



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:36 PM UTC

PDB ID : 4OD7 / pdb_00004od7
Title : Complex structure of Proteus mirabilis DsbA (C30S) with a non-covalently bound peptide PWATCDS
Authors : Kurth, F.; Premkumar, L.; Martin, J.L.
Deposited on : 2014-01-10
Resolution : 1.60 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	:	4-5-2 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

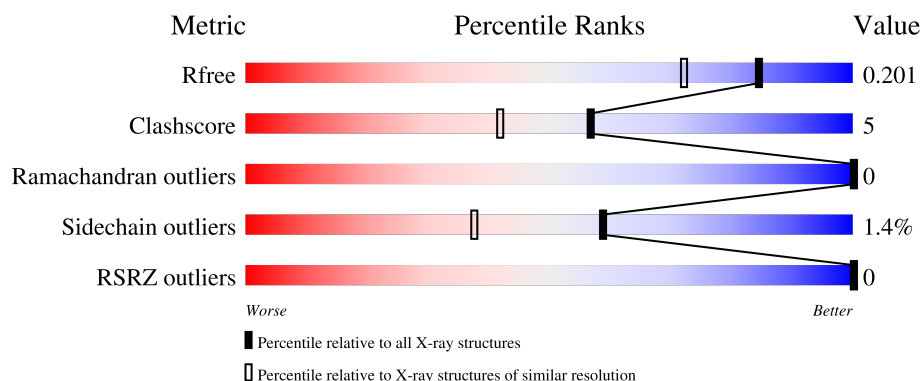
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 $\leq 5\%$. 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	190	94% 5% .
1	B	190	82% 16% ..
1	C	190	82% 16% .
2	D	9	89% 11%
2	E	9	89% 11%

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Mol	Chain	Length	Quality of chain
2	F	9	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9477 atoms, of which 4405 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 Thiol:disulfide interchange protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	187	Total	C	H	N	O	S	0	0	0
			2839	913	1402	237	281	6			
1	B	187	Total	C	H	N	O	S	0	1	0
			2885	925	1429	240	285	6			
1	C	187	Total	C	H	N	O	S	0	0	0
			2884	923	1430	240	285	6			

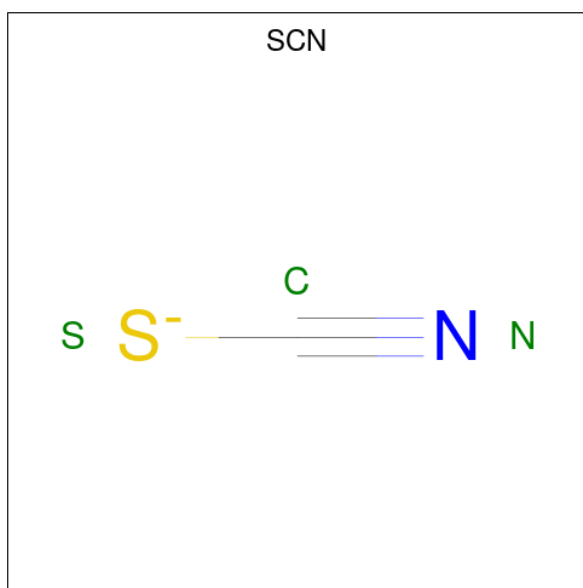
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP B4EZ68
A	0	ASN	-	expression tag	UNP B4EZ68
A	1	ALA	-	expression tag	UNP B4EZ68
A	30	SER	CYS	engineered mutation	UNP B4EZ68
B	-1	SER	-	expression tag	UNP B4EZ68
B	0	ASN	-	expression tag	UNP B4EZ68
B	1	ALA	-	expression tag	UNP B4EZ68
B	30	SER	CYS	engineered mutation	UNP B4EZ68
C	-1	SER	-	expression tag	UNP B4EZ68
C	0	ASN	-	expression tag	UNP B4EZ68
C	1	ALA	-	expression tag	UNP B4EZ68
C	30	SER	CYS	engineered mutation	UNP B4EZ68

- Molecule 2 is a protein called (ACE)PWATCDS(NH2) Peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	9	Total	C	H	N	O	S	0	0	1
			105	35	48	9	12	1			
2	E	9	Total	C	H	N	O	S	0	0	1
			105	35	48	9	12	1			
2	F	9	Total	C	H	N	O	S	0	0	1
			105	35	48	9	12	1			

- Molecule 3 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	A	1	Total	C	N	S	0	0
			3	1	1	1		
3	C	1	Total	C	N	S	0	0
			3	1	1	1		
3	C	1	Total	C	N	S	0	0
			3	1	1	1		

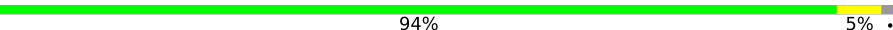
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	171	Total	O	0	0
			171	171		
4	C	173	Total	O	0	0
			173	173		
4	D	11	Total	O	0	0
			11	11		
4	E	10	Total	O	0	0
			10	10		
4	F	16	Total	O	0	0
			16	16		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

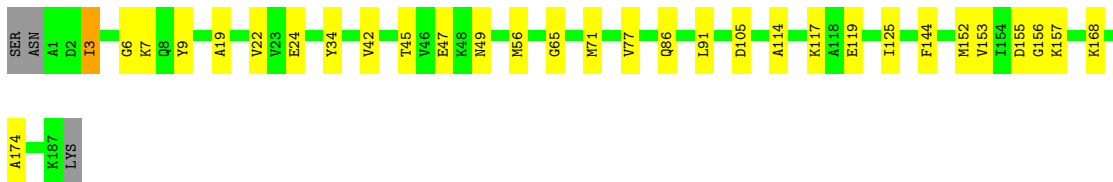
- Molecule 1: Thiol:disulfide interchange protein

Chain A:  94% 5% .



- Molecule 1: Thiol:disulfide interchange protein

Chain B:  82% 16% ..



- Molecule 1: Thiol:disulfide interchange protein

Chain C:  82% 16% .



- Molecule 2: (ACE)PWATCDS(NH2) Peptide

Chain D:  89% 11%



- Molecule 2: (ACE)PWATCDS(NH2) Peptide

Chain E:  89% 11%



- Molecule 2: (ACE)PWATCDS(NH2) Peptide

Chain F:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	74.06 Å 74.06 Å 93.27 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.72 – 1.60 37.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.72-1.60) 98.7 (37.72-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.172 , 0.200 0.172 , 0.201	Depositor DCC
R_{free} test set	3766 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9477	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: ACE, SCN, NH2

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	1.02	0/1466	0.99	0/1989
1	B	1.00	0/1488	1.07	3/2017 (0.1%)
1	C	1.03	0/1483	1.05	4/2010 (0.2%)
2	D	1.45	1/56 (1.8%)	0.89	0/78
2	E	1.30	1/56 (1.8%)	0.86	0/78
2	F	0.89	0/56	0.80	0/78
All	All	1.03	2/4605 (0.0%)	1.03	7/6250 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	65	ACE	C-N	8.47	1.51	1.43
2	E	65	ACE	C-N	-5.99	1.37	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	GLY	CA-C-N	7.03	127.01	119.28
1	B	65	GLY	C-N-CA	7.03	127.01	119.28
1	C	6	GLY	N-CA-C	-5.80	108.05	115.42
1	B	34	TYR	N-CA-C	-5.75	104.92	111.07
1	C	2	ASP	CA-C-N	5.36	130.02	123.10

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	1437	1402	1402	6	0
1	B	1456	1429	1432	19	1
1	C	1454	1430	1430	18	0
2	D	57	48	46	0	0
2	E	57	48	46	0	0
2	F	57	48	46	0	0
3	A	6	0	0	1	0
3	C	6	0	0	0	0
4	A	161	0	0	0	0
4	B	171	0	0	0	0
4	C	173	0	0	3	1
4	D	11	0	0	0	0
4	E	10	0	0	0	0
4	F	16	0	0	0	0
All	All	5072	4405	4402	41	1

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 5.

The worst 5 of 41 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:155:ASP:HB3	1:B:157:LYS:HE2	1.64	0.80
1:A:171:GLU:OE1	1:A:171:GLU:N	2.26	0.67
1:C:17:ALA:N	4:C:431:HOH:O	2.31	0.61
1:C:108:ARG:NH2	1:C:118:ALA:HB1	2.18	0.58
1:C:15:PRO:HB3	1:C:157:LYS:HG2	1.87	0.56

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASP:OD2	4:C:404:HOH:O[1_665]	2.19	0.01

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	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
1	B	186/190 (98%)	184 (99%)	2 (1%)	0	100	100
1	C	185/190 (97%)	183 (99%)	2 (1%)	0	100	100
2	D	7/9 (78%)	7 (100%)	0	0	100	100
2	E	7/9 (78%)	7 (100%)	0	0	100	100
2	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	577/597 (97%)	571 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	155/162 (96%)	154 (99%)	1 (1%)	78	66
1	B	159/162 (98%)	156 (98%)	3 (2%)	50	27
1	C	159/162 (98%)	156 (98%)	3 (2%)	50	27
2	D	6/6 (100%)	6 (100%)	0	100	100
2	E	6/6 (100%)	6 (100%)	0	100	100
2	F	6/6 (100%)	6 (100%)	0	100	100
All	All	491/504 (97%)	484 (99%)	7 (1%)	59	38

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	168	LYS
1	C	4	SER
1	C	52	GLU
1	C	14	LYS
1	B	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	136	GLN
1	B	138	GLN
1	C	136	GLN
1	C	35	GLN
1	A	139	ASN

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 [i](#)

4 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	$\# Z > 2$
3	SCN	A	202	-	1,2,2	0.97	0	0,1,1	-	-
3	SCN	C	201	-	1,2,2	0.23	0	0,1,1	-	-
3	SCN	A	201	-	1,2,2	1.16	0	0,1,1	-	-
3	SCN	C	202	-	1,2,2	0.78	0	0,1,1	-	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	SCN	1	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, 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	187/190 (98%)	-1.14	0 100 100	14, 24, 55, 81	0
1	B	187/190 (98%)	-1.22	0 100 100	15, 25, 47, 67	1 (0%)
1	C	187/190 (98%)	-1.17	0 100 100	14, 24, 50, 70	0
2	D	7/9 (77%)	-1.31	0 100 100	17, 18, 23, 26	0
2	E	7/9 (77%)	-1.31	0 100 100	17, 21, 22, 26	0
2	F	7/9 (77%)	-1.36	0 100 100	18, 19, 22, 23	0
All	All	582/597 (97%)	-1.18	0 100 100	14, 24, 50, 81	1 (0%)

There are no RSRZ outliers to report.

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, 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	B-factors(Å ²)	Q<0.9
3	SCN	A	201	3/3	1.00	0.03	12,12,18,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SCN	A	202	3/3	1.00	0.02	21,21,22,23	0
3	SCN	C	201	3/3	1.00	0.02	16,16,17,20	0
3	SCN	C	202	3/3	1.00	0.03	24,24,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.