



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 03:53 am GMT

PDB ID : 3OPO
Title : Crystal structure of the membrane fusion protein CusB from Escherichia coli
Authors : Su, C.-C.
Deposited on : 2010-09-01
Resolution : 3.85 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

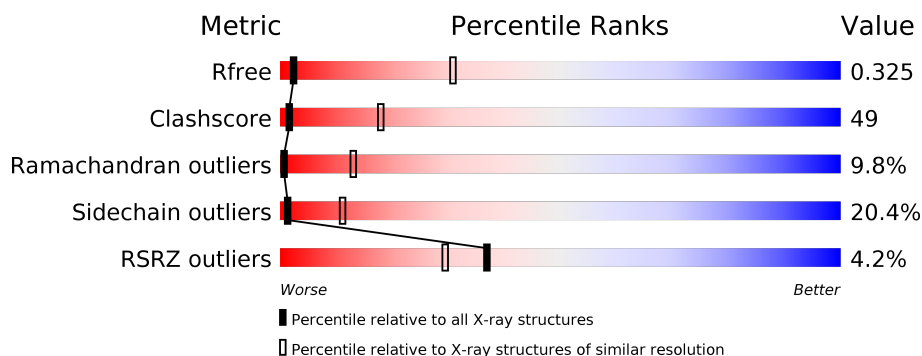
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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}	100719	1000 (4.12-3.56)
Clashscore	112137	1045 (4.10-3.58)
Ramachandran outliers	110173	1008 (4.10-3.58)
Sidechain outliers	110143	1001 (4.10-3.58)
RSRZ outliers	101464	1014 (4.12-3.56)

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. 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	<div> <div>2%</div> <div> <div></div> <div>22%</div> <div>36%</div> <div>12%</div> <div>•</div> <div>28%</div> </div> </div>
1	B	413	<div> <div>4%</div> <div> <div></div> <div>22%</div> <div>36%</div> <div>12%</div> <div>•</div> <div>28%</div> </div> </div>

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	414	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4543 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

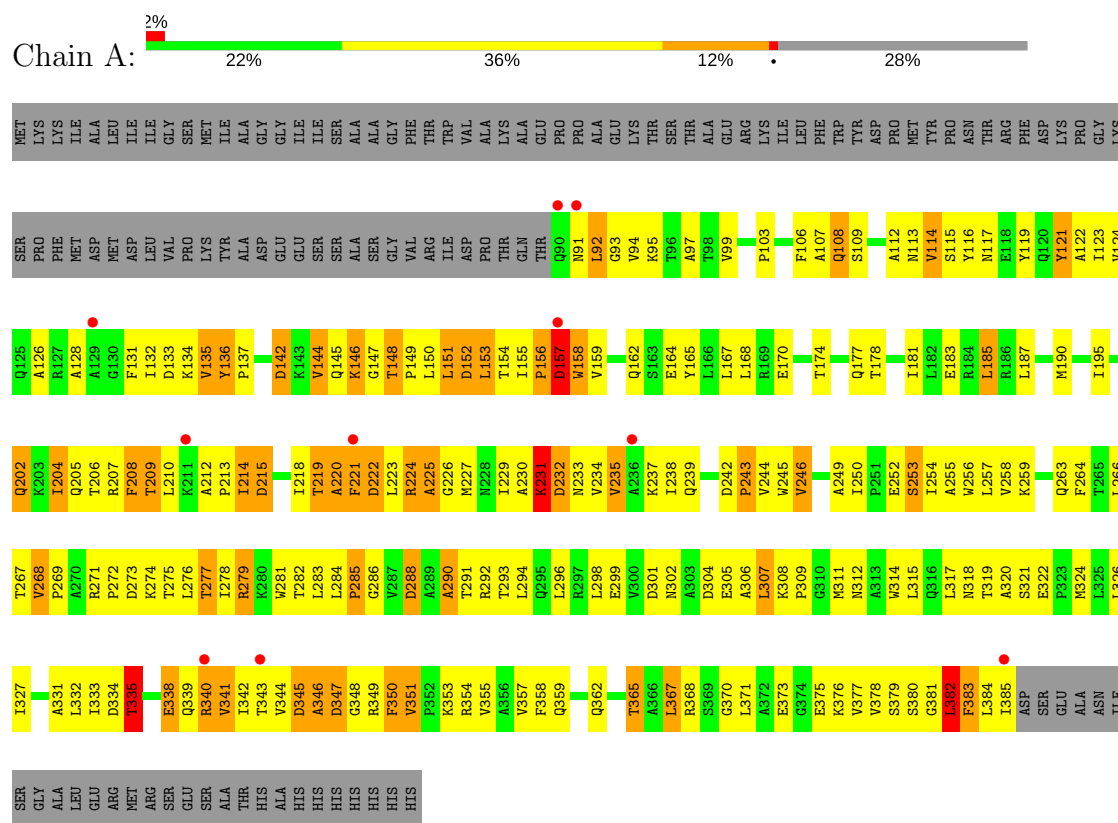
- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

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

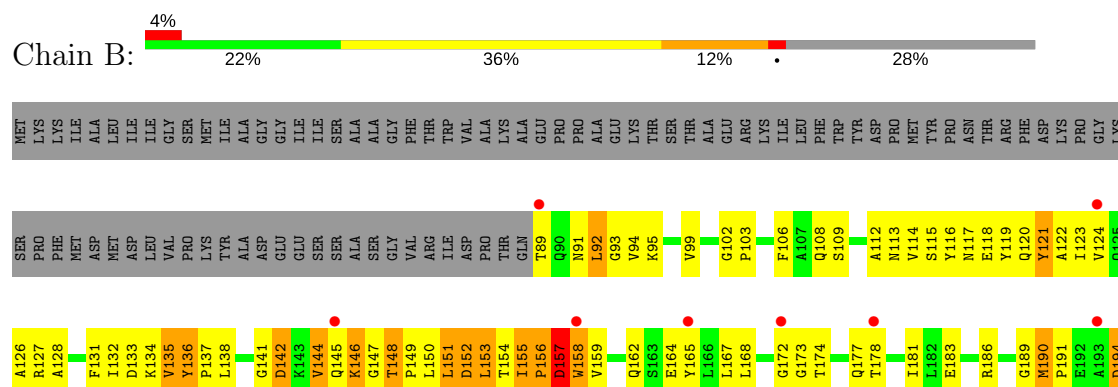
3 Residue-property plots

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



• Molecule 1: Cation efflux system protein cusB



GLU	I195	L257	I327
ARG	R196	V258	A331
MET	R197	K259	L332
ARG	L198	D260	I333
SER	I199	A261	D334
GLU	A200	F264	T335
SER	T201	T267	G336
ALA	Q202	V268	S337
THR	K203	P269	E338
HIS	I204	P270	Q339
ALA	Q205	A270	R340
HIS	T206	R271	V341
HIS	R207	P272	I342
HIS	F208	D273	T343
HIS	T209	K274	V344
HIS	L210	T275	D345
HIS	K211	L276	A346
	A212	T277	D347
	P213	I278	G348
	I214	R279	R349
	D215	K280	F350
	I218	W281	V351
	T219	T282	P352
	A220	L283	K353
	F221	L284	R354
	D222	P285	V355
	L223	G286	A356
	R224	V357	V357
	A225	A290	F358
	G226	T291	Q362
	M227	R292	T365
	N228	T293	A366
	A230	L294	L367
	K231	R297	R368
	D232	L298	L371
	N233	N302	A372
	V234	E305	V377
	V235	A306	V378
	A236	L307	S379
	K237	K308	S380
	I238	P309	G381
	Q239	N312	L382
	G240	A313	F383
	M241	W314	L384
	D242	L317	I385
	P243	N318	ASP
	V244	SER	SER
	W245	GLU	GLU
	V246	ALA	ALA
	A249	ALA	ASN
	I250	S321	ILE
	P251	E322	SER
	E252	P323	GLY
	S253	M324	ALA
	I254	L325	LEU
	A255	L326	
	W256		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.80Å 114.68Å 259.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.31 – 3.85 39.31 – 3.85	Depositor EDS
% Data completeness (in resolution range)	90.9 (39.31-3.85) 98.8 (39.31-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.295 , 0.340 0.275 , 0.325	Depositor DCC
R_{free} test set	585 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	159.3	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 239.3	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	0.91	EDS
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å ²)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.04% 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

5.1 Standard geometry

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	0.32	1/2306 (0.0%)	0.53	0/3142
1	B	0.27	0/2313	0.54	0/3152
All	All	0.30	1/4619 (0.0%)	0.53	0/6294

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	GLU	CB-CG	5.26	1.62	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2267	0	2336	233	0
1	B	2274	0	2343	227	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4543	0	4679	449	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 49.

The worst 5 of 449 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:332:LEU:HA	1:A:341:VAL:HG11	1.32	1.08
1:A:117:ASN:HD21	1:A:243:PRO:HG2	1.21	1.01
1:A:122:ALA:HB3	1:A:214:ILE:HD12	1.49	0.94
1:A:106:PHE:CD2	1:B:253:SER:HA	2.06	0.89
1:A:249:ALA:HB1	1:A:293:THR:HG21	1.52	0.89

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%)	220 (75%)	45 (15%)	29 (10%)	1	12
1	B	295/413 (71%)	218 (74%)	48 (16%)	29 (10%)	1	13
All	All	589/826 (71%)	438 (74%)	93 (16%)	58 (10%)	1	13

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	146	LYS
1	A	156	PRO
1	A	157	ASP
1	A	206	THR

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	242/338 (72%)	192 (79%)	50 (21%)	1	10
1	B	243/338 (72%)	194 (80%)	49 (20%)	1	11
All	All	485/676 (72%)	386 (80%)	99 (20%)	1	11

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	LEU
1	B	142	ASP
1	B	345	ASP
1	A	375	GLU
1	B	92	LEU

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

Mol	Chain	Res	Type
1	A	330	GLN
1	A	339	GLN
1	B	162	GLN
1	A	318	ASN
1	B	91	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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

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

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 [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%)	0.11	10 (3%) 46 36	112, 202, 318, 446	0
1	B	297/413 (71%)	0.28	15 (5%) 29 23	120, 214, 362, 581	0
All	All	593/826 (71%)	0.19	25 (4%) 37 29	112, 209, 343, 581	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	THR	7.6
1	B	200	ALA	3.3
1	A	90	GLN	3.2
1	B	158	TRP	3.0
1	B	223	LEU	2.8

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	AG	A	414	1/1	0.77	1.36	11.75	400,400,400,400	0
2	AG	B	414	1/1	0.80	1.08	-	268,268,268,268	0

6.5 Other polymers [i](#)

There are no such residues in this entry.