wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 04:51 AM EDT

PDB ID	:	6U3V
Title	:	Crystal structure of human alpha/epsilon-COP of the COPI vesicular coat bound to alpha-COP STM1
Authors	:	Travis, S.M.; Hughson, F.M.
Deposited on	:	2019-08-22
Resolution	:	2.96 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 2.96 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 2 unique types of molecules in this entry. The entry contains 9801 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 Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	1	0
			2332	1466	404	451	11			
1	C	290	Total	C	N	O	S	0	1	0
			2310	1453	400	446	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP O14579
A	-12	GLY	-	expression tag	UNP O14579
A	-11	SER	-	expression tag	UNP O14579
A	-10	SER	-	expression tag	UNP O14579
A	-9	HIS	-	expression tag	UNP O14579
A	-8	HIS	-	expression tag	UNP O14579
A	-7	HIS	-	expression tag	UNP O14579
A	-6	HIS	-	expression tag	UNP O14579
A	-5	HIS	-	expression tag	UNP O14579
A	-4	HIS	-	expression tag	UNP O14579
A	-3	SER	-	expression tag	UNP O14579
A	-2	GLN	-	expression tag	UNP O14579
A	-1	ASP	-	expression tag	UNP O14579
A	0	PRO	-	expression tag	UNP O14579
C	-13	MET	-	expression tag	UNP O14579
C	-12	GLY	-	expression tag	UNP O14579
C	-11	SER	-	expression tag	UNP O14579
C	-10	SER	-	expression tag	UNP O14579
C	-9	HIS	-	expression tag	UNP O14579
C	-8	HIS	-	expression tag	UNP O14579
C	-7	HIS	-	expression tag	UNP O14579
C	-6	HIS	-	expression tag	UNP O14579
C	-5	HIS	-	expression tag	UNP O14579
C	-4	HIS	-	expression tag	UNP O14579
C	-3	SER	-	expression tag	UNP O14579

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLN	-	expression tag	UNP O14579
C	-1	ASP	-	expression tag	UNP O14579
C	0	PRO	-	expression tag	UNP O14579

- Molecule 2 is a protein called Coatomer subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	332	Total	C	N	O	S	0	0	0
			2635	1691	456	473	15			
2	D	318	Total	C	N	O	S	0	0	0
			2524	1619	437	453	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	834	MET	-	initiating methionine	UNP P53621
B	?	-	ASP	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	ASP	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621
B	?	-	PHE	deletion	UNP P53621
B	?	-	VAL	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	ALA	deletion	UNP P53621
B	?	-	THR	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621
B	?	-	LEU	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621
B	?	-	ASP	deletion	UNP P53621
B	?	-	ASP	deletion	UNP P53621
B	?	-	ALA	deletion	UNP P53621
B	?	-	LEU	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621
B	?	-	LYS	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621
B	?	-	GLN	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621
B	?	-	GLY	deletion	UNP P53621

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	TRP	deletion	UNP P53621
B	?	-	ASP	deletion	UNP P53621
B	?	-	VAL	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	ASP	deletion	UNP P53621
B	?	-	LEU	deletion	UNP P53621
B	?	-	GLU	deletion	UNP P53621
B	?	-	LEU	deletion	UNP P53621
D	869	MET	-	initiating methionine	UNP P53621
D	?	-	ASP	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	ASP	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	PHE	deletion	UNP P53621
D	?	-	VAL	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	ALA	deletion	UNP P53621
D	?	-	THR	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	LEU	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	ASP	deletion	UNP P53621
D	?	-	ASP	deletion	UNP P53621
D	?	-	ALA	deletion	UNP P53621
D	?	-	LEU	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	LYS	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	GLN	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	GLY	deletion	UNP P53621
D	?	-	TRP	deletion	UNP P53621
D	?	-	ASP	deletion	UNP P53621
D	?	-	VAL	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	ASP	deletion	UNP P53621

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP P53621
D	?	-	GLU	deletion	UNP P53621
D	?	-	LEU	deletion	UNP P53621

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 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.10Å 138.10Å 192.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.55 – 2.96	Depositor
% Data completeness (in resolution range)	99.8 (29.55-2.96)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.13_2998: ???	Depositor
R, R_{free}	0.172 , 0.231	Depositor
Wilson B-factor (Å^2)	73.2	Xtriage
Anisotropy	0.048	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
Total number of atoms	9801	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

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.