Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 12:37 AM EDT

PDB ID	:	6VKE
Title	:	Crystal Structure of Inhibitor JNJ-40012665 in Complex with Prefusion RSV F Glycoprotein
Authors	:	McLellan, J.S.
Deposited on	:	2020-01-20
Resolution	:	2.10 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
buster-report	:	1.1.7 (2018)
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 2.10 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 6 unique types of molecules in this entry. The entry contains 3747 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	432	3343	2121	545	656	21	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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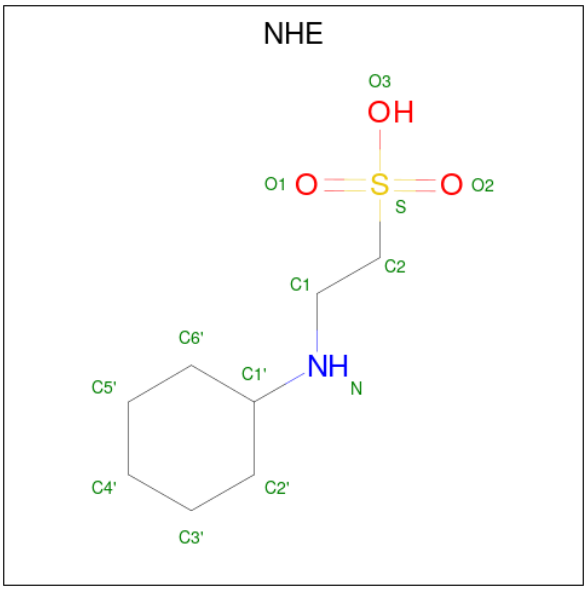
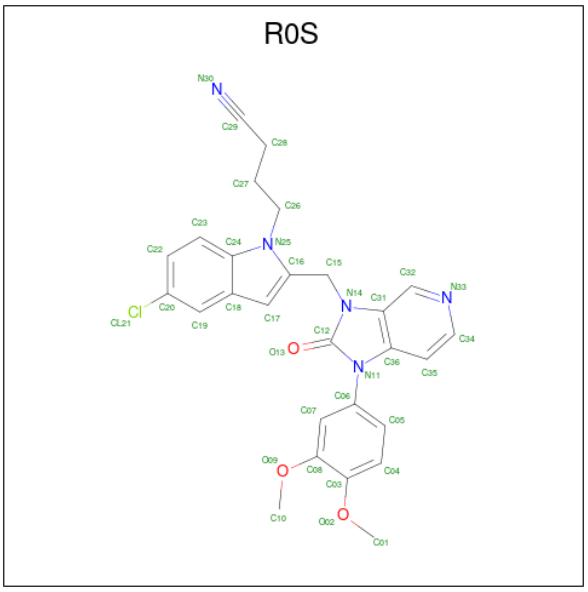
Chain	Residue	Modelled	Actual	Comment	Reference
F	564	PRO	-	expression tag	UNP M1E1E4
F	565	GLN	-	expression tag	UNP M1E1E4
F	566	PHE	-	expression tag	UNP M1E1E4
F	567	GLU	-	expression tag	UNP M1E1E4
F	568	LYS	-	expression tag	UNP M1E1E4

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 3 is 4-(5-chloro-2-{[1-(3,4-dimethoxyphenyl)-2-oxo-1,2-dihydro-3H-imidazo[4,5-c]pyridin-3-yl]methyl}-1H-indol-1-yl)butanenitrile (three-letter code: R0S) (formula: $C_{27}H_{24}ClN_5O_3$) (labeled as "Ligand of Interest" by depositor).

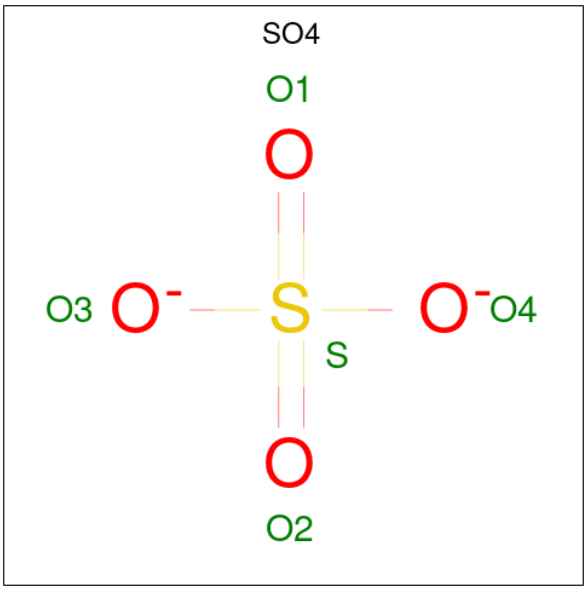


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	Cl	N	O	0	0
			36	27	1	5	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	333	Total O 333 333	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	168.77Å 168.77Å 168.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.93 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (40.93-2.10)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.178 , 0.199	Depositor
Wilson B-factor (Å^2)	32.7	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	3747	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	SO4	F	607	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	F	605	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	F	606	-	4,4,4	0.14	0	6,6,6	0.05	0
3	R0S	F	602	-	36,40,40	1.67	5 (13%)	50,57,57	1.89	16 (32%)
5	SO4	F	608	-	4,4,4	0.15	0	6,6,6	0.06	0
2	NHE	F	601	-	13,13,13	1.47	3 (23%)	16,17,17	1.77	4 (25%)

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
3	R0S	F	602	-	-	5/17/17/17	0/5/5/5
2	NHE	F	601	-	-	0/7/15/15	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	602	R0S	C36-N11	4.62	1.48	1.40
3	F	602	R0S	C12-N14	4.56	1.43	1.38
3	F	602	R0S	C31-N14	4.03	1.47	1.39
2	F	601	NHE	C2-S	2.92	1.81	1.77
2	F	601	NHE	O1-S	2.50	1.52	1.45
3	F	602	R0S	O02-C03	2.24	1.40	1.37
3	F	602	R0S	C20-CL21	2.16	1.79	1.74
2	F	601	NHE	O2-S	2.15	1.51	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	602	R0S	C16-C15-N14	-5.04	106.59	113.00
3	F	602	R0S	C36-N11-C12	-4.85	107.76	109.51
3	F	602	R0S	O02-C03-C08	3.77	120.66	115.41
3	F	602	R0S	C07-C06-N11	3.74	123.72	119.49
2	F	601	NHE	O2-S-C2	3.72	111.40	106.92
2	F	601	NHE	O3-S-O2	-3.60	102.47	111.27
3	F	602	R0S	C05-C06-N11	-3.05	116.45	119.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	NHE	O3-S-C2	3.04	110.69	105.77
3	F	602	R0S	C15-C16-N25	3.02	126.41	122.05
3	F	602	R0S	O02-C03-C04	-2.96	119.30	124.37
3	F	602	R0S	C01-O02-C03	-2.69	113.46	117.53
3	F	602	R0S	O09-C08-C03	2.67	119.13	115.41
3	F	602	R0S	C34-N33-C32	2.63	121.40	116.85
2	F	601	NHE	O1-S-C2	2.54	109.97	106.92
3	F	602	R0S	C15-C16-C17	-2.31	126.25	129.24
3	F	602	R0S	C15-N14-C12	2.28	126.47	122.81
3	F	602	R0S	C10-O09-C08	-2.20	114.20	117.53
3	F	602	R0S	O09-C08-C07	-2.20	120.33	124.12
3	F	602	R0S	C31-N14-C12	-2.08	107.89	110.05
3	F	602	R0S	C06-N11-C36	2.08	127.86	124.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

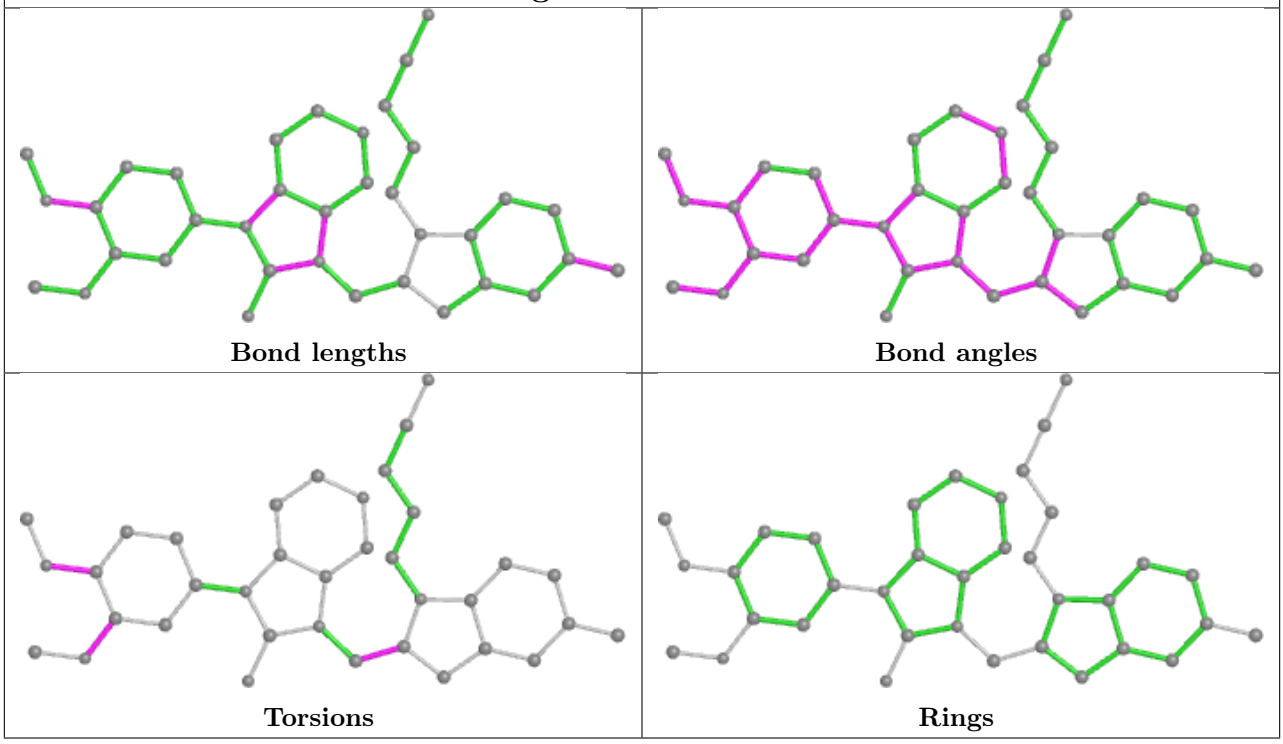
Mol	Chain	Res	Type	Atoms
3	F	602	R0S	C04-C03-O02-C01
3	F	602	R0S	C08-C03-O02-C01
3	F	602	R0S	C07-C08-O09-C10
3	F	602	R0S	C03-C08-O09-C10
3	F	602	R0S	N14-C15-C16-N25

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 R0S F 602



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.