



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2024 – 12:15 PM EST

PDB ID : 6DPS  
Title : Crystal Structure of Neisseria meningitidis DsbD n-terminal domain in the oxidised form  
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Deposited on : 2018-06-09  
Resolution : 2.56 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

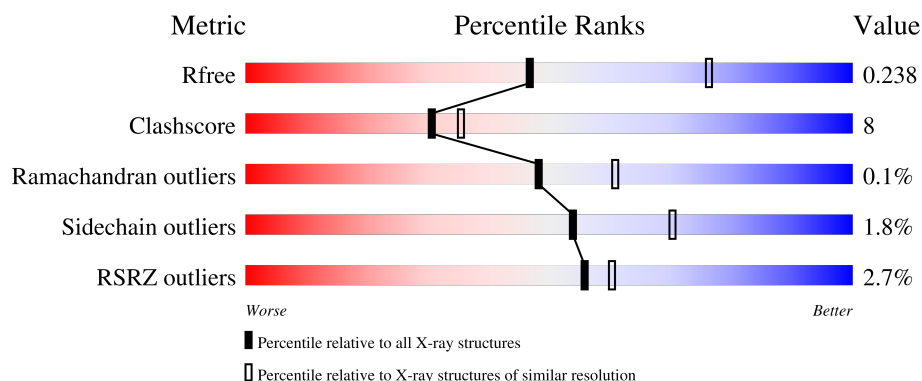
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*






The reported resolution of this entry is 2.56 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))
$R_{free}$	164625	1685 (2.58-2.54)
Clashscore	180529	1779 (2.58-2.54)
Ramachandran outliers	177936	1766 (2.58-2.54)
Sidechain outliers	177891	1766 (2.58-2.54)
RSRZ outliers	164620	1685 (2.58-2.54)

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	126	
1	B	126	
1	C	126	
1	D	126	
1	E	126	

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Mol	Chain	Length	Quality of chain
1	F	126	<div><div></div><div>4%</div><div>72%</div><div>23%</div><div>5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5960 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 Thiol:disulfide interchange protein DsbD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			956	615	152	186	3			
1	B	122	Total	C	N	O	S	0	0	0
			956	615	152	186	3			
1	C	123	Total	C	N	O	S	0	0	0
			964	619	154	188	3			
1	D	124	Total	C	N	O	S	0	1	0
			977	627	158	189	3			
1	E	121	Total	C	N	O	S	0	0	0
			949	611	151	184	3			
1	F	120	Total	C	N	O	S	0	0	0
			940	606	149	182	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP C6S7X6
A	0	ASN	-	expression tag	UNP C6S7X6
A	101	VAL	ALA	engineered mutation	UNP C6S7X6
B	-1	SER	-	expression tag	UNP C6S7X6
B	0	ASN	-	expression tag	UNP C6S7X6
B	101	VAL	ALA	engineered mutation	UNP C6S7X6
C	-1	SER	-	expression tag	UNP C6S7X6
C	0	ASN	-	expression tag	UNP C6S7X6
C	101	VAL	ALA	engineered mutation	UNP C6S7X6
D	-1	SER	-	expression tag	UNP C6S7X6
D	0	ASN	-	expression tag	UNP C6S7X6
D	101	VAL	ALA	engineered mutation	UNP C6S7X6
E	-1	SER	-	expression tag	UNP C6S7X6
E	0	ASN	-	expression tag	UNP C6S7X6
E	101	VAL	ALA	engineered mutation	UNP C6S7X6
F	-1	SER	-	expression tag	UNP C6S7X6
F	0	ASN	-	expression tag	UNP C6S7X6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	101	VAL	ALA	engineered mutation	UNP C6S7X6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Zn 3	0	0
2	B	8	Total 8	Zn 8	0	0
2	C	6	Total 6	Zn 6	0	0
2	D	7	Total 7	Zn 7	0	0
2	E	2	Total 2	Zn 2	0	0
2	F	6	Total 6	Zn 6	0	0


- Molecule 3 is water.

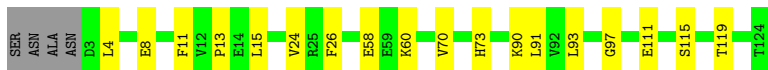
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	55	Total 55	O 55	0	0
3	C	18	Total 18	O 18	0	0
3	D	25	Total 25	O 25	0	0
3	E	19	Total 19	O 19	0	0
3	F	18	Total 18	O 18	0	0

### 3 Residue-property plots [i](#)


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 DsbD

Chain A: 




- Molecule 1: Thiol:disulfide interchange protein DsbD

Chain B: 




- Molecule 1: Thiol:disulfide interchange protein DsbD

Chain C: 



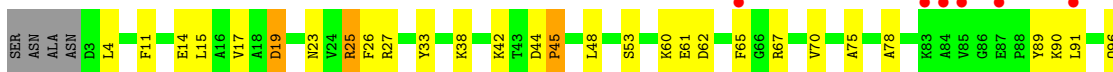
- Molecule 1: Thiol:disulfide interchange protein DsbD

Chain D: 



- Molecule 1: Thiol:disulfide interchange protein DsbD

Chain E: 





● Molecule 1: Thiol:disulfide interchange protein DsbD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.64Å 147.64Å 147.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.81 – 2.56 35.81 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.81-2.56) 99.8 (35.81-2.56)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.19 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.178 , 0.235 0.182 , 0.238	Depositor DCC
$R_{free}$ test set	1765 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.51	0/984	0.60	0/1340
1	B	0.51	0/984	0.64	0/1340
1	C	0.45	0/992	0.62	0/1351
1	D	0.49	0/1008	0.60	0/1372
1	E	0.47	0/977	0.65	2/1330 (0.2%)
1	F	0.46	0/968	0.62	0/1318
All	All	0.48	0/5913	0.62	2/8051 (0.0%)

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	E	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	E	25	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	E	25	ARG	NE-CZ-NH1	-5.40	117.60	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	44	ASP	Peptide

## 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	956	0	900	12	0
1	B	956	0	900	12	0
1	C	964	0	906	18	0
1	D	977	0	927	7	0
1	E	949	0	893	24	0
1	F	940	0	885	21	0
2	A	3	0	0	0	0
2	B	8	0	0	0	0
2	C	6	0	0	0	0
2	D	7	0	0	0	0
2	E	2	0	0	0	0
2	F	6	0	0	0	0
3	A	51	0	0	3	0
3	B	55	0	0	4	0
3	C	18	0	0	0	0
3	D	25	0	0	1	0
3	E	19	0	0	2	0
3	F	18	0	0	4	0
All	All	5960	0	5411	92	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 8.

The worst 5 of 92 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:C:83:LYS:HE3	1:C:84:ALA:O	1.52	1.07
1:E:45:PRO:HG2	1:E:48:LEU:HD11	1.49	0.94
1:F:114:ILE:HD12	1:F:120:TYR:CZ	2.03	0.93
1:E:38:LYS:NZ	1:E:96:GLN:OE1	2.01	0.93
1:C:83:LYS:CE	1:C:84:ALA:O	2.25	0.85

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	120/126 (95%)	117 (98%)	3 (2%)	0	100	100
1	B	120/126 (95%)	116 (97%)	4 (3%)	0	100	100
1	C	121/126 (96%)	111 (92%)	10 (8%)	0	100	100
1	D	123/126 (98%)	118 (96%)	5 (4%)	0	100	100
1	E	119/126 (94%)	111 (93%)	7 (6%)	1 (1%)	16	23
1	F	118/126 (94%)	109 (92%)	9 (8%)	0	100	100
All	All	721/756 (95%)	682 (95%)	38 (5%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	45	PRO

### 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	100/103 (97%)	100 (100%)	0	100	100
1	B	100/103 (97%)	98 (98%)	2 (2%)	50	67
1	C	101/103 (98%)	99 (98%)	2 (2%)	50	67
1	D	102/103 (99%)	101 (99%)	1 (1%)	73	83
1	E	99/103 (96%)	97 (98%)	2 (2%)	50	67
1	F	98/103 (95%)	94 (96%)	4 (4%)	26	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	600/618 (97%)	589 (98%)	11 (2%)	54 70

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	3	ASP
1	F	25	ARG
1	F	64	PHE
1	F	38	LYS
1	D	115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	E	23	ASN
1	F	76	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 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, 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	122/126 (96%)	-0.55	0 100 100	35, 49, 83, 104	0
1	B	122/126 (96%)	-0.38	1 (0%) 82 85	34, 51, 94, 140	0
1	C	123/126 (97%)	0.02	4 (3%) 49 54	40, 69, 109, 161	0
1	D	124/126 (98%)	-0.34	3 (2%) 59 64	37, 56, 96, 144	1 (0%)
1	E	121/126 (96%)	0.31	7 (5%) 30 34	38, 84, 159, 225	0
1	F	120/126 (95%)	0.26	5 (4%) 41 46	43, 92, 145, 176	0
All	All	732/756 (96%)	-0.12	20 (2%) 56 60	34, 63, 134, 225	1 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	VAL	4.8
1	F	64	PHE	3.7
1	C	85	VAL	3.5
1	E	84	ALA	3.3
1	F	122	PRO	3.2

### 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 monosaccharides 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. 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(Å <sup>2</sup> )	Q<0.9
2	ZN	F	206	1/1	-0.51	0.28	265,265,265,265	1
2	ZN	C	206	1/1	0.63	0.15	166,166,166,166	1
2	ZN	D	206	1/1	0.74	0.10	168,168,168,168	1
2	ZN	C	204	1/1	0.82	0.11	143,143,143,143	0
2	ZN	F	205	1/1	0.83	0.19	170,170,170,170	1
2	ZN	B	205	1/1	0.85	0.08	200,200,200,200	0
2	ZN	F	203	1/1	0.86	0.15	182,182,182,182	0
2	ZN	C	205	1/1	0.86	0.08	68,68,68,68	1
2	ZN	D	207	1/1	0.86	0.12	154,154,154,154	0
2	ZN	B	206	1/1	0.87	0.09	161,161,161,161	0
2	ZN	B	207	1/1	0.88	0.15	149,149,149,149	0
2	ZN	D	205	1/1	0.88	0.11	135,135,135,135	0
2	ZN	F	202	1/1	0.88	0.09	147,147,147,147	0
2	ZN	D	202	1/1	0.89	0.09	139,139,139,139	0
2	ZN	B	208	1/1	0.90	0.08	153,153,153,153	0
2	ZN	E	202	1/1	0.92	0.10	139,139,139,139	0
2	ZN	F	204	1/1	0.95	0.07	129,129,129,129	0
2	ZN	C	203	1/1	0.96	0.07	133,133,133,133	0
2	ZN	A	202	1/1	0.97	0.04	108,108,108,108	0
2	ZN	C	202	1/1	0.98	0.04	71,71,71,71	0
2	ZN	B	202	1/1	0.98	0.03	44,44,44,44	1
2	ZN	D	203	1/1	0.98	0.03	101,101,101,101	0
2	ZN	A	203	1/1	0.99	0.03	62,62,62,62	0
2	ZN	C	201	1/1	0.99	0.02	51,51,51,51	1
2	ZN	B	201	1/1	0.99	0.02	62,62,62,62	0
2	ZN	D	204	1/1	0.99	0.04	40,40,40,40	1
2	ZN	F	201	1/1	0.99	0.02	54,54,54,54	0
2	ZN	B	203	1/1	1.00	0.04	42,42,42,42	0
2	ZN	B	204	1/1	1.00	0.02	58,58,58,58	0
2	ZN	E	201	1/1	1.00	0.03	49,49,49,49	0
2	ZN	A	201	1/1	1.00	0.06	43,43,43,43	0
2	ZN	D	201	1/1	1.00	0.03	60,60,60,60	0

## 6.5 Other polymers

There are no such residues in this entry.