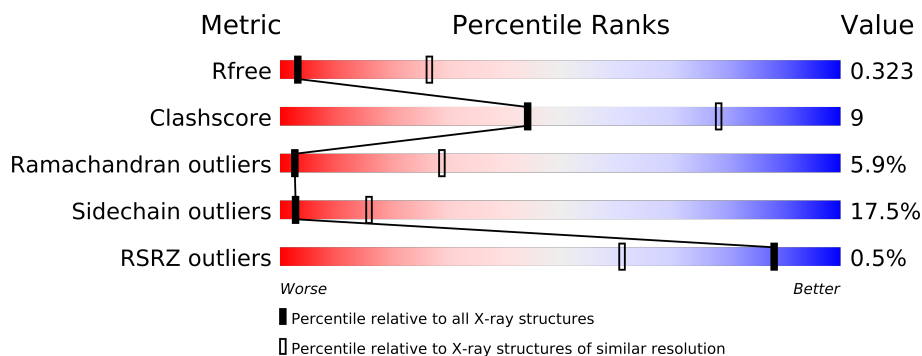
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.40 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}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	413	
1	B	413	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4548 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

There are 12 discrepancies between the modelled and reference sequences:

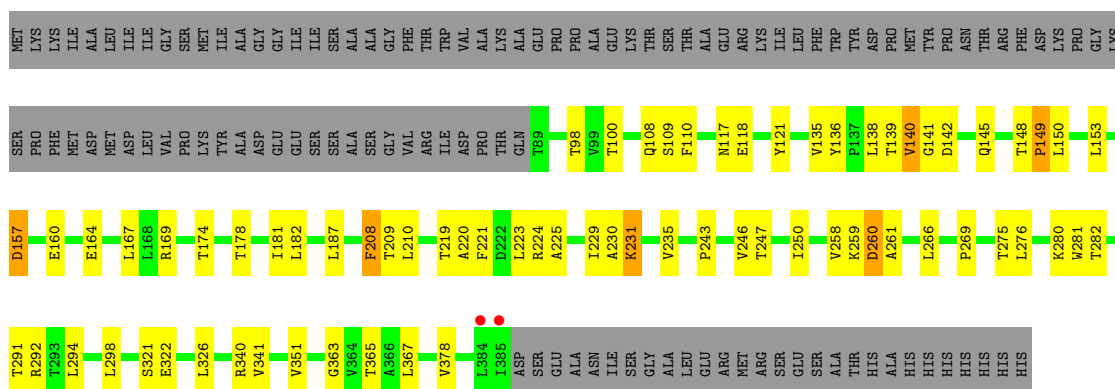
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	HIS	-	EXPRESSION TAG	UNP P77239
A	409	HIS	-	EXPRESSION TAG	UNP P77239
A	410	HIS	-	EXPRESSION TAG	UNP P77239
A	411	HIS	-	EXPRESSION TAG	UNP P77239
A	412	HIS	-	EXPRESSION TAG	UNP P77239
A	413	HIS	-	EXPRESSION TAG	UNP P77239
B	408	HIS	-	EXPRESSION TAG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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

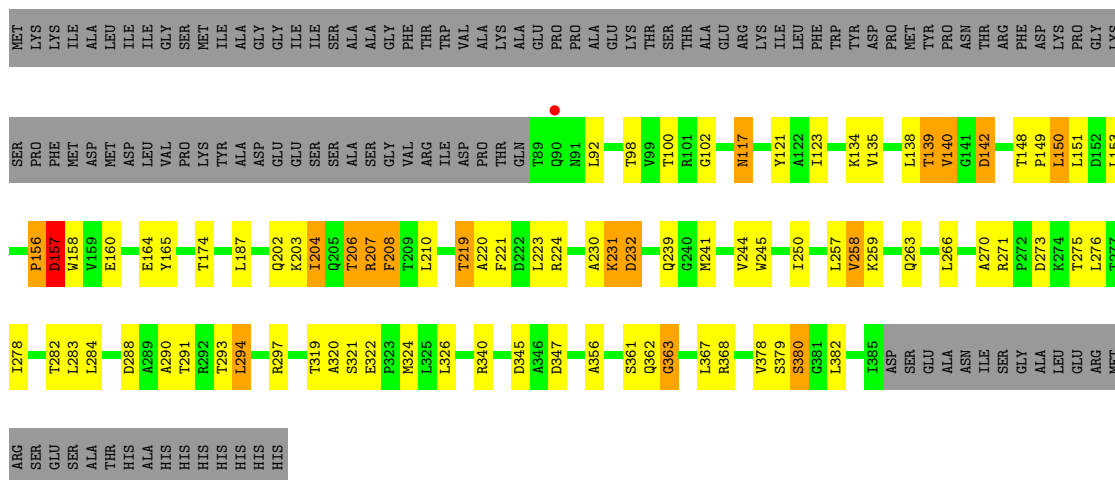
• Molecule 1: Cation efflux system protein cusB

Chain A:



• Molecule 1: Cation efflux system protein cusB

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.96Å 113.24Å 258.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 3.40 47.10 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.3 (47.10-3.40) 98.0 (47.10-3.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.261 , 0.318 0.276 , 0.323	Depositor DCC
R_{free} test set	867 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	132.2	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 145.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 17209 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4548	wwPDB-VP
Average B, all atoms (Å ²)	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.24	0/2313	0.50	0/3152
1	B	0.25	0/2313	0.50	0/3152
All	All	0.25	0/4626	0.50	0/6304

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2274	0	0	12	0
1	B	2274	0	0	27	0
All	All	4548	0	0	39	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (39) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:207:ARG:CG	1:B:207:ARG:NH1	2.60	0.63
1:B:156:PRO:O	1:B:158:TRP:N	2.33	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:117:ASN:OD1	1:B:117:ASN:N	2.34	0.61
1:B:379:SER:O	1:B:380:SER:CB	2.51	0.59
1:B:231:LYS:CG	1:B:232:ASP:N	2.67	0.56
1:B:208:PHE:N	1:B:208:PHE:CD1	2.72	0.55
1:B:270:ALA:O	1:B:271:ARG:C	2.45	0.54
1:A:208:PHE:N	1:A:208:PHE:CD1	2.75	0.54
1:A:157:ASP:N	1:A:157:ASP:OD2	2.40	0.54
1:B:230:ALA:O	1:B:231:LYS:C	2.48	0.53
1:B:319:THR:CG2	1:B:320:ALA:N	2.72	0.52
1:B:288:ASP:N	1:B:293:THR:O	2.43	0.52
1:A:229:ILE:CG2	1:A:230:ALA:N	2.73	0.52
1:A:250:ILE:O	1:A:294:LEU:N	2.44	0.50
1:A:230:ALA:O	1:A:231:LYS:C	2.49	0.49
1:B:121:TYR:CD2	1:B:121:TYR:C	2.88	0.47
1:B:356:ALA:O	1:B:368:ARG:N	2.49	0.46
1:B:156:PRO:O	1:B:157:ASP:C	2.55	0.45
1:A:261:ALA:CB	1:A:281:TRP:CD1	3.00	0.45
1:A:117:ASN:OD1	1:A:117:ASN:N	2.49	0.44
1:B:321:SER:O	1:B:322:GLU:C	2.53	0.44
1:A:139:THR:O	1:A:140:VAL:CB	2.65	0.44
1:A:148:THR:N	1:A:149:PRO:CD	2.82	0.43
1:B:142:ASP:OD2	1:B:142:ASP:N	2.51	0.43
1:B:203:LYS:CD	1:B:203:LYS:O	2.67	0.42
1:B:245:TRP:CH2	1:B:297:ARG:CZ	3.02	0.42
1:B:219:THR:O	1:B:220:ALA:CB	2.68	0.42
1:B:102:GLY:O	1:B:324:MET:N	2.52	0.42
1:B:361:SER:O	1:B:363:GLY:N	2.52	0.41
1:A:321:SER:O	1:A:322:GLU:C	2.57	0.41
1:B:250:ILE:O	1:B:294:LEU:N	2.54	0.41
1:A:110:PHE:CD2	1:A:110:PHE:N	2.89	0.41
1:B:219:THR:OG1	1:B:219:THR:O	2.37	0.41
1:A:259:LYS:O	1:A:260:ASP:O	2.38	0.41
1:B:202:GLN:CG	1:B:202:GLN:O	2.69	0.41
1:B:290:ALA:O	1:B:291:THR:OG1	2.38	0.41
1:B:258:VAL:O	1:B:263:GLN:NE2	2.54	0.40
1:B:345:ASP:C	1:B:347:ASP:N	2.75	0.40
1:B:139:THR:O	1:B:140:VAL:CB	2.68	0.40

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	295/413 (71%)	218 (74%)	60 (20%)	17 (6%)	3	29
1	B	295/413 (71%)	231 (78%)	46 (16%)	18 (6%)	2	28
All	All	590/826 (71%)	449 (76%)	106 (18%)	35 (6%)	2	29

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	140	VAL
1	A	149	PRO
1	A	150	LEU
1	A	221	PHE
1	A	225	ALA
1	A	231	LYS
1	A	258	VAL
1	A	260	ASP
1	B	135	VAL
1	B	140	VAL
1	B	156	PRO
1	B	157	ASP
1	B	380	SER
1	A	141	GLY
1	A	223	LEU
1	B	150	LEU
1	B	204	ILE
1	B	223	LEU
1	B	231	LYS
1	A	220	ALA
1	A	243	PRO
1	B	134	LYS
1	B	206	THR
1	B	362	GLN
1	A	363	GLY
1	B	151	LEU

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Mol	Chain	Res	Type
1	B	221	PHE
1	B	259	LYS
1	B	149	PRO
1	B	258	VAL
1	A	269	PRO
1	A	136	TYR
1	A	341	VAL
1	B	363	GLY

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	243/338 (72%)	201 (83%)	42 (17%)	3	16
1	B	243/338 (72%)	200 (82%)	43 (18%)	3	15
All	All	486/676 (72%)	401 (82%)	85 (18%)	3	16

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	THR
1	A	100	THR
1	A	108	GLN
1	A	109	SER
1	A	118	GLU
1	A	121	TYR
1	A	138	LEU
1	A	142	ASP
1	A	145	GLN
1	A	153	LEU
1	A	157	ASP
1	A	160	GLU
1	A	164	GLU
1	A	167	LEU
1	A	169	ARG
1	A	174	THR
1	A	178	THR

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Mol	Chain	Res	Type
1	A	181	ILE
1	A	182	LEU
1	A	187	LEU
1	A	208	PHE
1	A	209	THR
1	A	210	LEU
1	A	219	THR
1	A	224	ARG
1	A	235	VAL
1	A	246	VAL
1	A	247	THR
1	A	266	LEU
1	A	275	THR
1	A	276	LEU
1	A	280	LYS
1	A	282	THR
1	A	291	THR
1	A	292	ARG
1	A	298	LEU
1	A	326	LEU
1	A	340	ARG
1	A	351	VAL
1	A	365	THR
1	A	367	LEU
1	A	378	VAL
1	B	92	LEU
1	B	98	THR
1	B	100	THR
1	B	117	ASN
1	B	123	ILE
1	B	138	LEU
1	B	139	THR
1	B	142	ASP
1	B	148	THR
1	B	150	LEU
1	B	153	LEU
1	B	157	ASP
1	B	160	GLU
1	B	164	GLU
1	B	165	TYR
1	B	174	THR
1	B	187	LEU

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Mol	Chain	Res	Type
1	B	204	ILE
1	B	206	THR
1	B	207	ARG
1	B	208	PHE
1	B	210	LEU
1	B	219	THR
1	B	224	ARG
1	B	232	ASP
1	B	239	GLN
1	B	241	MET
1	B	244	VAL
1	B	257	LEU
1	B	266	LEU
1	B	273	ASP
1	B	275	THR
1	B	276	LEU
1	B	278	ILE
1	B	282	THR
1	B	283	LEU
1	B	284	LEU
1	B	294	LEU
1	B	326	LEU
1	B	340	ARG
1	B	367	LEU
1	B	378	VAL
1	B	382	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	297/413 (71%)	0.25	2 (0%)	84 52	136, 169, 291, 372	0
1	B	297/413 (71%)	0.23	1 (0%)	91 73	133, 182, 279, 427	0
All	All	594/826 (71%)	0.24	3 (0%)	88 61	133, 175, 284, 427	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ILE	4.7
1	B	90	GLN	3.5
1	A	384	LEU	2.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.