



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 07:12 PM EDT

PDB ID : 3H94
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 : 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

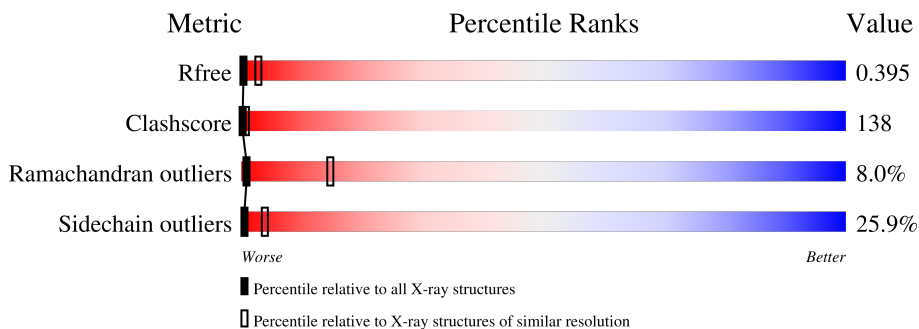
1 Overall quality at a glance

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}	130704	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	407	
1	B	407	

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 (three-letter code: 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		

V244	L307	R368
W245	K308	S369
V246	P309	G370
T247	G310	L371
A248	M311	A372
A249	N312	E373
I250	G313	G374
P251	W314	E375
E252	L315	R376
S253	Q316	V377
I254	L317	V378
A255	N318	S379
W256	T319	S380
L257	A320	G381
V258	S321	L382
K259	E322	F383
D260	P323	L384
	M324	I385
	L325	ASP
T265	L326	SER
L266	L327	GLU
T267	P328	ALA
V268	S329	ASN
P269	Q330	ILE
A270	A331	SER
R271	L332	GLY
P272	I333	ALA
D273	D334	LEU
K274	T335	GLU
T275	G336	ARG
L276	S337	MET
T277	E338	ARG
I278	Q339	SER
R279	R340	GLU
K280	V341	SER
W281	I342	ALA
T282	T343	THR
L283	V344	HIS
L284	D345	ALA
P285	A346	
G286	D347	
V287	G348	
D288	R349	
A289	F350	
A290	V351	
T291	P352	
R292	K353	
T293	R354	
L294	V355	
Q295		
L296		
R297	F358	
L298	Q359	
E299	A360	
V300	S361	
D301	Q362	
N302	G363	
A303	V364	
D304	T365	
E305	A366	
A306	L367	

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 – 3.71	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
$\langle I/\sigma(I) \rangle$ ¹	4.96 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.300 0.396 , 0.395	Depositor DCC
R_{free} test set	675 reflections (4.98%)	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 , 231.4	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

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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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%)	1	13
1	B	295/407 (72%)	248 (84%)	26 (9%)	21 (7%)	1	17
All	All	590/814 (72%)	490 (83%)	53 (9%)	47 (8%)	1	15

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%)	186 (76%)	57 (24%)	1	5
1	B	243/332 (73%)	174 (72%)	69 (28%)	0	2
All	All	486/664 (73%)	360 (74%)	126 (26%)	0	4

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

Mol	Chain	Res	Type
1	B	98	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	327	ILE
1	B	164	GLU
1	B	324	MET
1	B	361	SER

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

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

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 monosaccharides 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 [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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.