wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	3H94
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

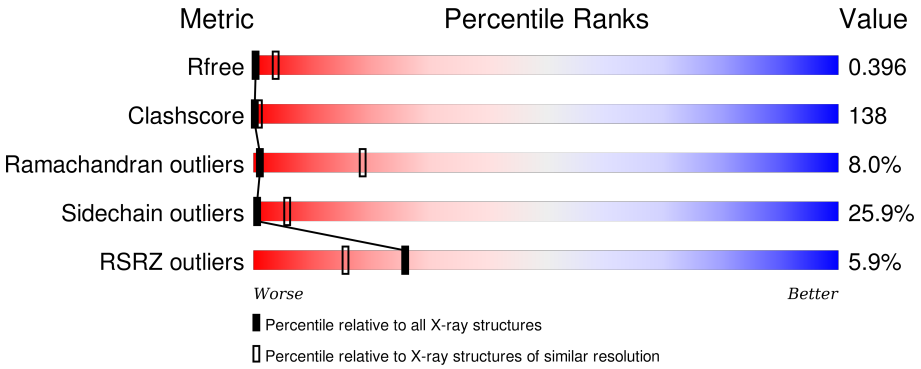
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1334 (4.18-3.50)
Clashscore	102246	1036 (4.16-3.52)
Ramachandran outliers	100387	1415 (4.18-3.50)
Sidechain outliers	100360	1410 (4.18-3.50)
RSRZ outliers	91569	1342 (4.18-3.50)

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 <=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	5% 14% 38% 20% • 27%
1	B	407	4% 13% 40% 18% • 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	B	408	-	-	-	X

2 Entry composition (i)

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 (three-letter code: AG) (formula: Ag).

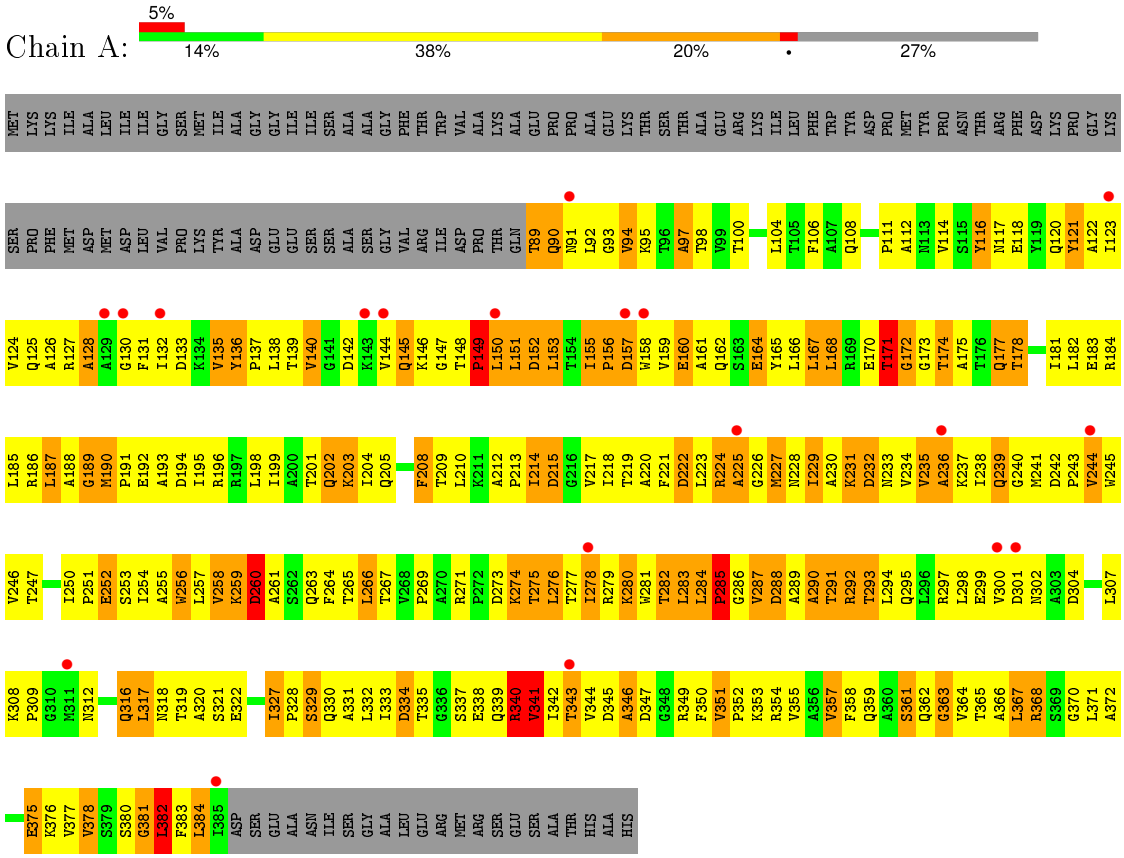
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ag	0	0
			1	1		
2	A	1	Total	Ag	0	0
			1	1		

3 Residue-property plots (i)

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.

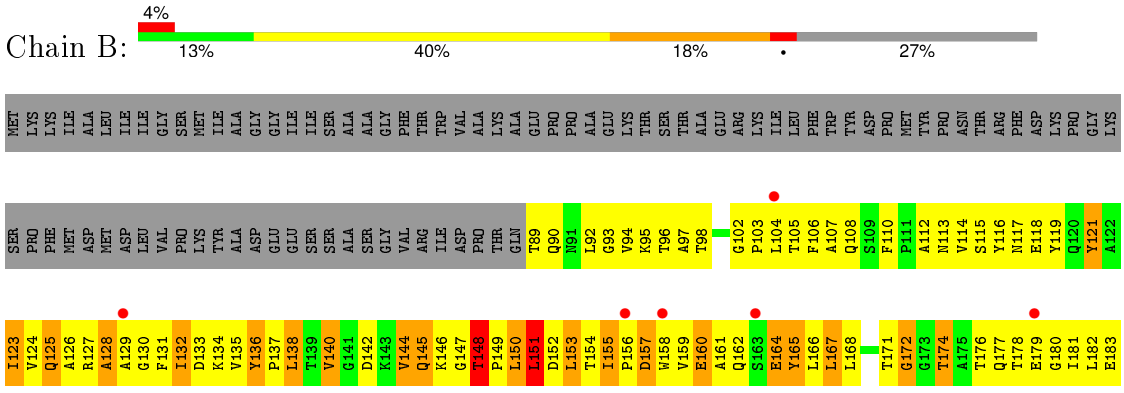
- Molecule 1: Cation efflux system protein cusB

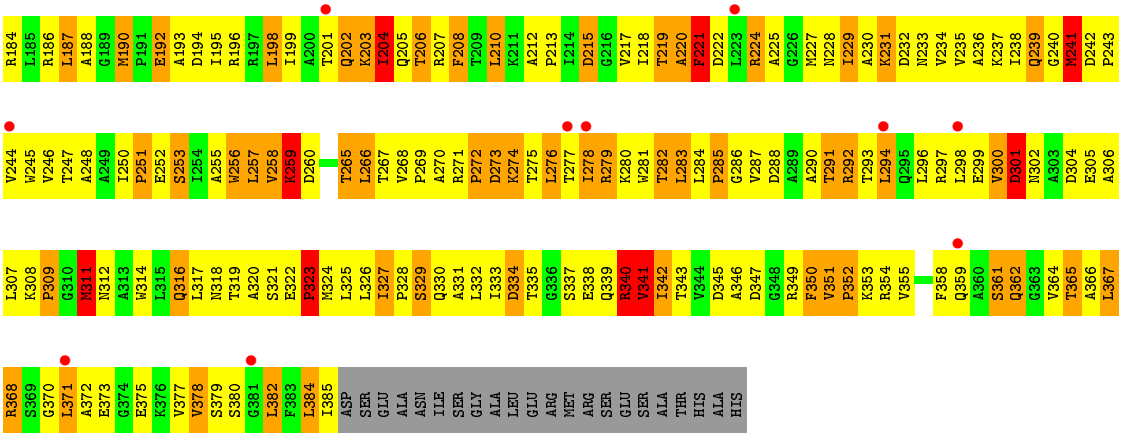
Chain A:



- Molecule 1: Cation efflux system protein cusB

Chain B:




R184 L185 R186 L187 A188 G189 M190 P191 E192 A193 D194 I195 R196 R197 L198 I199 A200 T201 Q202 K203 I204 Q205 T206 R207 F208 T209 L210 K211 A212 P213 I214 D215 G216 V217 I218 T219 A220 F221 D222 L223 R224 A225 G226 M227 N228 I229 A230 K231 D232 N233 V234 V235 A236 K237 I238 Q239 G240 M241 D242 P243
V244 W245 V246 T247 A248 A249 I250 P251 E252 S253 I254 A255 W256 L257 V258 K259 D260 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 F358 Q359 A360 S361 Q362 G363 V364 T365 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

4 Data and refinement statistics (i)

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 – 3.71	Depositor EDS
% Data completeness (in resolution range)	87.3 (47.20-3.84) 98.1 (47.20-3.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.96 (at 3.66Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.280 , 0.300 0.398 , 0.396	Depositor DCC
R_{free} test set	611 reflections (5.17%)	DCC
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 , 231.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 13543 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	5/2313 (0.2%)	1.25	25/3152 (0.8%)
1	B	0.85	3/2313 (0.1%)	1.34	32/3152 (1.0%)
All	All	0.84	8/4626 (0.2%)	1.29	57/6304 (0.9%)

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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	ALA	C-O	-9.88	1.04	1.23
1	A	94	VAL	C-N	8.15	1.52	1.34
1	A	89	THR	C-N	7.67	1.51	1.34
1	A	149	PRO	C-N	7.35	1.50	1.34
1	A	377	VAL	C-O	-6.94	1.10	1.23

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	119	TYR	N-CA-CB	-16.57	80.77	110.60
1	A	94	VAL	O-C-N	15.20	147.02	122.70
1	A	94	VAL	CA-C-N	-14.14	86.08	117.20
1	B	323	PRO	O-C-N	-11.99	103.51	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	VAL	C-N-CA	-11.00	94.20	121.70

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 (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	2274	0	2341	658	0
1	B	2274	0	2341	648	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	4550	0	4682	1274	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 138.

The worst 5 of 1274 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: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
1:B:244:VAL:HG21	1:B:307:LEU:CD1	1.53	1.38

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	295/407 (72%)	242 (82%)	27 (9%)	26 (9%)	1 16
1	B	295/407 (72%)	248 (84%)	26 (9%)	21 (7%)	1 22
All	All	590/814 (72%)	490 (83%)	53 (9%)	47 (8%)	1 19

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 (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	243/332 (73%)	186 (76%)	57 (24%)	1 7
1	B	243/332 (73%)	174 (72%)	69 (28%)	0 4
All	All	486/664 (73%)	360 (74%)	126 (26%)	0 6

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	LEU

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Mol	Chain	Res	Type
1	B	160	GLU
1	B	350	PHE
1	B	121	TYR
1	B	144	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	B	339	GLN
1	B	145	GLN
1	A	239	GLN
1	B	125	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 carbohydrates 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

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, 95^{th} 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%)	0.47	19 (6%)	23	13	20, 161, 275, 353	0
1	B	297/407 (72%)	0.42	16 (5%)	29	19	20, 167, 274, 377	0
All	All	594/814 (72%)	0.45	35 (5%)	26	16	20, 164, 275, 377	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	VAL	3.9
1	B	158	TRP	3.8
1	A	144	VAL	3.5
1	A	91	ASN	3.3
1	A	129	ALA	3.3

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

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, 95^{th} 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(Å^2)	Q<0.9
2	AG	B	408	1/1	0.91	0.43	0.40	30,30,30,30	0
2	AG	A	408	1/1	0.83	0.58	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.