W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 09:08 AM EDT

PDB ID	:	6N20
Title	:	Structure of L509V CAO1 - growth condition 2
Authors	:	Khadka, N.; Shi, W.; Kiser, P.D.
Deposited on	:	2018-11-12
Resolution	:	1.95 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.

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 1.95 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 16739 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 oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	501	Total	C	N	O	S	0	2	0
			4019	2578	680	741	20			
1	A	497	Total	C	N	O	S	0	1	0
			3987	2558	678	731	20			
1	C	497	Total	C	N	O	S	0	0	0
			3976	2550	675	731	20			
1	B	480	Total	C	N	O	S	0	1	0
			3847	2463	653	711	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8
A	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8
C	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8
B	509	VAL	LEU	engineered mutation	UNP A0A0B0DIC8

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	252	Total 252	O 252	0	0
4	A	231	Total 231	O 231	0	0
4	C	207	Total 207	O 207	0	0
4	B	212	Total 212	O 212	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 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.55Å　99.55Å　447.49Å 90.00°　90.00°　120.00°	Depositor
Resolution (Å)	49.47　–　1.95	Depositor
% Data completeness (in resolution range)	100.0 (49.47-1.95)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.32 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187　,　0.205	Depositor
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.513	Xtriage
L-test for twinning[2]	$<|L|> = 0.51$, $<L^2> = 0.35$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l	Xtriage
Total number of atoms	16739	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 8 ligands modelled in this entry, 8 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 ⓘ

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.