WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 04:05 AM EDT

PDB ID	:	6VKD
Title	:	Crystal Structure of Inhibitor JNJ-36689282 in Complex with Prefusion RSV F Glycoprotein
Authors	:	McLellan, J.S.
Deposited on	:	2020-01-20
Resolution	:	2.50 Å(reported)

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 2.50 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 ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3558 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 Prefusion RSV F (DS-Cav1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	441	3411	2160	558	671	22	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	66	GLU	LYS	conflict	UNP W8RJF9
F	155	CYS	SER	conflict	UNP W8RJF9
F	190	PHE	SER	conflict	UNP W8RJF9
F	207	LEU	VAL	conflict	UNP W8RJF9
F	290	CYS	SER	conflict	UNP W8RJF9
F	514	SER	-	linker	UNP W8RJF9
F	515	ALA	-	linker	UNP W8RJF9
F	516	ILE	-	linker	UNP W8RJF9
F	517	GLY	-	linker	UNP W8RJF9
F	546	GLY	-	expression tag	UNP M1E1E4
F	547	LEU	-	expression tag	UNP M1E1E4
F	548	VAL	-	expression tag	UNP M1E1E4
F	549	PRO	-	expression tag	UNP M1E1E4
F	550	ARG	-	expression tag	UNP M1E1E4
F	551	GLY	-	expression tag	UNP M1E1E4
F	552	SER	-	expression tag	UNP M1E1E4
F	553	HIS	-	expression tag	UNP M1E1E4
F	554	HIS	-	expression tag	UNP M1E1E4
F	555	HIS	-	expression tag	UNP M1E1E4
F	556	HIS	-	expression tag	UNP M1E1E4
F	557	HIS	-	expression tag	UNP M1E1E4
F	558	HIS	-	expression tag	UNP M1E1E4
F	559	SER	-	expression tag	UNP M1E1E4
F	560	ALA	-	expression tag	UNP M1E1E4
F	561	TRP	-	expression tag	UNP M1E1E4
F	562	SER	-	expression tag	UNP M1E1E4
F	563	HIS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	564	PRO	-	expression tag	UNP M1E1E4
F	565	GLN	-	expression tag	UNP M1E1E4
F	566	PHE	-	expression tag	UNP M1E1E4
F	567	GLU	-	expression tag	UNP M1E1E4
F	568	LYS	-	expression tag	UNP M1E1E4

- Molecule 2 is 1-cyclopropyl-3-({1-[3-(methylsulfonyl)propyl]-1H-pyrrolo[3,2-c]pyridin-2-yl}methyl)-1,3-dihydro-2H-imidazo[4,5-c]pyridin-2-one (three-letter code: R0P) (formula: $C_{21}H_{23}N_5O_3S$) (labeled as "Ligand of Interest" by depositor).
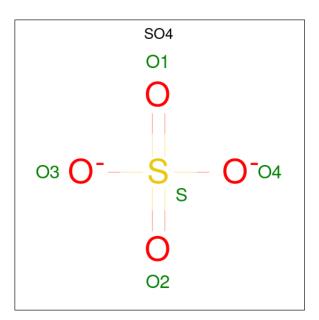

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total 30	C 21	N 5	O 3	S 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Cl 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	86	Total 86	O 86	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	168.61Å 168.61Å 168.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.06 – 2.50	Depositor
% Data completeness (in resolution range)	100.0 (45.06-2.50)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.197 , 0.229	Depositor
Wilson B-factor (Å^2)	53.3	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	3558	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	#$|Z| > 2$
4	SO4	F	603	-	4,4,4	0.13	0	6,6,6	0.10	0
2	R0P	F	601	-	30,34,34	2.21	11 (36%)	45,51,51	3.63	11 (24%)
4	SO4	F	604	-	4,4,4	0.16	0	6,6,6	0.06	0
4	SO4	F	605	-	4,4,4	0.14	0	6,6,6	0.14	0
4	SO4	F	607	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	F	608	-	4,4,4	0.16	0	6,6,6	0.04	0
4	SO4	F	606	-	4,4,4	0.14	0	6,6,6	0.09	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	R0P	F	601	-	-	6/15/17/17	0/5/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	R0P	C12-N11	5.07	1.44	1.38
2	F	601	R0P	C23-N11	4.43	1.48	1.39
2	F	601	R0P	C18-N14	4.20	1.48	1.40
2	F	601	R0P	C05-S02	3.85	1.83	1.78
2	F	601	R0P	C12-N14	3.55	1.44	1.38

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	R0P	C17-C15-N14	20.30	138.79	118.29
2	F	601	R0P	O04-S02-O03	-7.18	101.75	117.09
2	F	601	R0P	O04-S02-C05	5.29	112.05	108.34
2	F	601	R0P	O03-S02-C05	3.06	110.48	108.34
2	F	601	R0P	C10-C09-N08	3.02	126.41	122.05

There are no chirality outliers.
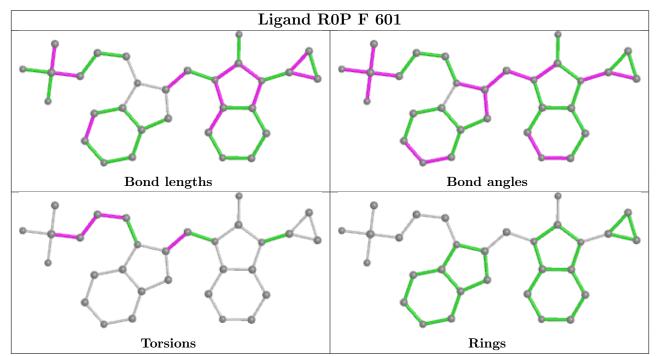
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	R0P	S02-C05-C06-C07
2	F	601	R0P	C06-C05-S02-O03
2	F	601	R0P	C06-C05-S02-O04
2	F	601	R0P	C05-C06-C07-N08
2	F	601	R0P	C06-C05-S02-C01

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand R0P F 601

Bond lengths

Bond angles

Torsions

Rings

4.7 Other polymers ⓘ

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.