wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 04:16 AM EDT

PDB ID	:	6Q0S
Title	:	Crystal Structure of RSV strain B18537 Prefusion-stabilized glycoprotein F Variant DS-Cav1
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Deposited on	:	2019-08-02
Resolution	:	1.94 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
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 (i)

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

The reported resolution of this entry is 1.94 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 4 unique types of molecules in this entry. The entry contains 7442 atoms, of which 3590 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	F	454	7109	2237	3563	592	692	25	0	3	0

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	155	CYS	SER	engineered mutation	UNP P13843
F	190	PHE	SER	engineered mutation	UNP P13843
F	207	LEU	VAL	engineered mutation	UNP P13843
F	290	CYS	SER	engineered mutation	UNP P13843
F	514	SER	-	expression tag	UNP P13843
F	515	ALA	-	expression tag	UNP P13843
F	516	ILE	-	expression tag	UNP P13843
F	517	GLY	-	expression tag	UNP P13843
F	518	GLY	-	expression tag	UNP P13843
F	519	TYR	-	expression tag	UNP P13843
F	520	ILE	-	expression tag	UNP P13843
F	521	PRO	-	expression tag	UNP P13843
F	522	GLU	-	expression tag	UNP P13843
F	523	ALA	-	expression tag	UNP P13843
F	524	PRO	-	expression tag	UNP P13843
F	525	ARG	-	expression tag	UNP P13843
F	526	ASP	-	expression tag	UNP P13843
F	527	GLY	-	expression tag	UNP P13843
F	528	GLN	-	expression tag	UNP P13843
F	529	ALA	-	expression tag	UNP P13843
F	530	TYR	-	expression tag	UNP P13843
F	531	VAL	-	expression tag	UNP P13843
F	532	ARG	-	expression tag	UNP P13843
F	533	LYS	-	expression tag	UNP P13843
F	534	ASP	-	expression tag	UNP P13843
F	535	GLY	-	expression tag	UNP P13843
F	536	GLU	-	expression tag	UNP P13843

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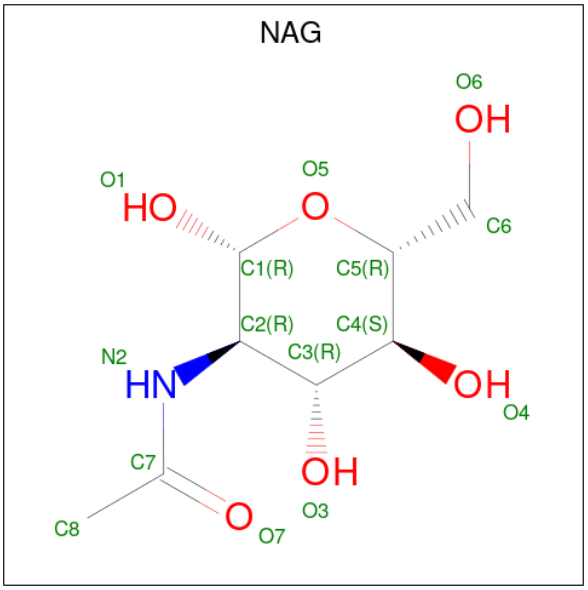
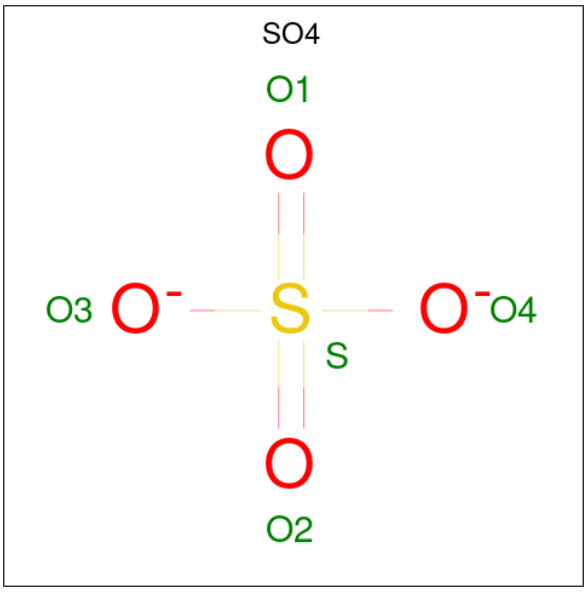
Chain	Residue	Modelled	Actual	Comment	Reference
F	537	TRP	-	expression tag	UNP P13843
F	538	VAL	-	expression tag	UNP P13843
F	539	LEU	-	expression tag	UNP P13843
F	540	LEU	-	expression tag	UNP P13843
F	541	SER	-	expression tag	UNP P13843
F	542	THR	-	expression tag	UNP P13843
F	543	PHE	-	expression tag	UNP P13843
F	544	LEU	-	expression tag	UNP P13843
F	545	GLY	-	expression tag	UNP P13843
F	546	GLY	-	expression tag	UNP P13843
F	547	LEU	-	expression tag	UNP P13843
F	548	VAL	-	expression tag	UNP P13843
F	549	PRO	-	expression tag	UNP P13843
F	550	ARG	-	expression tag	UNP P13843

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
2	F	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	263	Total O 263 263	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	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	167.87Å 167.87Å 167.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.27 – 1.94	Depositor
% Data completeness (in resolution range)	95.9 (34.27-1.94)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.187 , 0.212	Depositor
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7442	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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

5 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	F	604	-	4,4,4	0.26	0	6,6,6	0.37	0
3	SO4	F	605	-	4,4,4	0.14	0	6,6,6	0.18	0
2	NAG	F	601	-	14,14,15	0.65	1 (7%)	17,19,21	0.76	1 (5%)
3	SO4	F	603	-	4,4,4	0.17	0	6,6,6	1.05	0
2	NAG	F	602	1	14,14,15	0.47	0	17,19,21	0.80	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
2	NAG	F	601	-	-	2/6/23/26	0/1/1/1
2	NAG	F	602	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	NAG	O5-C1	2.28	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	NAG	C1-O5-C5	2.79	115.98	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	NAG	O5-C5-C6-O6
2	F	601	NAG	C4-C5-C6-O6

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.