



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 12:03 am BST

PDB ID : 1TJR  
Title : Crystal structure of wild-type BX1 complexed with a sulfate ion  
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Deposited on : 2004-06-07  
Resolution : 2.30 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

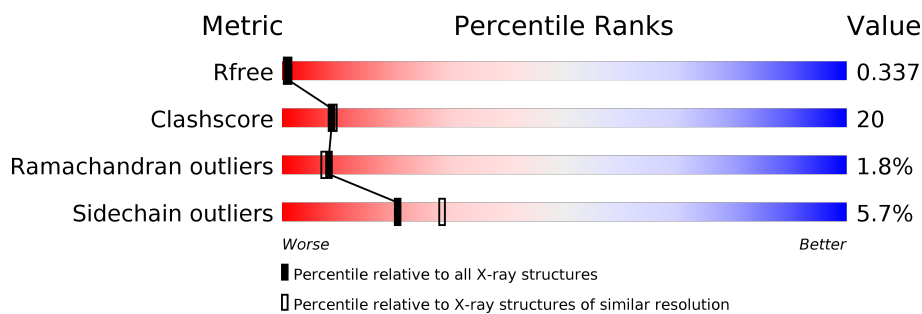
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 on 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3819 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 BX1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	Se	0	0	0
			1924	1217	329	366	3	9			
1	B	255	Total	C	N	O	S	Se	0	0	0
			1812	1152	301	347	3	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	97	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	163	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	169	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	191	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	198	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	243	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	317	MSE	MET	MODIFIED RESIDUE	UNP P42390
A	341	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	93	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	97	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	163	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	169	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	191	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	198	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	243	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	317	MSE	MET	MODIFIED RESIDUE	UNP P42390
B	341	MSE	MET	MODIFIED RESIDUE	UNP P42390

- Molecule 2 is SULFATE ION (three-letter code: 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	B	1	Total	O	S	0	0
			5	4	1		

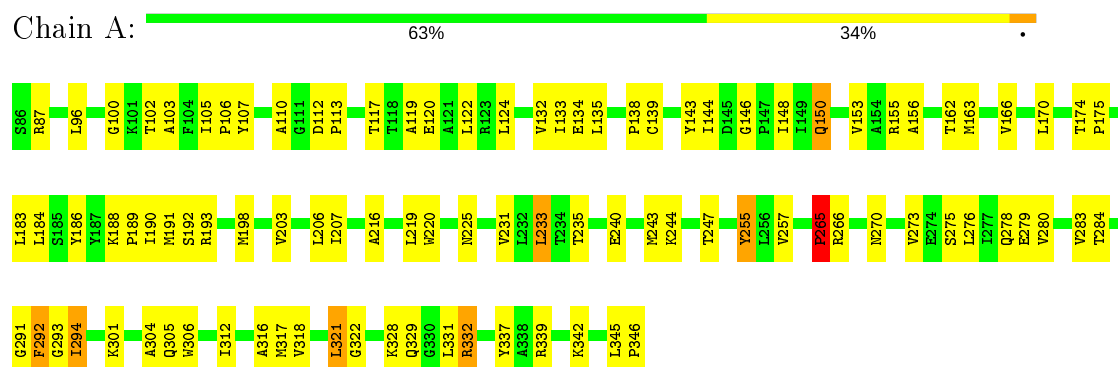
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	23	Total	O	0	0
			23	23		

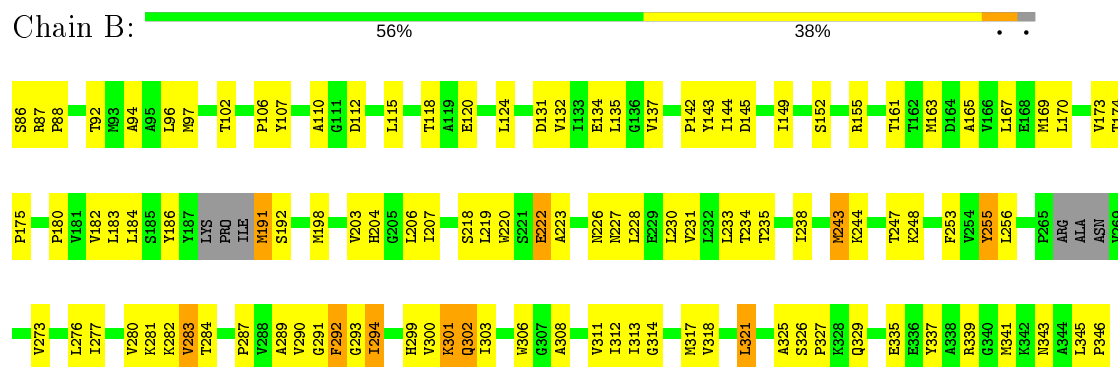
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: BX1



#### • Molecule 1: BX1



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.00 Å   123.00 Å   98.80 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	19.72 – 2.30 19.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.72-2.30) 99.6 (19.73-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.19 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.285   ,   0.338 0.286   ,   0.337	Depositor DCC
$R_{free}$ test set	2726 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 9.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.287 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0/1950	0.62	0/2642
1	B	0.38	0/1836	0.60	0/2496
All	All	0.39	0/3786	0.61	0/5138

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	1924	0	1951	70	0
1	B	1812	0	1783	83	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	50	0	0	5	0
3	B	23	0	0	1	0
All	All	3819	0	3734	153	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 20.

The worst 5 of 153 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:B:124:LEU:HD11	1:B:335:GLU:HG3	1.45	0.98
1:B:124:LEU:HD21	1:B:335:GLU:HB2	1.53	0.90
1:A:244:LYS:O	1:A:247:THR:HG22	1.71	0.89
1:B:198:MSE:HE3	1:B:203:VAL:HG11	1.65	0.79
1:B:290:VAL:HG21	1:B:303:ILE:HG21	1.65	0.77

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	259/261 (99%)	233 (90%)	22 (8%)	4 (2%)	10	10
1	B	249/261 (95%)	220 (88%)	24 (10%)	5 (2%)	7	6
All	All	508/522 (97%)	453 (89%)	46 (9%)	9 (2%)	8	7

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	PRO
1	A	294	ILE
1	B	143	TYR
1	B	294	ILE
1	B	282	LYS

### 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	204/202 (101%)	195 (96%)	9 (4%)	28	39
1	B	184/202 (91%)	171 (93%)	13 (7%)	14	19
All	All	388/404 (96%)	366 (94%)	22 (6%)	20	28

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ARG
1	B	191	MSE
1	B	321	LEU
1	B	118	THR
1	B	120	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	B	343	ASN
1	B	225	ASN
1	A	204	HIS
1	B	226	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	B	347	-	4,4,4	2.43	2 (50%)	6,6,6	0.90	0
2	SO4	A	347	-	4,4,4	2.17	2 (50%)	6,6,6	0.81	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	347	SO4	O2-S	4.23	1.69	1.46
2	A	347	SO4	O2-S	3.80	1.66	1.46
2	B	347	SO4	O3-S	2.39	1.67	1.47
2	A	347	SO4	O3-S	2.07	1.64	1.47

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.