



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3PPO / pdb\_00003ppo  
Title : Structures of the substrate-binding protein provide insights into the multiple compatible solutes binding specificities of *Bacillus subtilis* ABC transporter OpuC  
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Deposited on : 2010-11-24  
Resolution : 2.70 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

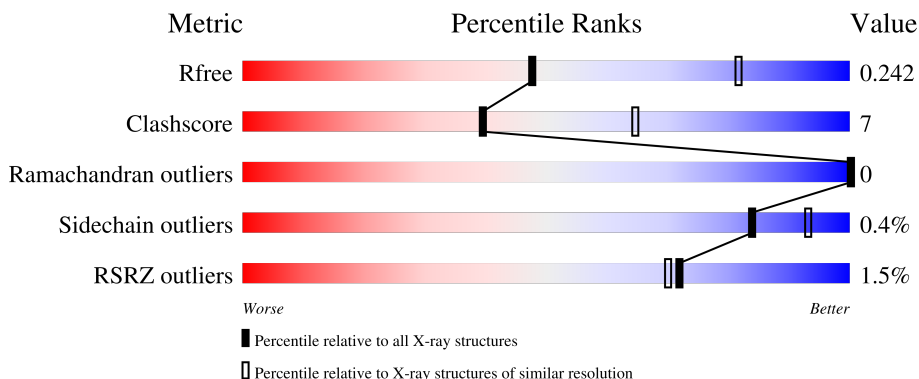
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	311	 2% 70% 17% 13%
1	B	311	 2% 75% 12% 13%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4496 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.

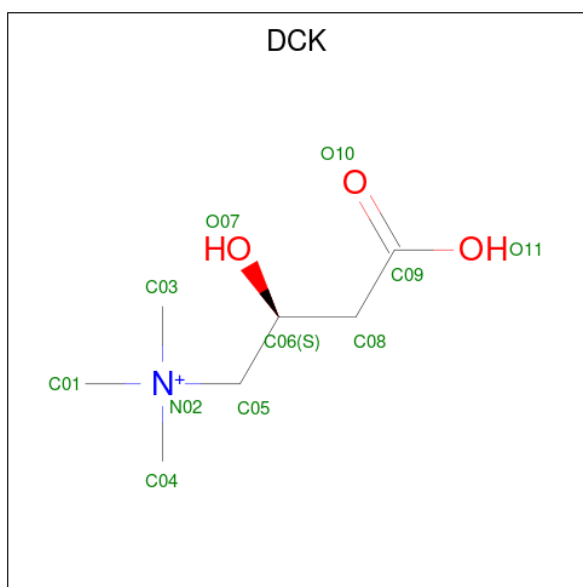
- Molecule 1 is a protein called Glycine betaine/carnitine/choline-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	Total	C	N	O	S	0	0	0
			2173	1388	354	424	7			
1	B	272	Total	C	N	O	S	0	0	0
			2173	1388	354	424	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP O32243
A	-6	GLY	-	expression tag	UNP O32243
A	-5	HIS	-	expression tag	UNP O32243
A	-4	HIS	-	expression tag	UNP O32243
A	-3	HIS	-	expression tag	UNP O32243
A	-2	HIS	-	expression tag	UNP O32243
A	-1	HIS	-	expression tag	UNP O32243
A	0	HIS	-	expression tag	UNP O32243
B	-7	MET	-	expression tag	UNP O32243
B	-6	GLY	-	expression tag	UNP O32243
B	-5	HIS	-	expression tag	UNP O32243
B	-4	HIS	-	expression tag	UNP O32243
B	-3	HIS	-	expression tag	UNP O32243
B	-2	HIS	-	expression tag	UNP O32243
B	-1	HIS	-	expression tag	UNP O32243
B	0	HIS	-	expression tag	UNP O32243

- Molecule 2 is (2S)-3-carboxy-2-hydroxy-N,N,N-trimethylpropan-1-aminium (CCD ID: DCK) (formula: C<sub>7</sub>H<sub>16</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	11	7	1	3	0	0
2	B	1	11	7	1	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	61	61	61	0	0
3	B	67	67	67	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.89Å 91.07Å 115.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.70 29.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	78.8 (29.92-2.70) 78.8 (29.92-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.29 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.212 , 0.238 0.212 , 0.242	Depositor DCC
$R_{free}$ test set	742 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4496	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DCK

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	0.90	5/2218 (0.2%)	0.92	1/2991 (0.0%)
1	B	0.98	6/2218 (0.3%)	0.95	3/2991 (0.1%)
All	All	0.94	11/4436 (0.2%)	0.94	4/5982 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	C-O	-6.81	1.16	1.24
1	B	242	ASP	C-O	-6.33	1.16	1.23
1	B	240	PRO	C-O	-5.64	1.17	1.23
1	A	116	GLN	CD-OE1	5.62	1.34	1.23
1	B	258	LEU	C-O	-5.51	1.17	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ILE	N-CA-C	7.64	118.86	108.17
1	B	259	GLU	N-CA-C	5.92	117.41	111.07
1	B	259	GLU	CA-C-N	5.48	126.17	120.03
1	B	259	GLU	C-N-CA	5.48	126.17	120.03

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	2173	0	2141	36	0
1	B	2173	0	2141	19	0
2	A	11	0	14	3	0
2	B	11	0	14	4	0
3	A	61	0	0	2	0
3	B	67	0	0	2	0
All	All	4496	0	4310	58	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 7.

The worst 5 of 58 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:269:ILE:HG21	1:B:274:MET:HE2	1.46	0.97
1:A:269:ILE:HG21	1:A:274:MET:HE2	1.44	0.97
1:A:134:ASP:HB3	3:A:351:HOH:O	1.68	0.92
1:A:114:ILE:O	1:A:118:GLU:HG2	1.73	0.89
2:B:401:DCK:H04A	2:B:401:DCK:O07	1.78	0.84

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	270/311 (87%)	265 (98%)	5 (2%)	0	100	100
1	B	270/311 (87%)	266 (98%)	4 (2%)	0	100	100
All	All	540/622 (87%)	531 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	236/265 (89%)	236 (100%)	0	100	100
1	B	236/265 (89%)	234 (99%)	2 (1%)	73	88
All	All	472/530 (89%)	470 (100%)	2 (0%)	84	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	115	VAL
1	B	224	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	B	113	ASN
1	B	152	ASN
1	A	152	ASN
1	A	76	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DCK	A	401	-	10,10,10	2.19	2 (20%)	13,14,14	2.40	4 (30%)
2	DCK	B	401	-	10,10,10	1.74	2 (20%)	13,14,14	2.18	4 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DCK	A	401	-	-	6/9/9/9	-
2	DCK	B	401	-	-	2/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	DCK	O07-C06	-5.12	1.28	1.43
2	B	401	DCK	O07-C06	-3.91	1.32	1.43
2	A	401	DCK	C05-N02	-3.23	1.45	1.52
2	B	401	DCK	C05-N02	-3.17	1.45	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	DCK	C06-C05-N02	5.08	126.05	116.70
2	B	401	DCK	C05-C06-C08	5.04	117.19	107.79
2	A	401	DCK	C05-C06-C08	3.98	115.22	107.79
2	A	401	DCK	O07-C06-C05	3.84	123.11	110.68
2	B	401	DCK	O07-C06-C08	3.62	119.04	109.64

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	DCK	C06-C05-N02-C04
2	A	401	DCK	C05-C06-C08-C09
2	A	401	DCK	O07-C06-C08-C09
2	B	401	DCK	N02-C05-C06-O07
2	B	401	DCK	O07-C06-C08-C09

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	DCK	3	0
2	B	401	DCK	4	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	272/311 (87%)	-0.13	1 (0%) 88 87	12, 25, 40, 50	0
1	B	272/311 (87%)	0.03	7 (2%) 57 54	16, 28, 45, 86	0
All	All	544/622 (87%)	-0.05	8 (1%) 72 70	12, 27, 43, 86	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	PRO	3.3
1	B	303	ASP	3.3
1	B	300	HIS	2.5
1	B	170	ASN	2.4
1	B	73	TYR	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, 95<sup>th</sup> 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	DCK	B	401	11/11	0.92	0.12	5,7,11,12	0
2	DCK	A	401	11/11	0.96	0.07	4,7,9,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.