wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 12:43 AM EDT

PDB ID	:	6URI
Title	:	HIV-1 Nef in complex with the CD4 cytoplasmic domain and the AP2 clathrin adaptor complex
Authors	:	Jia, X.; Kwon, Y.
Deposited on	:	2019-10-23
Resolution	:	3.00 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
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

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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 7 unique types of molecules in this entry. The entry contains 12263 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 AP-2 complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	611	4823	3073	830	899	21	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q66HM2
A	-12	GLY	-	expression tag	UNP Q66HM2
A	-11	SER	-	expression tag	UNP Q66HM2
A	-10	SER	-	expression tag	UNP Q66HM2
A	-9	HIS	-	expression tag	UNP Q66HM2
A	-8	HIS	-	expression tag	UNP Q66HM2
A	-7	HIS	-	expression tag	UNP Q66HM2
A	-6	HIS	-	expression tag	UNP Q66HM2
A	-5	HIS	-	expression tag	UNP Q66HM2
A	-4	HIS	-	expression tag	UNP Q66HM2
A	-3	SER	-	expression tag	UNP Q66HM2
A	-2	GLN	-	expression tag	UNP Q66HM2
A	-1	ASP	-	expression tag	UNP Q66HM2
A	0	PRO	-	expression tag	UNP Q66HM2
A	622	GLU	-	expression tag	UNP Q66HM2
A	623	ASN	-	expression tag	UNP Q66HM2
A	624	LEU	-	expression tag	UNP Q66HM2
A	625	TYR	-	expression tag	UNP Q66HM2
A	626	PHE	-	expression tag	UNP Q66HM2
A	627	GLN	-	expression tag	UNP Q66HM2

- Molecule 2 is a protein called AP-2 complex subunit sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	S	142	1202	778	202	215	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	45	ARG	LYS	conflict	UNP P53680

- Molecule 3 is a protein called Protein Nef.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	164	Total	C	N	O	S	0	0	0
			1346	861	233	248	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	21	ALA	-	expression tag	UNP Q90VU7
N	22	GLY	-	expression tag	UNP Q90VU7
N	23	PHE	-	expression tag	UNP Q90VU7
N	24	SER	-	expression tag	UNP Q90VU7
N	25	MET	-	expression tag	UNP Q90VU7

- Molecule 4 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	480	Total	C	N	O	S	0	0	0
			3797	2414	639	727	17			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	initiating methionine	UNP P63010
B	-22	GLY	-	expression tag	UNP P63010
B	-21	SER	-	expression tag	UNP P63010
B	-20	SER	-	expression tag	UNP P63010
B	-19	HIS	-	expression tag	UNP P63010
B	-18	HIS	-	expression tag	UNP P63010
B	-17	HIS	-	expression tag	UNP P63010
B	-16	HIS	-	expression tag	UNP P63010
B	-15	HIS	-	expression tag	UNP P63010
B	-14	HIS	-	expression tag	UNP P63010
B	-13	SER	-	expression tag	UNP P63010
B	-12	GLN	-	expression tag	UNP P63010
B	-11	ASP	-	expression tag	UNP P63010
B	-10	PRO	-	expression tag	UNP P63010
B	-9	ASN	-	expression tag	UNP P63010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	SER	-	expression tag	UNP P63010
B	-7	SER	-	expression tag	UNP P63010
B	-6	SER	-	expression tag	UNP P63010
B	-5	ALA	-	expression tag	UNP P63010
B	-4	ARG	-	expression tag	UNP P63010
B	-3	LEU	-	expression tag	UNP P63010
B	-2	GLN	-	expression tag	UNP P63010
B	-1	VAL	-	expression tag	UNP P63010
B	0	ASP	-	expression tag	UNP P63010
B	16	SER	PHE	variant	UNP P63010
B	421	HIS	TYR	variant	UNP P63010
B	434	GLY	GLU	variant	UNP P63010

- Molecule 5 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	120	Total	C	N	O	S	0	0	0
			975	631	167	172	5			

- Molecule 6 is a protein called cDNA FLJ50658, highly similar to T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	14	Total	C	N	O	S	0	0	0
			118	73	24	20	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	358	GLY	-	expression tag	UNP B4DT49
D	359	VAL	-	expression tag	UNP B4DT49
D	360	ASP	-	expression tag	UNP B4DT49
D	361	GLY	-	expression tag	UNP B4DT49
D	362	SER	-	expression tag	UNP B4DT49
D	363	ASP	-	expression tag	UNP B4DT49
D	364	GLU	-	expression tag	UNP B4DT49
D	365	ALA	-	expression tag	UNP B4DT49
D	366	SER	-	expression tag	UNP B4DT49
D	367	GLU	-	expression tag	UNP B4DT49
D	368	LEU	-	expression tag	UNP B4DT49
D	369	ALA	-	expression tag	UNP B4DT49
D	370	CYS	-	expression tag	UNP B4DT49

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Chain	Residue	Modelled	Actual	Comment	Reference
D	371	PRO	-	expression tag	UNP B4DT49
D	372	THR	-	expression tag	UNP B4DT49
D	373	PRO	-	expression tag	UNP B4DT49
D	374	LYS	-	expression tag	UNP B4DT49
D	375	GLU	-	expression tag	UNP B4DT49
D	376	ASP	-	expression tag	UNP B4DT49
D	377	GLY	-	expression tag	UNP B4DT49
D	378	LEU	-	expression tag	UNP B4DT49
D	379	ALA	-	expression tag	UNP B4DT49
D	380	GLN	-	expression tag	UNP B4DT49
D	381	GLN	-	expression tag	UNP B4DT49
D	382	GLN	-	expression tag	UNP B4DT49
D	383	THR	-	expression tag	UNP B4DT49
D	384	GLN	-	expression tag	UNP B4DT49
D	385	LEU	-	expression tag	UNP B4DT49
D	386	ASN	-	expression tag	UNP B4DT49
D	387	LEU	-	expression tag	UNP B4DT49
D	388	ARG	-	expression tag	UNP B4DT49
D	389	GLY	-	expression tag	UNP B4DT49
D	390	SER	-	expression tag	UNP B4DT49
D	391	GLY	-	expression tag	UNP B4DT49
D	392	SER	-	expression tag	UNP B4DT49
D	393	GLY	-	expression tag	UNP B4DT49

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	N	1	Total O 1 1	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	Depositor
Cell constants a, b, c, α, β, γ	109.15Å 109.15Å 178.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.82 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (48.82-3.00)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.241 , 0.277	Depositor
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.106	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
Total number of atoms	12263	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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

There are no ligands in this entry.

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.