



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 01:16 AM EDT

PDB ID : 6V3P
Title : The B1gI domain of beta protein from *S. agalactiae* bound to CEACAM1
Authors : Bonsor, D.A.; McCarthy, A.J.
Deposited on : 2019-11-26
Resolution : 3.25 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

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>.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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 5 unique types of molecules in this entry. The entry contains 3349 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 Carcinoembryonic antigen-related cell adhesion molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	108	846	535	143	167	1	0	0	0
1	B	107	841	532	142	166	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P13688
B	-1	MET	-	initiating methionine	UNP P13688

- Molecule 2 is a protein called IgA FC receptor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	103	812	507	132	173	0	0	0
2	D	103	812	507	132	173	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

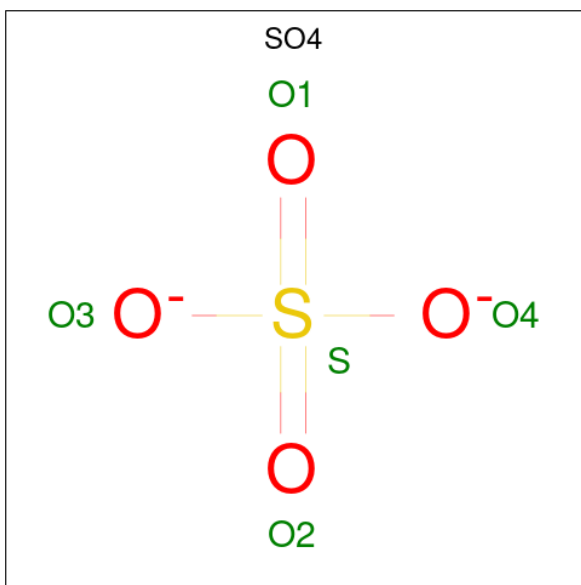
Chain	Residue	Modelled	Actual	Comment	Reference
C	113	LEU	-	expression tag	UNP P27951
C	114	PRO	-	expression tag	UNP P27951
C	115	SER	-	expression tag	UNP P27951
C	116	THR	-	expression tag	UNP P27951
C	117	GLY	-	expression tag	UNP P27951
C	118	GLY	-	expression tag	UNP P27951
C	119	SER	-	expression tag	UNP P27951
C	120	HIS	-	expression tag	UNP P27951
C	121	HIS	-	expression tag	UNP P27951
C	122	HIS	-	expression tag	UNP P27951

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Chain	Residue	Modelled	Actual	Comment	Reference
C	123	HIS	-	expression tag	UNP P27951
C	124	HIS	-	expression tag	UNP P27951
C	125	HIS	-	expression tag	UNP P27951
D	113	LEU	-	expression tag	UNP P27951
D	114	PRO	-	expression tag	UNP P27951
D	115	SER	-	expression tag	UNP P27951
D	116	THR	-	expression tag	UNP P27951
D	117	GLY	-	expression tag	UNP P27951
D	118	GLY	-	expression tag	UNP P27951
D	119	SER	-	expression tag	UNP P27951
D	120	HIS	-	expression tag	UNP P27951
D	121	HIS	-	expression tag	UNP P27951
D	122	HIS	-	expression tag	UNP P27951
D	123	HIS	-	expression tag	UNP P27951
D	124	HIS	-	expression tag	UNP P27951
D	125	HIS	-	expression tag	UNP P27951

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



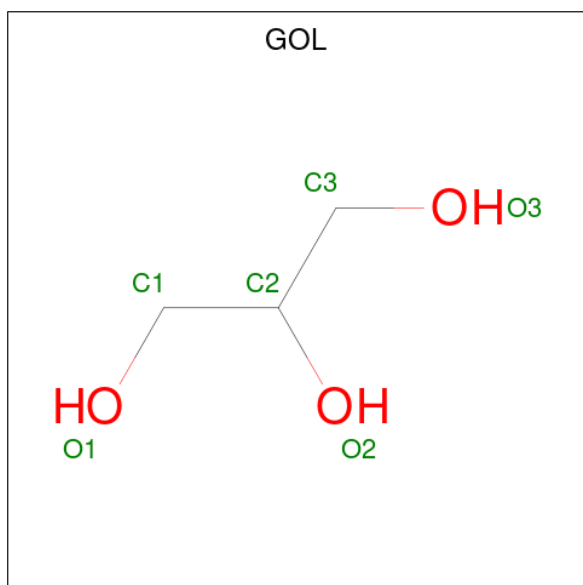
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O 1 1	0	0

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.62Å 131.62Å 257.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.95 – 3.25	Depositor
% Data completeness (in resolution range)	99.7 (38.95-3.25)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.218 , 0.244	Depositor
Wilson B-factor (Å ²)	126.9	Xtriage
Anisotropy	0.591	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3349	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 monosaccharides in this entry.

4.6 Ligand geometry [i](#)

7 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
3	SO4	D	201	-	4,4,4	0.37	0	6,6,6	0.06	0
3	SO4	A	203	-	4,4,4	0.40	0	6,6,6	0.06	0
4	GOL	A	204	-	5,5,5	0.11	0	5,5,5	0.37	0
3	SO4	A	202	-	4,4,4	0.38	0	6,6,6	0.05	0
3	SO4	B	201	-	4,4,4	0.39	0	6,6,6	0.04	0
4	GOL	A	205	-	5,5,5	0.13	0	5,5,5	0.38	0
3	SO4	A	201	-	4,4,4	0.37	0	6,6,6	0.06	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
4	GOL	A	204	-	-	2/4/4/4	-
4	GOL	A	205	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	205	GOL	C1-C2-C3-O3
4	A	204	GOL	O1-C1-C2-O2
4	A	204	GOL	O1-C1-C2-C3
4	A	205	GOL	O1-C1-C2-C3
4	A	205	GOL	O2-C2-C3-O3
4	A	205	GOL	O1-C1-C2-O2

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

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.