



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 08:02 AM EDT

PDB ID : 7M6U
Title : Crystal structure of a circular permutation and computationally designed pro-enzyme of carboxypeptidase G2
Authors : Yachnin, B.J.; Khare, S.D.
Deposited on : 2021-03-26
Resolution : 2.59 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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) : 2.27

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 2.59 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

There are 4 unique types of molecules in this entry. The entry contains 11105 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 Carboxypeptidase G2 circular permutation pro-domain fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2854	1793	491	564	6			
1	B	392	Total	C	N	O	S	0	0	0
			2849	1786	491	566	6			
1	C	389	Total	C	N	O	S	0	0	0
			2772	1731	477	558	6			
1	D	356	Total	C	N	O	S	0	0	0
			2473	1537	425	507	4			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP P06621
A	-24	GLY	-	expression tag	UNP P06621
A	-23	SER	-	expression tag	UNP P06621
A	-22	SER	-	expression tag	UNP P06621
A	-21	HIS	-	expression tag	UNP P06621
A	-20	HIS	-	expression tag	UNP P06621
A	-19	HIS	-	expression tag	UNP P06621
A	-18	HIS	-	expression tag	UNP P06621
A	-17	HIS	-	expression tag	UNP P06621
A	-16	HIS	-	expression tag	UNP P06621
A	-15	SER	-	expression tag	UNP P06621
A	-14	SER	-	expression tag	UNP P06621
A	-13	GLY	-	expression tag	UNP P06621
A	-12	LEU	-	expression tag	UNP P06621
A	-11	VAL	-	expression tag	UNP P06621
A	-10	PRO	-	expression tag	UNP P06621
A	-9	ARG	-	expression tag	UNP P06621
A	-8	GLY	-	expression tag	UNP P06621
A	-7	SER	-	expression tag	UNP P06621
A	-6	HIS	-	expression tag	UNP P06621
A	-5	MET	-	expression tag	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P06621
A	-3	SER	-	expression tag	UNP P06621
A	86	ALA	LYS	engineered mutation	UNP P06621
A	325	GLY	-	linker	UNP P06621
A	326	THR	-	linker	UNP P06621
A	327	ALA	-	linker	UNP P06621
A	328	SER	-	linker	UNP P06621
B	-25	MET	-	initiating methionine	UNP P06621
B	-24	GLY	-	expression tag	UNP P06621
B	-23	SER	-	expression tag	UNP P06621
B	-22	SER	-	expression tag	UNP P06621
B	-21	HIS	-	expression tag	UNP P06621
B	-20	HIS	-	expression tag	UNP P06621
B	-19	HIS	-	expression tag	UNP P06621
B	-18	HIS	-	expression tag	UNP P06621
B	-17	HIS	-	expression tag	UNP P06621
B	-16	HIS	-	expression tag	UNP P06621
B	-15	SER	-	expression tag	UNP P06621
B	-14	SER	-	expression tag	UNP P06621
B	-13	GLY	-	expression tag	UNP P06621
B	-12	LEU	-	expression tag	UNP P06621
B	-11	VAL	-	expression tag	UNP P06621
B	-10	PRO	-	expression tag	UNP P06621
B	-9	ARG	-	expression tag	UNP P06621
B	-8	GLY	-	expression tag	UNP P06621
B	-7	SER	-	expression tag	UNP P06621
B	-6	HIS	-	expression tag	UNP P06621
B	-5	MET	-	expression tag	UNP P06621
B	-4	GLY	-	expression tag	UNP P06621
B	-3	SER	-	expression tag	UNP P06621
B	86	ALA	LYS	engineered mutation	UNP P06621
B	325	GLY	-	linker	UNP P06621
B	326	THR	-	linker	UNP P06621
B	327	ALA	-	linker	UNP P06621
B	328	SER	-	linker	UNP P06621
C	-25	MET	-	initiating methionine	UNP P06621
C	-24	GLY	-	expression tag	UNP P06621
C	-23	SER	-	expression tag	UNP P06621
C	-22	SER	-	expression tag	UNP P06621
C	-21	HIS	-	expression tag	UNP P06621
C	-20	HIS	-	expression tag	UNP P06621
C	-19	HIS	-	expression tag	UNP P06621

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP P06621
C	-17	HIS	-	expression tag	UNP P06621
C	-16	HIS	-	expression tag	UNP P06621
C	-15	SER	-	expression tag	UNP P06621
C	-14	SER	-	expression tag	UNP P06621
C	-13	GLY	-	expression tag	UNP P06621
C	-12	LEU	-	expression tag	UNP P06621
C	-11	VAL	-	expression tag	UNP P06621
C	-10	PRO	-	expression tag	UNP P06621
C	-9	ARG	-	expression tag	UNP P06621
C	-8	GLY	-	expression tag	UNP P06621
C	-7	SER	-	expression tag	UNP P06621
C	-6	HIS	-	expression tag	UNP P06621
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C	-4	GLY	-	expression tag	UNP P06621
C	-3	SER	-	expression tag	UNP P06621
C	86	ALA	LYS	engineered mutation	UNP P06621
C	325	GLY	-	linker	UNP P06621
C	326	THR	-	linker	UNP P06621
C	327	ALA	-	linker	UNP P06621
C	328	SER	-	linker	UNP P06621
D	-25	MET	-	initiating methionine	UNP P06621
D	-24	GLY	-	expression tag	UNP P06621
D	-23	SER	-	expression tag	UNP P06621
D	-22	SER	-	expression tag	UNP P06621
D	-21	HIS	-	expression tag	UNP P06621
D	-20	HIS	-	expression tag	UNP P06621
D	-19	HIS	-	expression tag	UNP P06621
D	-18	HIS	-	expression tag	UNP P06621
D	-17	HIS	-	expression tag	UNP P06621
D	-16	HIS	-	expression tag	UNP P06621
D	-15	SER	-	expression tag	UNP P06621
D	-14	SER	-	expression tag	UNP P06621
D	-13	GLY	-	expression tag	UNP P06621
D	-12	LEU	-	expression tag	UNP P06621
D	-11	VAL	-	expression tag	UNP P06621
D	-10	PRO	-	expression tag	UNP P06621
D	-9	ARG	-	expression tag	UNP P06621
D	-8	GLY	-	expression tag	UNP P06621
D	-7	SER	-	expression tag	UNP P06621
D	-6	HIS	-	expression tag	UNP P06621
D	-5	MET	-	expression tag	UNP P06621

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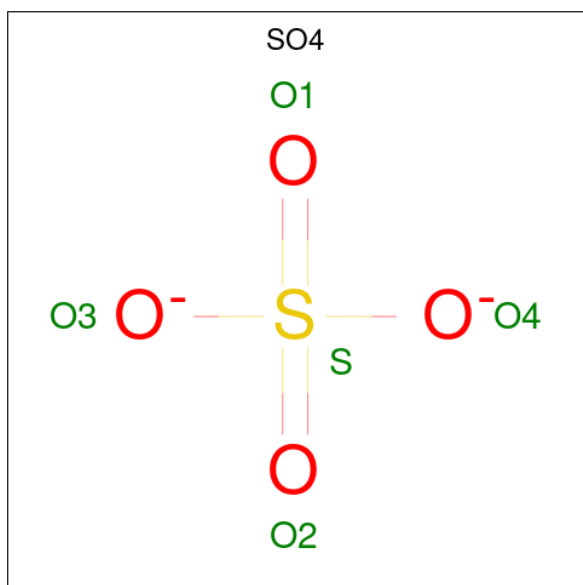
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP P06621
D	-3	SER	-	expression tag	UNP P06621
D	86	ALA	LYS	engineered mutation	UNP P06621
D	325	GLY	-	linker	UNP P06621
D	326	THR	-	linker	UNP P06621
D	327	ALA	-	linker	UNP P06621
D	328	SER	-	linker	UNP P06621

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Zn	0	0
			7	7		
2	B	5	Total	Zn	0	0
			5	5		
2	C	4	Total	Zn	0	0
			4	4		
2	D	4	Total	Zn	0	0
			4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total 54	O 54	0	0
4	B	43	Total 43	O 43	0	0
4	C	22	Total 22	O 22	0	0
4	D	13	Total 13	O 13	0	0

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

3 Data and refinement statistics

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	78.54Å 106.36Å 121.93Å 90.00° 107.48° 90.00°	Depositor
Resolution (Å)	39.27 – 2.59	Depositor
% Data completeness (in resolution range)	80.9 (39.27-2.59)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.222 , 0.279	Depositor
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.574	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
Total number of atoms	11105	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Of 21 ligands modelled in this entry, 20 are 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	$\# Z > 2$
3	SO4	A	507	-	4,4,4	0.32	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.