Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 08:04 AM EDT

PDB ID	:	6NYX
Title	:	Human parainfluenza virus type 3 fusion protein N-terminal heptad repeat domain+VI
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Deposited on	:	2019-02-12
Resolution	:	1.85 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 1.85 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 12093 atoms, of which 5994 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	46	705	217	357	59	72	0	0	0
1	B	48	737	226	375	62	74	0	0	0
1	C	48	704	219	353	61	71	0	0	0
1	D	49	762	233	389	65	75	0	0	0
1	E	48	744	227	381	62	74	0	0	0
1	F	49	753	231	384	63	75	0	0	0
1	H	51	746	230	378	64	74	0	0	1
1	J	48	743	227	380	62	74	0	0	0
1	L	48	749	227	381	66	75	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ACE	-	acetylation	UNP Q84193
A	190	NH2	-	amidation	UNP Q84193
B	138	ACE	-	acetylation	UNP Q84193
B	190	NH2	-	amidation	UNP Q84193
C	138	ACE	-	acetylation	UNP Q84193
C	190	NH2	-	amidation	UNP Q84193
D	138	ACE	-	acetylation	UNP Q84193
D	190	NH2	-	amidation	UNP Q84193
E	138	ACE	-	acetylation	UNP Q84193
E	190	NH2	-	amidation	UNP Q84193
F	138	ACE	-	acetylation	UNP Q84193

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Chain	Residue	Modelled	Actual	Comment	Reference
F	190	NH2	-	amidation	UNP Q84193
H	138	ACE	-	acetylation	UNP Q84193
H	190	NH2	-	amidation	UNP Q84193
J	138	ACE	-	acetylation	UNP Q84193
J	190	NH2	-	amidation	UNP Q84193
L	138	ACE	-	acetylation	UNP Q84193
L	190	NH2	-	amidation	UNP Q84193

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	G	35	570	177	288	48	57	0	0	0
2	I	35	583	179	298	49	57	0	0	0
2	K	35	558	174	279	48	57	0	0	0
2	M	35	561	173	284	48	56	0	0	1
2	N	34	555	172	281	48	54	0	0	0
2	O	34	546	171	274	47	54	0	0	0
2	P	35	575	176	294	49	56	0	0	1
2	Q	35	585	181	297	50	57	0	1	1
2	T	34	573	176	293	48	56	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	448	ACE	-	acetylation	UNP Q84193
G	459	VAL	GLU	engineered mutation	UNP Q84193
G	463	ILE	ALA	engineered mutation	UNP Q84193
G	485	NH2	-	amidation	UNP Q84193
I	448	ACE	-	acetylation	UNP Q84193
I	459	VAL	GLU	engineered mutation	UNP Q84193
I	463	ILE	ALA	engineered mutation	UNP Q84193
I	485	NH2	-	amidation	UNP Q84193
K	441	ACE	-	acetylation	UNP Q84193

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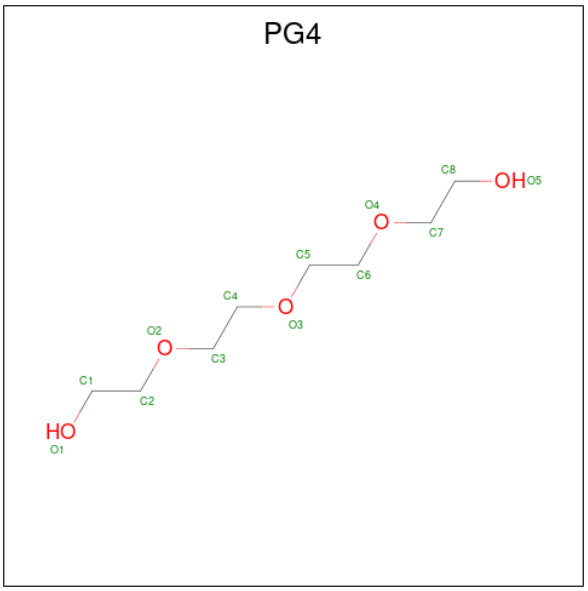
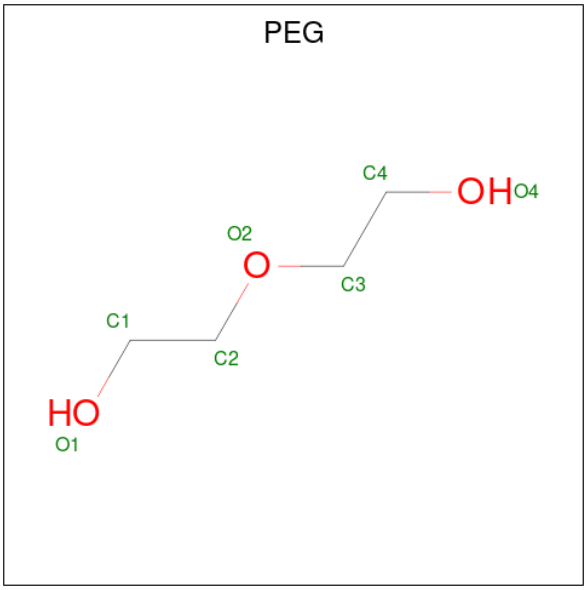
Chain	Residue	Modelled	Actual	Comment	Reference
K	452	VAL	GLU	engineered mutation	UNP Q84193
K	456	ILE	ALA	engineered mutation	UNP Q84193
K	478	NH2	-	amidation	UNP Q84193
M	448	ACE	-	acetylation	UNP Q84193
M	459	VAL	GLU	engineered mutation	UNP Q84193
M	463	ILE	ALA	engineered mutation	UNP Q84193
M	485	NH2	-	amidation	UNP Q84193
N	448	ACE	-	acetylation	UNP Q84193
N	459	VAL	GLU	engineered mutation	UNP Q84193
N	463	ILE	ALA	engineered mutation	UNP Q84193
N	485	NH2	-	amidation	UNP Q84193
O	448	ACE	-	acetylation	UNP Q84193
O	459	VAL	GLU	engineered mutation	UNP Q84193
O	463	ILE	ALA	engineered mutation	UNP Q84193
O	485	NH2	-	amidation	UNP Q84193
P	448	ACE	-	acetylation	UNP Q84193
P	459	VAL	GLU	engineered mutation	UNP Q84193
P	463	ILE	ALA	engineered mutation	UNP Q84193
P	485	NH2	-	amidation	UNP Q84193
Q	448	ACE	-	acetylation	UNP Q84193
Q	459	VAL	GLU	engineered mutation	UNP Q84193
Q	463	ILE	ALA	engineered mutation	UNP Q84193
Q	485	NH2	-	amidation	UNP Q84193
T	448	ACE	-	acetylation	UNP Q84193
T	459	VAL	GLU	engineered mutation	UNP Q84193
T	463	ILE	ALA	engineered mutation	UNP Q84193
T	485	NH2	-	amidation	UNP Q84193

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	G	1	31	8	18	5	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	L	1	17	4	10	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	14	14	14	0	0
			Total	O		
5	B	17	17	17	0	0
			Total	O		
5	C	15	15	15	0	0
			Total	O		
5	D	14	14	14	0	0
			Total	O		
5	E	14	14	14	0	0
			Total	O		
5	F	20	21	21	0	1
			Total	O		
5	G	19	19	19	0	0
			Total	O		
5	H	17	17	17	0	0
			Total	O		
5	I	19	19	19	0	0
			Total	O		
5	J	15	15	15	0	0
			Total	O		
5	K	14	14	14	0	0
			Total	O		
5	L	12	12	12	0	0
			Total	O		
5	M	17	17	17	0	0
			Total	O		
5	N	29	29	29	0	0
			Total	O		
5	O	15	15	15	0	0
			Total	O		
5	P	20	21	21	0	1
			Total	O		
5	Q	18	18	18	0	0
			Total	O		
5	T	5	5	5	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 3	Depositor
Cell constants a, b, c, α, β, γ	88.03Å 88.03Å 75.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.12 – 1.85	Depositor
% Data completeness (in resolution range)	99.8 (38.12-1.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.198 , 0.229	Depositor
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.059	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l 0.013 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Total number of atoms	12093	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 16.57% 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 (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)

2 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	$\#\|Z\| > 2$
4	PEG	L	201	-	6,6,6	0.60	0	5,5,5	0.43	0
3	PG4	G	501	-	12,12,12	0.59	0	11,11,11	0.95	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	PEG	L	201	-	-	2/4/4/4	-
3	PG4	G	501	-	-	5/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	501	PG4	O4-C7-C8-O5
3	G	501	PG4	O1-C1-C2-O2
4	L	201	PEG	O2-C3-C4-O4
3	G	501	PG4	C8-C7-O4-C6
4	L	201	PEG	C4-C3-O2-C2
3	G	501	PG4	C3-C4-O3-C5
3	G	501	PG4	O2-C3-C4-O3

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 (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.