



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2022 – 02:45 pm BST

PDB ID : 7PPA  
Title : High resolution structure of bone morphogenetic protein receptor type II (BMPRII) extracellular domain in complex with BMP10  
Authors : Guo, J.; Yu, M.; Read, R.J.; Li, W.  
Deposited on : 2021-09-13  
Resolution : 1.48 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.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

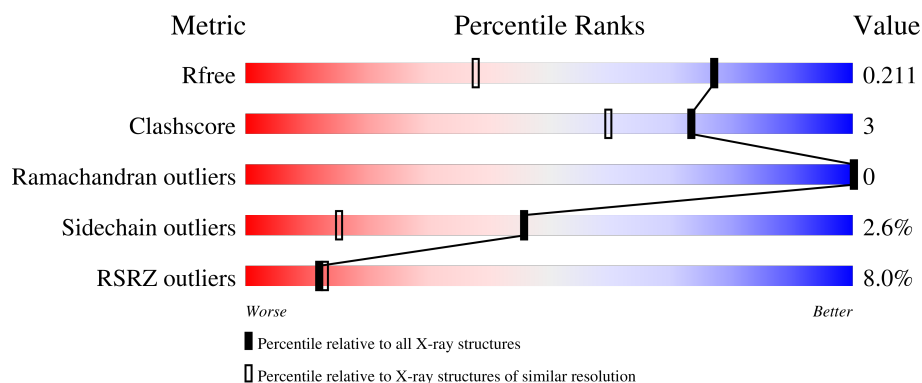
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 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))
$R_{free}$	130704	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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>85%</div> <div>11%</div> <div>.</div> </div>
1	B	108	<div> <div>86%</div> <div>10%</div> <div>..</div> </div>
2	C	125	<div> <div>4%</div> <div>71%</div> <div>10%</div> <div>..</div> <div>16%</div> </div>
2	D	125	<div> <div>22%</div> <div>74%</div> <div>.</div> <div>22%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6812 atoms, of which 3167 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	104	Total	C	H	N	O	S	26	6	0
			1747	564	875	142	157	9			
1	B	105	Total	C	H	N	O	S	26	1	0
			1667	539	833	137	149	9			

- Molecule 2 is a protein called Bone morphogenetic protein receptor type-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	105	Total	C	H	N	O	S	33	10	0
			1719	547	832	152	178	10			
2	D	98	Total	C	H	N	O	S	37	1	0
			1313	430	619	118	136	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	26	GLY	-	expression tag	UNP Q13873
D	26	GLY	-	expression tag	UNP Q13873

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	2	0
			14	3	8	3		

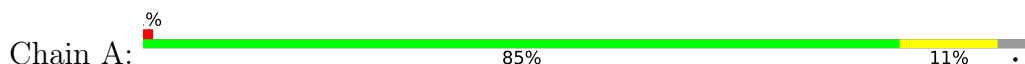
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	84	Total	O	0	0
			84	84		
4	C	133	Total	O	0	0
			133	133		
4	D	22	Total	O	0	0
			22	22		

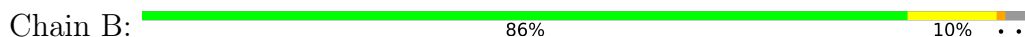
### 3 Residue-property plots [i](#)

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



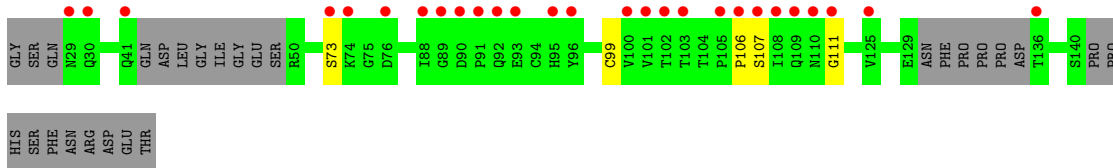
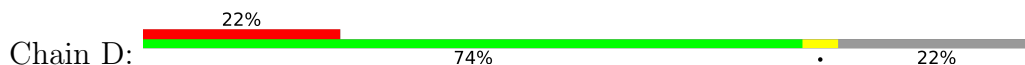
- Molecule 1: Bone morphogenetic protein 10



- Molecule 2: Bone morphogenetic protein receptor type-2



- Molecule 2: Bone morphogenetic protein receptor type-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.72Å 47.23Å 250.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.04 – 1.48 125.04 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (125.04-1.48) 99.9 (125.04-1.48)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.165 , 0.207 0.168 , 0.211	Depositor DCC
$R_{free}$ test set	4383 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.21% 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: 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	0.90	2/898 (0.2%)	1.00	2/1216 (0.2%)
1	B	0.82	1/860 (0.1%)	0.94	1/1165 (0.1%)
2	C	1.03	3/908 (0.3%)	1.11	5/1234 (0.4%)
2	D	0.67	0/707	0.74	0/960
All	All	0.87	6/3373 (0.2%)	0.97	8/4575 (0.2%)

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
2	C	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	140	SER	C-O	8.93	1.40	1.23
1	A	351	GLU	CD-OE1	-6.08	1.19	1.25
2	C	31	GLU	CD-OE2	5.91	1.32	1.25
2	C	129	GLU	CD-OE2	-5.51	1.19	1.25
1	B	320	GLY	C-O	5.29	1.32	1.23
1	A	405	GLY	C-O	5.16	1.31	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	32	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	424	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	408	THR	CA-CB-CG2	-6.12	103.83	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	96	TYR	CB-CG-CD2	5.70	124.42	121.00
1	A	347	TYR	CB-CG-CD2	-5.62	117.62	121.00
2	C	38	ASP	CB-CG-OD1	-5.57	113.28	118.30
2	C	32	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	C	135	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	135	ASP	Sidechain

## 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	872	875	866	8	0
1	B	834	833	829	7	0
2	C	887	832	817	9	0
2	D	694	619	583	1	0
3	C	6	8	8	0	0
4	A	113	0	0	2	0
4	B	84	0	0	0	0
4	C	133	0	0	1	0
4	D	22	0	0	0	0
All	All	3645	3167	3103	21	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 3.

All (21) 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:338[B]:ASP:OD2	4:A:501:HOH:O	2.00	0.79
4:A:539:HOH:O	2:C:108[B]:ILE:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342[B]:ILE:HD11	1:A:402:LEU:HG	1.72	0.71
1:A:333[A]:LYS:HG3	1:A:338[A]:ASP:OD2	1.94	0.67
1:B:331:ASP:HB3	1:B:334:GLU:HG3	1.87	0.57
1:A:348[B]:GLU:HG3	1:A:350:TYR:CE2	2.39	0.57
2:C:139:LEU:O	2:C:140:SER:HB2	2.05	0.56
1:B:378:LEU:C	1:B:378:LEU:HD23	2.26	0.55
2:C:137:THR:HB	2:C:138:PRO:HD2	1.91	0.52
1:A:339:SER:HA	2:C:108[B]:ILE:HG21	1.92	0.51
2:C:31:GLU:HB3	2:C:59:LEU:HD11	1.92	0.50
2:D:106:PRO:O	2:D:111:GLY:HA2	2.13	0.49
1:A:333[A]:LYS:NZ	2:C:104:THR:HB	2.28	0.48
2:C:50:ARG:NH2	4:C:305:HOH:O	2.46	0.48
1:B:364:LEU:HD13	1:B:423:CYS:SG	2.54	0.47
1:B:326:THR:HB	1:B:327:PRO:HD2	1.97	0.45
1:A:402:LEU:HD12	2:C:108[B]:ILE:HD12	1.99	0.44
1:B:378:LEU:HD23	1:B:378:LEU:O	2.18	0.43
1:B:378:LEU:C	1:B:378:LEU:CD2	2.87	0.43
1:B:320:GLY:HA3	1:B:322:TYR:CZ	2.56	0.41
1:A:339:SER:HA	2:C:108[B]:ILE:CG2	2.51	0.40

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	108/108 (100%)	106 (98%)	2 (2%)	0	100	100
1	B	104/108 (96%)	103 (99%)	1 (1%)	0	100	100
2	C	111/125 (89%)	106 (96%)	5 (4%)	0	100	100
2	D	92/125 (74%)	89 (97%)	3 (3%)	0	100	100
All	All	415/466 (89%)	404 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	96/92 (104%)	95 (99%)	1 (1%)	76	54
1	B	91/92 (99%)	89 (98%)	2 (2%)	52	20
2	C	106/114 (93%)	103 (97%)	3 (3%)	43	13
2	D	70/114 (61%)	67 (96%)	3 (4%)	29	5
All	All	363/412 (88%)	354 (98%)	9 (2%)	46	16

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	GLU
1	B	324	LYS
1	B	385	SER
2	C	99	CYS
2	C	121	ASP
2	C	140	SER
2	D	73	SER
2	D	99	CYS
2	D	107	SER

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

Mol	Chain	Res	Type
2	C	130	ASN
2	D	41	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	C	201	-	5,5,5	0.13	0	5,5,5	0.32	0

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	C	201	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	201	GOL	O1-C1-C2-C3
3	C	201	GOL	C1-C2-C3-O3
3	C	201	GOL	O1-C1-C2-O2
3	C	201	GOL	O2-C2-C3-O3

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

### 6.1 Protein, DNA and RNA chains

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	104/108 (96%)	0.02	1 (0%) 82 84	12, 24, 62, 80	0
1	B	105/108 (97%)	-0.04	0 100 100	13, 34, 68, 98	0
2	C	105/125 (84%)	0.28	5 (4%) 30 33	12, 19, 79, 145	0
2	D	98/125 (78%)	1.45	27 (27%) 0 0	27, 54, 99, 135	0
All	All	412/466 (88%)	0.41	33 (8%) 12 13	12, 31, 85, 145	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	90	ASP	9.4
2	D	92	GLN	7.6
2	D	105	PRO	6.4
2	D	110	ASN	6.3
2	D	107	SER	4.8
2	D	102	THR	4.8
2	D	93	GLU	4.7
2	D	100	VAL	4.6
2	D	89	GLY	4.6
2	D	88	ILE	4.3
2	D	108	ILE	4.2
2	C	136	THR	3.7
2	D	106	PRO	3.7
2	C	133	PRO	3.4
2	D	95	HIS	3.3
2	C	134	PRO	2.9
2	D	111	GLY	2.8
2	D	73	SER	2.8
2	D	101	VAL	2.7
2	C	135	ASP	2.7
2	D	29	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	74	LYS	2.6
2	D	109	GLN	2.6
2	D	96	TYR	2.6
2	D	91	PRO	2.5
1	A	382	GLN	2.3
2	D	76	ASP	2.3
2	C	50	ARG	2.3
2	D	125	VAL	2.2
2	D	103	THR	2.2
2	D	136	THR	2.1
2	D	41	GLN	2.1
2	D	30	GLN	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(Å <sup>2</sup> )	Q<0.9
3	GOL	C	201	6/6	0.75	0.13	56,59,69,69	2

## 6.5 Other polymers [i](#)

There are no such residues in this entry.