



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4FFJ / pdb\_00004ffj  
Title : The crystal structure of spDHBP from S.pneumoniae  
Authors : Wang, D.  
Deposited on : 2012-06-01  
Resolution : 1.95 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

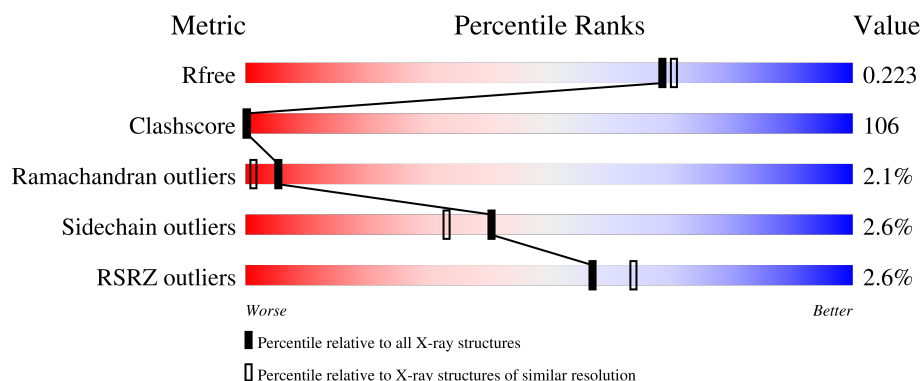
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	210	

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	SO4	A	302	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	303	-	X	-	-
3	GOL	A	304	-	X	X	-
3	GOL	A	305	-	X	X	-
3	GOL	A	306	-	X	X	-
3	GOL	A	307	-	X	X	-
3	GOL	A	308	-	X	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1636 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 Riboflavin biosynthesis protein ribBA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	7	1	0
			1470	919	249	285	17			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

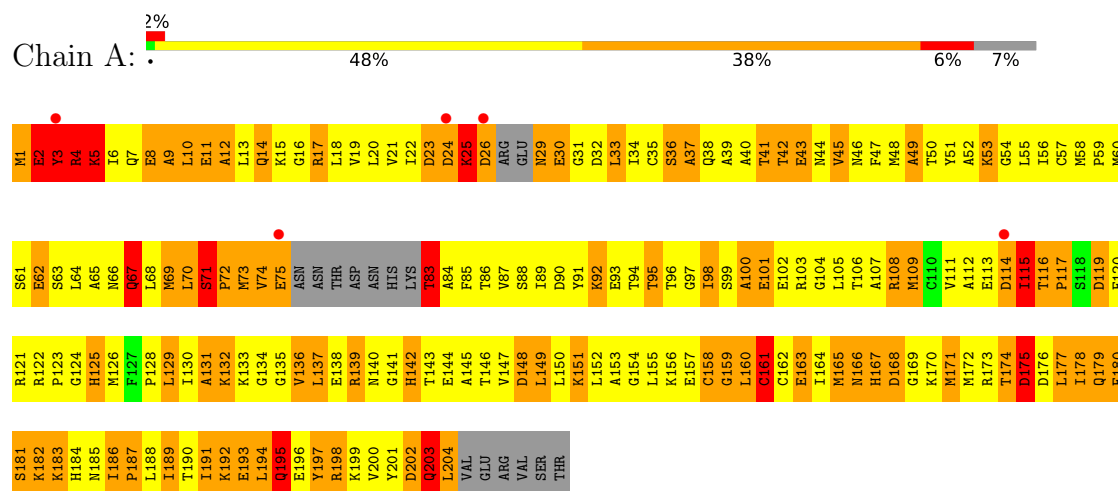
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		

### 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: Riboflavin biosynthesis protein ribBA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.01Å 78.01Å 87.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.20 – 1.95 38.20 – 1.95	Depositor EDS
% Data completeness (in resolution range)	84.4 (38.20-1.95) 84.5 (38.20-1.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.187 , 0.244 (Not available) , 0.223	Depositor DCC
$R_{free}$ test set	1037 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% 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: SO4, GOL

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	7.98	644/1485 (43.4%)	3.74	321/1998 (16.1%)

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	10

The worst 5 of 644 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	ASP	C-N	43.14	1.94	1.33
1	A	4	ARG	C-O	40.87	2.05	1.23
1	A	5	LYS	CA-C	40.69	2.09	1.52
1	A	4	ARG	NE-CZ	33.67	1.70	1.33
1	A	198	ARG	CD-NE	-32.21	1.01	1.46

The worst 5 of 321 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CA-C-O	20.01	141.99	120.58
1	A	185	ASN	OD1-CG-ND2	-17.00	105.60	122.60
1	A	203	GLN	O-C-N	16.89	143.43	122.65
1	A	3	TYR	O-C-N	15.20	142.81	122.59
1	A	193	GLU	CA-C-O	14.44	135.85	120.55

There are no chirality outliers.

5 of 10 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	100	ALA	Mainchain
1	A	2	GLU	Mainchain
1	A	4	ARG	Sidechain
1	A	5	LYS	Peptide,Mainchain
1	A	67	GLN	Sidechain

## 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	1470	0	1437	294	0
2	A	15	0	0	0	0
3	A	30	0	36	31	0
4	A	121	0	0	15	2
All	All	1636	0	1473	316	2

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 106.

The worst 5 of 316 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:A:95:THR:CA	1:A:95:THR:CB	1.75	1.64
1:A:189:ILE:CG2	1:A:189:ILE:CB	1.75	1.63
1:A:49:ALA:CA	1:A:49:ALA:CB	1.75	1.63
1:A:194:LEU:CB	1:A:194:LEU:CA	1.77	1.63
1:A:45:VAL:CB	1:A:45:VAL:CA	1.74	1.62

All (2) 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)
4:A:418:HOH:O	4:A:495:HOH:O[7_555]	0.57	1.63
4:A:410:HOH:O	4:A:497:HOH:O[7_555]	0.94	1.26

## 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	188/210 (90%)	177 (94%)	7 (4%)	4 (2%)	5 1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	25	LYS
1	A	2	GLU
1	A	4	ARG

### 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	154/183 (84%)	150 (97%)	4 (3%)	40 33

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	83	THR
1	A	115	ILE
1	A	203	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	142	HIS
1	A	167	HIS
1	A	203	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](#)

8 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	SO4	A	301	-	4,4,4	1.35	1 (25%)	6,6,6	1.57	2 (33%)
3	GOL	A	307	-	5,5,5	5.27	4 (80%)	5,5,5	1.30	1 (20%)
2	SO4	A	303	-	4,4,4	4.65	3 (75%)	6,6,6	1.77	2 (33%)
3	GOL	A	308	-	5,5,5	5.65	4 (80%)	5,5,5	1.92	2 (40%)
3	GOL	A	305	-	5,5,5	3.69	2 (40%)	5,5,5	2.29	3 (60%)
3	GOL	A	306	-	5,5,5	9.26	3 (60%)	5,5,5	4.34	5 (100%)
3	GOL	A	304	-	5,5,5	5.60	5 (100%)	5,5,5	3.24	3 (60%)
2	SO4	A	302	-	4,4,4	2.04	2 (50%)	6,6,6	3.68	4 (66%)

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
3	GOL	A	307	-	-	2/4/4/4	-
3	GOL	A	308	-	-	2/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	A	306	-	-	0/4/4/4	-
3	GOL	A	304	-	-	2/4/4/4	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	306	GOL	C3-C2	18.65	2.22	1.51
3	A	307	GOL	O2-C2	9.21	1.70	1.43
3	A	308	GOL	C3-C2	7.61	1.80	1.51
2	A	303	SO4	O2-S	7.47	1.89	1.44
3	A	305	GOL	O1-C1	7.06	1.72	1.42

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	SO4	O3-S-O2	-6.89	73.56	109.56
3	A	306	GOL	O3-C3-C2	-6.54	80.95	110.38
3	A	304	GOL	C3-C2-C1	4.87	129.65	111.80
3	A	304	GOL	O1-C1-C2	-4.72	89.12	110.38
3	A	306	GOL	C3-C2-C1	-4.17	96.49	111.80

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	307	GOL	O1-C1-C2-C3
3	A	308	GOL	O1-C1-C2-C3
3	A	305	GOL	O1-C1-C2-C3
3	A	305	GOL	O1-C1-C2-O2
3	A	307	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	307	GOL	4	0
3	A	308	GOL	5	0
3	A	305	GOL	7	0
3	A	306	GOL	5	0
3	A	304	GOL	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	12

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	23:ASP	C	24:ASP	N	2.09
1	A	24:ASP	C	25:LYS	N	1.94
1	A	74:VAL	C	75:GLU	N	1.61
1	A	2:GLU	C	3:TYR	N	1.60
1	A	176:ASP	C	177:LEU	N	1.60

## 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	195/210 (92%)	-0.39	5 (2%) 57 64	14, 29, 48, 76	6 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	ASP	4.0
1	A	24	ASP	3.2
1	A	114	ASP	2.8
1	A	3	TYR	2.1
1	A	75	GLU	2.0

### 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(Å <sup>2</sup> )	Q<0.9
2	SO4	A	303	5/5	0.58	0.13	128,132,150,159	0
3	GOL	A	306	6/6	0.76	0.18	65,72,81,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	307	6/6	0.84	0.15	60,65,78,79	0
3	GOL	A	304	6/6	0.89	0.15	46,48,55,56	0
2	SO4	A	302	5/5	0.91	0.10	67,74,87,91	0
3	GOL	A	305	6/6	0.91	0.13	38,49,55,60	0
3	GOL	A	308	6/6	0.91	0.11	50,53,63,77	0
2	SO4	A	301	5/5	0.98	0.05	38,45,49,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.