wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 08:33 AM EDT

PDB ID	:	6NKQ
Title	:	The structure of bovine beta-lactoglobulin in novel crystals grown at pH 3.8
Authors	:	McPherson, A.
Deposited on	:	2019-01-07
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS 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 7617 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 Beta-lactoglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	160	Total	C	N	O	S	0	0	0
			1260	802	204	245	9			
1	C	159	Total	C	N	O	S	0	2	0
			1262	806	201	246	9			
1	D	159	Total	C	N	O	S	0	2	0
			1267	807	203	248	9			
1	E	159	Total	C	N	O	S	0	0	0
			1250	796	201	244	9			
1	F	159	Total	C	N	O	S	0	1	0
			1261	803	203	246	9			
1	A	158	Total	C	N	O	S	0	0	0
			1248	794	202	243	9			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	16	Total	O	0	0
			16	16		
3	C	12	Total	O	0	0
			12	12		
3	D	8	Total	O	0	1
			9	9		
3	E	7	Total	O	0	0
			7	7		
3	F	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0

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

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	65.89Å 114.12Å 140.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.06 – 2.30	Depositor
% Data completeness (in resolution range)	99.5 (57.06-2.30)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	4.16 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.207 , 0.261	Depositor
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.956	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.448 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.439 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.447 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.437 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.467 for -h,-k,l	Xtriage
Reported twinning fraction	0.162 for H, K, L 0.159 for -h,-k,l 0.164 for -1/2H-1/2K, 3/2H-1/2K, L 0.175 for 1/2H-1/2K, 3/2H+1/2K, L 0.158 for 1/2H+1/2K, -3/2H+1/2K, L 0.183 for -1/2H+1/2K, -3/2H-1/2K, L	Depositor
Outliers	1 of 49499 reflections (0.002%)	Xtriage
Total number of atoms	7617	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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