



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2024 – 12:06 AM EDT

PDB ID : 8GD8  
Title : Porous framework formed by assembly of a bipyridyl-conjugated helical peptide  
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Deposited on : 2023-03-03  
Resolution : 1.04 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

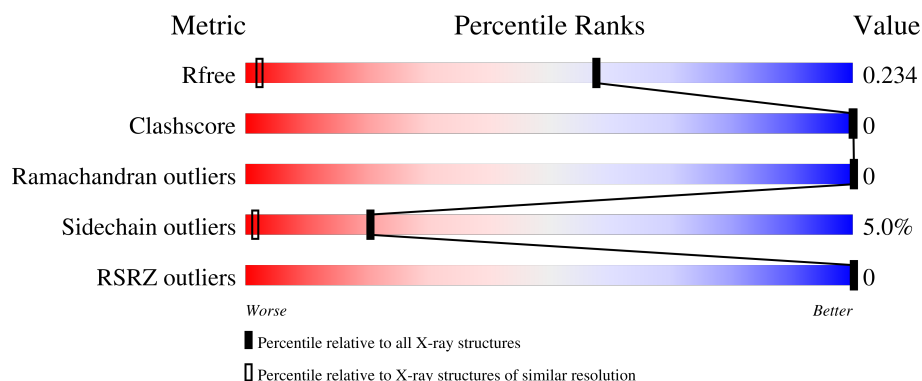
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.04 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	1633 (1.08-1.00)
Clashscore	180529	1019 (1.06-1.02)
Ramachandran outliers	177936	1780 (1.08-1.00)
Sidechain outliers	177891	1781 (1.08-1.00)
RSRZ outliers	164620	1632 (1.08-1.00)

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	11	 100%
1	B	11	 91% 9%
1	C	11	 100%
1	D	11	 100%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 742 atoms, of which 352 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 bipyridyl-conjugated helical peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	11	Total	C	H	N	O	S	0	1	0
			183	62	88	17	14	2			
1	B	11	Total	C	H	N	O	S	0	1	0
			183	62	88	17	14	2			
1	C	11	Total	C	H	N	O	S	0	1	0
			183	62	88	17	14	2			
1	D	11	Total	C	H	N	O	S	0	1	0
			183	62	88	17	14	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	1	Total	O	0	0
			1	1		
2	C	2	Total	O	0	0
			2	2		
2	D	3	Total	O	0	0
			3	3		

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- Molecule 1: bipyridyl-conjugated helical peptide

100%

- Molecule 1: bipyridyl-conjugated helical peptide

91%

9%



- Molecule 1: bipyridyl-conjugated helical peptide

100%

- Molecule 1: bipyridyl-conjugated helical peptide

100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	8.79Å 16.59Å 51.15Å 89.99° 89.97° 90.01°	Depositor
Resolution (Å)	16.59 – 1.04 16.59 – 1.04	Depositor EDS
% Data completeness (in resolution range)	79.7 (16.59-1.04) 81.1 (16.59-1.04)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.82 (at 0.83Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.206 , 0.231 0.206 , 0.234	Depositor DCC
$R_{free}$ test set	10208 reflections (9.43%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	5.1	Xtriage
Anisotropy	0.940	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.64 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l 0.438 for -h,k,-l 0.436 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9241e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NIO, AIB, I77

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	0.39	0/49	0.77	0/65
1	B	0.44	0/49	0.65	0/65
1	C	0.36	0/49	0.71	0/65
1	D	0.37	0/49	0.81	0/65
All	All	0.39	0/196	0.74	0/260

There are no bond length outliers.

There are no bond angle outliers.

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	95	88	79	0	0
1	B	95	88	79	0	0
1	C	95	88	79	0	0
1	D	95	88	79	0	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
All	All	390	352	316	0	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 0.

There are no clashes within the asymmetric unit.

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	5/11 (46%)	5 (100%)	0	0	100	100
1	B	5/11 (46%)	5 (100%)	0	0	100	100
1	C	5/11 (46%)	5 (100%)	0	0	100	100
1	D	5/11 (46%)	5 (100%)	0	0	100	100
All	All	20/44 (46%)	20 (100%)	0	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	6/5 (120%)	6 (100%)	0	100	100
1	B	6/5 (120%)	4 (67%)	2 (33%)	0	0
1	C	6/5 (120%)	6 (100%)	0	100	100
1	D	6/5 (120%)	6 (100%)	0	100	100
All	All	24/20 (120%)	22 (92%)	2 (8%)	20	0

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

Mol	Chain	Res	Type
1	B	5[A]	CYS
1	B	5[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	AIB	D	9	1	1,5,6	1.10	0	0,7,9	-	-
1	AIB	C	9	1	1,5,6	1.24	0	0,7,9	-	-
1	AIB	C	7	1	1,5,6	1.03	0	0,7,9	-	-
1	AIB	A	3	1	1,5,6	1.07	0	0,7,9	-	-
1	AIB	B	7	1	1,5,6	1.04	0	0,7,9	-	-
1	AIB	A	7	1	1,5,6	1.23	0	0,7,9	-	-
1	AIB	B	9	1	1,5,6	0.94	0	0,7,9	-	-
1	AIB	C	3	1	1,5,6	0.78	0	0,7,9	-	-
1	AIB	D	3	1	1,5,6	0.79	0	0,7,9	-	-
1	AIB	B	3	1	1,5,6	0.71	0	0,7,9	-	-
1	AIB	D	7	1	1,5,6	1.36	0	0,7,9	-	-
1	AIB	A	9	1	1,5,6	1.13	0	0,7,9	-	-

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
1	AIB	D	9	1	-	0/2/3/6	-
1	AIB	C	9	1	-	0/2/3/6	-
1	AIB	C	7	1	-	0/2/3/6	-
1	AIB	A	3	1	-	0/2/3/6	-
1	AIB	B	7	1	-	0/2/3/6	-
1	AIB	A	7	1	-	0/2/3/6	-
1	AIB	B	9	1	-	0/2/3/6	-
1	AIB	C	3	1	-	0/2/3/6	-
1	AIB	D	3	1	-	0/2/3/6	-
1	AIB	B	3	1	-	0/2/3/6	-
1	AIB	D	7	1	-	0/2/3/6	-
1	AIB	A	9	1	-	0/2/3/6	-

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.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	6/11 (54%)	-1.23	0 100 100	4, 7, 8, 11	1 (16%)
1	B	6/11 (54%)	-1.27	0 100 100	4, 7, 7, 11	1 (16%)
1	C	6/11 (54%)	-1.18	0 100 100	4, 7, 8, 11	1 (16%)
1	D	6/11 (54%)	-1.20	0 100 100	4, 8, 8, 12	1 (16%)
All	All	24/44 (54%)	-1.22	0 100 100	4, 7, 11, 12	4 (16%)

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	AIB	D	3	6/7	0.99	0.02	4,6,7,7	0
1	AIB	A	9	6/7	0.99	0.02	4,6,8,8	0
1	AIB	C	3	6/7	1.00	0.02	5,6,7,7	0
1	AIB	A	3	6/7	1.00	0.02	4,6,7,7	0
1	AIB	A	7	6/7	1.00	0.02	4,6,8,8	0
1	AIB	B	7	6/7	1.00	0.01	4,7,9,9	0
1	AIB	C	7	6/7	1.00	0.02	5,6,8,8	0
1	AIB	D	7	6/7	1.00	0.02	5,6,7,7	0
1	AIB	B	3	6/7	1.00	0.02	5,6,7,7	0
1	AIB	B	9	6/7	1.00	0.02	4,6,7,7	0
1	AIB	C	9	6/7	1.00	0.03	4,6,10,10	0
1	AIB	D	9	6/7	1.00	0.02	4,6,7,7	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.