



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2025 – 04:46 PM EST

PDB ID : 9DPY  
Title : BMP-10 with BMP-9 Crystal Contacts  
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Deposited on : 2024-09-23  
Resolution : 1.77 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

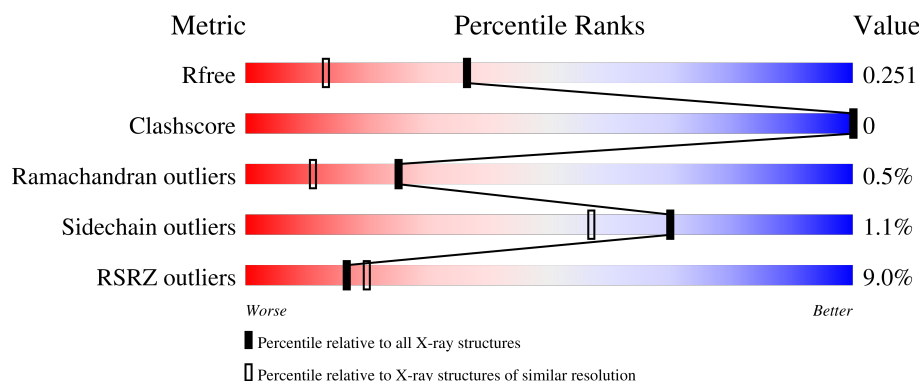
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	108	<div> <div>9%</div> <div>95%</div> <div>..</div> </div>
1	B	108	<div> <div>8%</div> <div>96%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3538 atoms, of which 1663 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 Bone morphogenetic protein 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	105	Total	C	H	N	O	S	0	0	0
			1663	540	831	136	148	8			
1	B	105	Total	C	H	N	O	S	0	0	0
			1664	540	832	136	148	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	GLY	-	expression tag	UNP O95393
A	318	ASP	-	expression tag	UNP O95393
A	319	ASP	-	expression tag	UNP O95393
A	357	PHE	ASN	engineered mutation	UNP O95393
A	358	PHE	TYR	engineered mutation	UNP O95393
A	374	THR	ALA	engineered mutation	UNP O95393
A	409	LEU	TYR	engineered mutation	UNP O95393
A	411	TYR	PHE	engineered mutation	UNP O95393
B	317	GLY	-	expression tag	UNP O95393
B	318	ASP	-	expression tag	UNP O95393
B	319	ASP	-	expression tag	UNP O95393
B	357	PHE	ASN	engineered mutation	UNP O95393
B	358	PHE	TYR	engineered mutation	UNP O95393
B	374	THR	ALA	engineered mutation	UNP O95393
B	409	LEU	TYR	engineered mutation	UNP O95393
B	411	TYR	PHE	engineered mutation	UNP O95393

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0

- Molecule 4 is water.

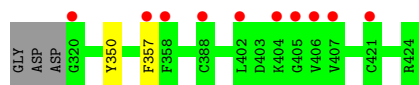
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total 68	O 68	0	0
4	B	76	Total 76	O 76	0	0

### 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.

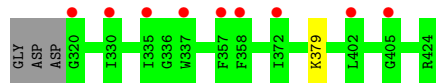
- Molecule 1: Bone morphogenetic protein 10

Chain A: 9% 95%



- Molecule 1: Bone morphogenetic protein 10

Chain B: 8% 96%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.75Å 123.04Å 120.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.52 – 1.77 61.52 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.3 (61.52-1.77) 98.5 (61.52-1.77)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.214 , 0.251 0.214 , 0.251	Depositor DCC
$R_{free}$ test set	29025 reflections (6.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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: NA, PO4

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	0.40	0/855	0.60	0/1158
1	B	0.43	0/855	0.59	0/1158
All	All	0.42	0/1710	0.59	0/2316

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

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	832	831	831	0	0
1	B	832	832	831	0	0
2	A	30	0	0	0	0
2	B	35	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	68	0	0	0	0
4	B	76	0	0	0	0
All	All	1875	1663	1662	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 [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	103/108 (95%)	101 (98%)	1 (1%)	1 (1%)	13	3
1	B	103/108 (95%)	101 (98%)	2 (2%)	0	100	100
All	All	206/216 (95%)	202 (98%)	3 (2%)	1 (0%)	25	11

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	TYR

### 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	91/93 (98%)	90 (99%)	1 (1%)	70	57
1	B	91/93 (98%)	90 (99%)	1 (1%)	70	57
All	All	182/186 (98%)	180 (99%)	2 (1%)	70	57

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

Mol	Chain	Res	Type
1	A	357	PHE

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Mol	Chain	Res	Type
1	B	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN
1	B	382	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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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	PO4	A	506	-	4,4,4	0.89	0	6,6,6	0.57	0
2	PO4	A	503	-	4,4,4	1.04	0	6,6,6	0.60	0
2	PO4	A	504	-	4,4,4	0.94	0	6,6,6	0.35	0
2	PO4	B	502	-	4,4,4	0.70	0	6,6,6	0.66	0
2	PO4	A	501	-	4,4,4	1.69	1 (25%)	6,6,6	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	A	502	-	4,4,4	0.94	0	6,6,6	0.35	0
2	PO4	B	505	-	4,4,4	0.94	0	6,6,6	0.53	0
2	PO4	A	505	-	4,4,4	0.71	0	6,6,6	0.60	0
2	PO4	B	503	-	4,4,4	0.92	0	6,6,6	0.51	0
2	PO4	B	501	-	4,4,4	0.90	0	6,6,6	1.07	0
2	PO4	B	506	-	4,4,4	1.00	0	6,6,6	0.45	0
2	PO4	B	507	-	4,4,4	1.03	0	6,6,6	0.89	0
2	PO4	B	504	-	4,4,4	0.83	0	6,6,6	0.66	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PO4	P-O4	-2.91	1.46	1.54

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 [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	105/108 (97%)	0.62	10 (9%) 15 18	46, 61, 110, 169	0
1	B	105/108 (97%)	0.56	9 (8%) 18 20	42, 60, 94, 130	0
All	All	210/216 (97%)	0.59	19 (9%) 17 20	42, 61, 106, 169	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	GLY	4.4
1	B	320	GLY	3.5
1	A	358	PHE	3.1
1	A	405	GLY	3.0
1	A	388	CYS	2.7
1	B	405	GLY	2.7
1	B	372	ILE	2.7
1	A	406	VAL	2.6
1	B	335	ILE	2.5
1	A	357	PHE	2.5
1	B	357	PHE	2.3
1	B	358	PHE	2.3
1	B	337	TRP	2.3
1	B	402	LEU	2.3
1	B	330	ILE	2.3
1	A	402	LEU	2.2
1	A	421	CYS	2.1
1	A	407	VAL	2.0
1	A	404	LYS	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 monosaccharides 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	PO4	A	504	5/5	0.68	0.21	59,59,59,59	5
3	NA	B	508	1/1	0.70	0.29	93,93,93,93	0
2	PO4	B	505	5/5	0.77	0.24	63,63,63,64	5
2	PO4	A	502	5/5	0.77	0.12	68,68,68,69	5
2	PO4	A	505	5/5	0.80	0.21	61,61,61,61	5
2	PO4	B	503	5/5	0.81	0.14	63,63,63,63	5
2	PO4	A	506	5/5	0.83	0.23	64,64,64,64	5
2	PO4	B	504	5/5	0.85	0.16	69,69,69,69	5
3	NA	A	507	1/1	0.89	0.13	77,77,77,77	0
2	PO4	A	503	5/5	0.89	0.18	59,59,59,59	5
2	PO4	B	506	5/5	0.90	0.18	58,59,59,59	5
2	PO4	A	501	5/5	0.91	0.14	60,60,60,61	5
2	PO4	B	502	5/5	0.94	0.15	55,55,55,55	5
2	PO4	B	507	5/5	0.96	0.15	61,61,61,61	5
2	PO4	B	501	5/5	0.99	0.05	47,47,47,47	5

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

There are no such residues in this entry.