wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 03:00 PM EDT

PDB ID	:	6NRO
Title	:	Human parainfluenza virus type 3 fusion protein N-terminal heptad repeat domain+VIQKI
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Deposited on	:	2019-01-23
Resolution	:	1.75 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 1.75 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 4017 atoms, of which 2003 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 Human parainfluenza virus type 3 fusion glycoprotein N-terminal heptad repeat domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	50	Total	C	H	N	O	0	0	1
			745	230	379	63	73			
1	E	49	Total	C	H	N	O	0	0	0
			710	222	356	61	71			
1	C	49	Total	C	H	N	O	0	0	0
			750	230	382	63	75			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	ACE	-	acetylation	UNP A0A1V0E102
A	165	ILE	VAL	engineered mutation	UNP A0A1V0E102
A	190	NH2	-	amidation	UNP A0A1V0E102
E	138	ACE	-	acetylation	UNP A0A1V0E102
E	165	ILE	VAL	engineered mutation	UNP A0A1V0E102
E	190	NH2	-	amidation	UNP A0A1V0E102
C	138	ACE	-	acetylation	UNP A0A1V0E102
C	165	ILE	VAL	engineered mutation	UNP A0A1V0E102
C	190	NH2	-	amidation	UNP A0A1V0E102

- Molecule 2 is a protein called Human parainfluenza virus type 3 fusion glycoprotein C-terminal heptad repeat domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	34	Total	C	H	N	O	0	0	0
			568	176	291	47	54			
2	B	35	Total	C	H	N	O	0	0	0
			590	181	305	49	55			
2	F	34	Total	C	H	N	O	0	0	0
			553	173	280	46	54			

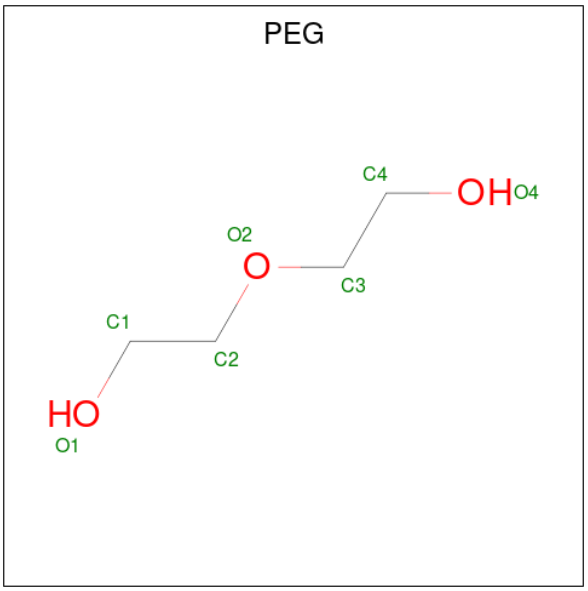
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	448	ACE	-	acetylation	UNP A0A023PHT3
D	459	VAL	GLU	engineered mutation	UNP A0A023PHT3
D	463	ILE	ALA	engineered mutation	UNP A0A023PHT3
D	466	GLN	ASP	engineered mutation	UNP A0A023PHT3
D	479	LYS	GLN	engineered mutation	UNP A0A023PHT3
D	480	ILE	LYS	engineered mutation	UNP A0A023PHT3
D	485	NH2	-	amidation	UNP A0A023PHT3
B	448	ACE	-	acetylation	UNP A0A023PHT3
B	459	VAL	GLU	engineered mutation	UNP A0A023PHT3
B	463	ILE	ALA	engineered mutation	UNP A0A023PHT3
B	466	GLN	ASP	engineered mutation	UNP A0A023PHT3
B	479	LYS	GLN	engineered mutation	UNP A0A023PHT3
B	480	ILE	LYS	engineered mutation	UNP A0A023PHT3
B	485	NH2	-	amidation	UNP A0A023PHT3
F	448	ACE	-	acetylation	UNP A0A023PHT3
F	459	VAL	GLU	engineered mutation	UNP A0A023PHT3
F	463	ILE	ALA	engineered mutation	UNP A0A023PHT3
F	466	GLN	ASP	engineered mutation	UNP A0A023PHT3
F	479	LYS	GLN	engineered mutation	UNP A0A023PHT3
F	480	ILE	LYS	engineered mutation	UNP A0A023PHT3
F	485	NH2	-	amidation	UNP A0A023PHT3

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total O 14 14	0	0
5	E	10	Total O 10 10	0	0
5	C	16	Total O 16 16	0	0
5	D	16	Total O 16 16	0	0
5	B	16	Total O 16 16	0	0
5	F	11	Total O 11 11	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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.97Å 52.25Å 54.11Å 90.00° 100.56° 90.00°	Depositor
Resolution (Å)	39.29 – 1.75	Depositor
% Data completeness (in resolution range)	99.5 (39.29-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.217 , 0.244	Depositor
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.364	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	4017	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.61% 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	PEG	F	501	-	6,6,6	0.65	0	5,5,5	0.37	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	F	501	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	501	PEG	O2-C3-C4-O4
4	F	501	PEG	O1-C1-C2-O2
4	F	501	PEG	C1-C2-O2-C3

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.