



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 06:53 PM EDT

PDB ID : 3HZB  
Title : Crystal structure of a betagamma-crystallin domain from *Flavobacterium johnsoniae*  
Authors : Aravind, P.; Sankaranarayanan, R.  
Deposited on : unknown  
Resolution : 1.74 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	<b>FAILED</b>
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

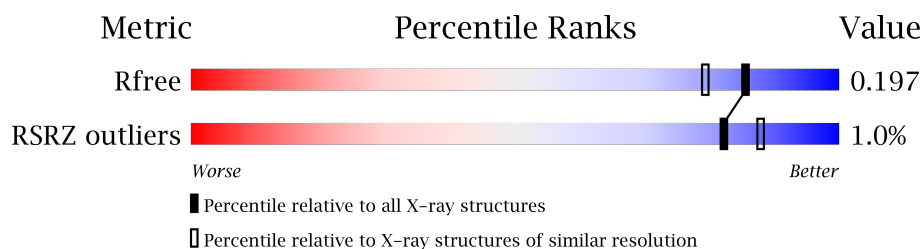
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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))
$R_{free}$	100719	2694 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6301 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 Carbohydrate binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	0	0
			655	406	110	137	2			
1	B	87	Total	C	N	O	S	0	0	0
			663	410	112	139	2			
1	C	88	Total	C	N	O	S	0	0	0
			667	412	113	140	2			
1	D	90	Total	C	N	O	S	0	0	0
			682	420	115	145	2			
1	E	90	Total	C	N	O	S	0	0	0
			682	420	115	145	2			
1	F	88	Total	C	N	O	S	0	0	0
			667	412	113	140	2			
1	G	87	Total	C	N	O	S	0	0	0
			663	410	112	139	2			
1	H	87	Total	C	N	O	S	0	0	0
			663	410	112	139	2			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Ca	0	0
			3	3		
2	D	2	Total	Ca	0	0
			2	2		
2	E	3	Total	Ca	0	0
			3	3		
2	H	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		
2	C	3	Total	Ca	0	0
			3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Ca 3	0	0
2	F	2	Total 2	Ca 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	114	Total 114	O 114	0	0
3	C	131	Total 131	O 131	0	0
3	D	128	Total 128	O 128	0	0
3	E	112	Total 112	O 112	0	0
3	F	116	Total 116	O 116	0	0
3	G	105	Total 105	O 105	0	0
3	H	112	Total 112	O 112	0	0

MolProbity failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.65Å 99.28Å 64.10Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	30.00 – 1.74 16.02 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-1.74) 99.3 (16.02-1.73)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 1.73Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.192 , 0.223 0.194 , 0.197	Depositor DCC
$R_{free}$ test set	3467 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6301	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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 77.46 % 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 8.4735e-07. 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.

## 4 Model quality [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 4.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

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.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 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	86/90 (95%)	-0.22	0 100 100	11, 16, 25, 32	0
1	B	87/90 (96%)	-0.24	0 100 100	11, 16, 23, 37	0
1	C	88/90 (97%)	-0.10	2 (2%) 61 68	9, 15, 26, 48	0
1	D	90/90 (100%)	-0.24	0 100 100	12, 15, 22, 36	0
1	E	90/90 (100%)	-0.26	1 (1%) 80 86	12, 15, 23, 34	0
1	F	88/90 (97%)	-0.18	2 (2%) 61 68	9, 15, 24, 47	0
1	G	87/90 (96%)	-0.06	1 (1%) 80 86	11, 16, 23, 37	0
1	H	87/90 (96%)	-0.17	1 (1%) 80 86	10, 16, 26, 45	0
All	All	703/720 (97%)	-0.18	7 (0%) 82 88	9, 15, 25, 48	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	GLY	8.5
1	F	88	GLY	7.1
1	C	87	ASN	3.6
1	H	87	ASN	3.1
1	G	87	ASN	2.6
1	F	87	ASN	2.2
1	E	90	THR	2.1

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 5.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	107	1/1	1.00	0.07	-0.13	13,13,13,13	0
2	CA	H	115	1/1	1.00	0.07	-0.82	12,12,12,12	0
2	CA	H	116	1/1	0.99	0.06	-1.01	14,14,14,14	0
2	CA	A	101	1/1	1.00	0.07	-1.08	12,12,12,12	0
2	CA	F	113	1/1	1.00	0.06	-1.29	12,12,12,12	0
2	CA	C	118	1/1	0.99	0.03	-1.30	17,17,17,17	0
2	CA	E	119	1/1	0.99	0.04	-1.43	17,17,17,17	0
2	CA	D	105	1/1	1.00	0.06	-1.46	12,12,12,12	0
2	CA	E	109	1/1	1.00	0.05	-1.60	12,12,12,12	0
2	CA	A	102	1/1	0.99	0.05	-1.61	13,13,13,13	0
2	CA	A	117	1/1	1.00	0.02	-1.73	17,17,17,17	0
2	CA	C	103	1/1	1.00	0.07	-1.77	12,12,12,12	0
2	CA	G	120	1/1	1.00	0.03	-1.79	17,17,17,17	0
2	CA	G	111	1/1	0.99	0.05	-1.97	14,14,14,14	0
2	CA	F	114	1/1	0.99	0.05	-2.26	12,12,12,12	0
2	CA	C	104	1/1	0.99	0.05	-2.32	12,12,12,12	0
2	CA	E	110	1/1	0.99	0.05	-2.37	13,13,13,13	0
2	CA	B	108	1/1	0.99	0.04	-2.49	14,14,14,14	0
2	CA	G	112	1/1	1.00	0.04	-3.18	14,14,14,14	0
2	CA	D	106	1/1	0.99	0.04	-3.61	14,14,14,14	0

## 5.5 Other polymers [i](#)

There are no such residues in this entry.