

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 06:15 AM EDT

PDB ID : 6VCG

Title : Crystal structure of Nitrosotalea devanaterra carotenoid cleavage dioxygenase,

cobalt form

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Deposited on : 2019-12-20

Resolution : 2.30 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 (1)) 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 (i)

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

The reported resolution of this entry is 2.30 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 21658 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 carotenoid cleavage dioxygenase.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1 Λ	453	Total	С	N	О	S	0	2	0	
1	1 A	455	3624	2335	589	693	7	0	2	
1	В	453	Total	С	N	О	S	0	2	0
1	Ъ	455	3643	2351	595	690	7	0		0
1	С	453	Total	С	N	О	S	0	1	0
1			3604	2326	588	683	7			
1	1 D	453	Total	С	N	О	S	0	0	0
1	ט	400	3597	2320	586	684	7	0		
1	Е	423	Total	С	N	О	S	0	0	0
	l Li		3348	2161	541	639	7		0	
1	1 F	F 430	Total	С	N	О	S	0	0	0
1			3372	2179	551	634	8			

• Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Co 1 1	0	0
2	В	1	Total Co 1 1	0	0
2	С	1	Total Co 1 1	0	0
2	D	1	Total Co 1 1	0	0
2	E	1	Total Co 1 1	0	0
2	F	1	Total Co 1 1	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Na 1 1	0	0
3	С	1	Total Na 1 1	0	0

 \bullet Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total Cl 1 1	0	0
4	Е	1	Total Cl 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	110	Total O	0	0
F	D	105	110 110 Total O	0	0
5	В	135	135 135	0	0
5	С	89	Total O 89 89	0	0
	D	0.4	Total O	0	0
5	D	84	84 84	0	0
5	E	21	Total O 21 21	0	0
			Total O		
5	F	21	21 21	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 61	Depositor
Cell constants	108.01Å 108.01Å 491.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.44 - 2.30	Depositor
% Data completeness	99.8 (49.44-2.30)	Depositor
(in resolution range)	, ,	-
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.97 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.254	Depositor
Wilson B-factor $(Å^2)$	56.4	Xtriage
Anisotropy	0.229	Xtriage
L-test for twinning ²	$< L > = 0.51, < L^2> = 0.35$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
Total number of atoms	21658	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.16% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

