Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 04:43 PM EDT

PDB ID	:	6NTX
Title	:	Respiratory syncytial virus fusion protein N-terminal heptad repeat domain+VIQKI
Authors	:	Outlaw, V.K.; Kreitler, D.F.; Gellman, S.H.
Deposited on	:	2019-01-30
Resolution	:	2.20 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 (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 2.20 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 2029 atoms, of which 982 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			
1	A	43	633	196	322	52	63	0	0	0
1	B	40	494	160	238	42	54	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ACE	-	acetylation	UNP A0A1U8ZTH8
A	210	NH2	-	amidation	UNP A0A1U8ZTH8
B	158	ACE	-	acetylation	UNP A0A1U8ZTH8
B	210	NH2	-	amidation	UNP A0A1U8ZTH8

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	35	490	159	234	43	54	0	0	1
2	D	27	392	128	188	38	38	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	448	ACE	-	acetylation	UNP A0A1V0BZ41
C	459	VAL	GLU	engineered mutation	UNP A0A1V0BZ41
C	463	ILE	ALA	engineered mutation	UNP A0A1V0BZ41
C	466	GLN	ASP	engineered mutation	UNP A0A1V0BZ41
C	479	LYS	GLN	engineered mutation	UNP A0A1V0BZ41
C	480	ILE	LYS	engineered mutation	UNP A0A1V0BZ41
C	485	NH2	-	amidation	UNP A0A1V0BZ41
D	448	ACE	-	acetylation	UNP A0A1V0BZ41

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Chain	Residue	Modelled	Actual	Comment	Reference
D	459	VAL	GLU	engineered mutation	UNP A0A1V0BZ41
D	463	ILE	ALA	engineered mutation	UNP A0A1V0BZ41
D	466	GLN	ASP	engineered mutation	UNP A0A1V0BZ41
D	479	LYS	GLN	engineered mutation	UNP A0A1V0BZ41
D	480	ILE	LYS	engineered mutation	UNP A0A1V0BZ41
D	485	NH2	-	amidation	UNP A0A1V0BZ41

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	5	5	5	0	0
			Total	O		
3	B	6	6	6	0	0
			Total	O		
3	C	5	5	5	0	0
			Total	O		
3	D	4	4	4	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	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	51.97Å 51.97Å 299.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.76 – 2.20	Depositor
% Data completeness (in resolution range)	99.8 (28.76-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.232 , 0.285	Depositor
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.152	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2029	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3256e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (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)

There are no ligands in this entry.

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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