

wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 12:33 AM EDT

PDB ID	:	4FFU
Title	:	CRYSTAL STRUCTURE OF putative MaoC-like (monoamine oxidase-like)
		protein, similar to NodN from Sinorhizo Bium meliloti 1021
Authors	:	Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth,
		S.; Kar, A.; Chan, M.K.; Lafluer, J.; Patel, H.; Matikainen, B.; Chamala, S.;
		Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser,
		A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural
		Genomics Research Consortium (NYSGRC)
Deposited on	:	2012-06-01
Resolution	:	1.80 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 (1)) were used in the production of this report:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.35
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
	: : : : :

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	5950(1.80-1.80)		
Clashscore	141614	6793 (1.80-1.80)		
Ramachandran outliers	138981	6697 (1.80-1.80)		
Sidechain outliers	138945	6696 (1.80-1.80)		
RSRZ outliers	127900	5850 (1.80-1.80)		

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	176	5% 82%	6%	12%
1	В	176	3% 82%	•	15%
1	С	176	6% 75% 10%)	15%
			Continued o	n ne	xt page

Ideal geometry (DNA, RNA) : Parkinson et al. (1996) Validation Pipeline (wwPDB-VP) : 2.35



IVIOI	Chain	Length	Quality of chain	
- 1	D	150	7%	
1	D	176	78%	5% • 16%
_		1 - 0	5%	
1	E	176	82%	•• 14%
			10%	
1	F	176	77%	••• 18%
			14%	
1	G	176	70%	11% • 18%
			2%	
1	Н	176	84%	5% 11%
			6%	
1	Ι	176	81%	7% • 11%
			15%	
1	J	176	72%	9% • 19%
			13%	
1	K	176	71%	5% • 23%
			9%	
1	L	176	78%	7% • 14%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16207 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.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
1	Δ	155	Total	С	Ν	0	S	Se	0	5	0
	A	100	1248	790	224	229	1	4	0	0	0
1	В	150	Total	С	Ν	0	S	Se	0	4	0
	D	150	1199	755	219	220	1	4	0	4	0
1	С	150	Total	С	Ν	Ο	\mathbf{S}	Se	0	8	0
	U	100	1232	778	230	221	1	2	0	0	0
1	а	147	Total	С	Ν	Ο	\mathbf{S}	Se	0	7	0
1	D	147	1197	756	218	219	1	3	0	1	0
1	E	151	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	Ο
1		101	1196	752	220	221	1	2	0	T	0
1	F	145	Total	С	Ν	Ο	\mathbf{S}	Se	0	4	0
	1	140	1167	736	215	212	1	3	0	1	0
1	G	145	Total	С	Ν	Ο	\mathbf{S}	Se	0	5	0
	ŭ	140	1171	741	214	212	1	3	0		0
1	н	156	Total	С	Ν	Ο	\mathbf{S}	Se	0	3	0
	11	100	1246	787	223	230	1	5	0		0
1	т	157	Total	С	Ν	Ο	\mathbf{S}	Se	0	8	0
	-	101	1286	814	231	235	1	5	0		0
1	I	143	Total	С	Ν	Ο	\mathbf{S}	Se	0	4	0
	0	110	1145	722	210	210	1	2	0	1	0
1	K	135	Total	С	Ν	Ο	\mathbf{S}	Se	0	3	0
	13	100	1082	685	198	195	1	3		0	0
1	L	151	Total	С	Ν	Ο	\mathbf{S}	Se	0	2	0
1		101	1201	756	220	221	1	3			U

• Molecule 1 is a protein called oxidase.

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-22	MSE	-	expression tag	UNP Q92VL2
А	-21	HIS	-	expression tag	UNP Q92VL2
А	-20	HIS	-	expression tag	UNP Q92VL2
А	-19	HIS	-	expression tag	UNP Q92VL2
А	-18	HIS	-	expression tag	UNP Q92VL2



Continu	eu from pre	vious puye			
Chain	Residue	Modelled	Actual	Comment	Reference
А	-17	HIS	-	expression tag	UNP Q92VL2
А	-16	HIS	-	expression tag	UNP Q92VL2
А	-15	SER	-	expression tag	UNP Q92VL2
А	-14	SER	-	expression tag	UNP Q92VL2
А	-13	GLY	-	expression tag	UNP Q92VL2
А	-12	VAL	_	expression tag	UNP Q92VL2
А	-11	ASP	_	expression tag	UNP Q92VL2
А	-10	LEU	-	expression tag	UNP Q92VL2
А	-9	GLY	-	expression tag	UNP Q92VL2
А	-8	THR	-	expression tag	UNP Q92VL2
А	-7	GLU	-	expression tag	UNP Q92VL2
А	-6	ASN	-	expression tag	UNP Q92VL2
А	-5	LEU	-	expression tag	UNP Q92VL2
А	-4	TYR	-	expression tag	UNP Q92VL2
А	-3	PHE	-	expression tag	UNP Q92VL2
А	-2	GLN	-	expression tag	UNP Q92VL2
А	-1	SER	-	expression tag	UNP Q92VL2
А	0	MSE	-	expression tag	UNP Q92VL2
В	-22	MSE	-	expression tag	UNP Q92VL2
В	-21	HIS	-	expression tag	UNP Q92VL2
В	-20	HIS	-	expression tag	UNP Q92VL2
В	-19	HIS	-	expression tag	UNP Q92VL2
В	-18	HIS	-	expression tag	UNP Q92VL2
В	-17	HIS	-	expression tag	UNP Q92VL2
В	-16	HIS	-	expression tag	UNP Q92VL2
В	-15	SER	-	expression tag	UNP Q92VL2
В	-14	SER	-	expression tag	UNP Q92VL2
В	-13	GLY	-	expression tag	UNP Q92VL2
В	-12	VAL	-	expression tag	UNP Q92VL2
В	-11	ASP	-	expression tag	UNP Q92VL2
В	-10	LEU	-	expression tag	UNP Q92VL2
В	-9	GLY	-	expression tag	UNP Q92VL2
В	-8	THR	-	expression tag	UNP Q92VL2
В	-7	GLU	-	expression tag	UNP Q92VL2
В	-6	ASN	-	expression tag	UNP Q92VL2
В	-5	LEU	-	expression tag	UNP Q92VL2
В	-4	TYR	-	expression tag	UNP Q92VL2
В	-3	PHE	-	expression tag	UNP Q92VL2
В	-2	GLN	-	expression tag	UNP Q92VL2
В	-1	SER	-	expression tag	UNP Q92VL2
В	0	MSE	-	expression tag	UNP Q92VL2
С	-22	MSE	-	expression tag	UNP Q92VL2



Continu	ieu jioni pre	vious puye			
Chain	Residue	Modelled	Actual	Comment	Reference
С	-21	HIS	-	expression tag	UNP Q92VL2
С	-20	HIS	-	expression tag	UNP Q92VL2
С	-19	HIS	-	expression tag	UNP Q92VL2
С	-18	HIS	-	expression tag	UNP Q92VL2
С	-17	HIS	-	expression tag	UNP Q92VL2
С	-16	HIS	-	expression tag	UNP Q92VL2
С	-15	SER	-	expression tag	UNP Q92VL2
С	-14	SER	-	expression tag	UNP Q92VL2
С	-13	GLY	-	expression tag	UNP Q92VL2
С	-12	VAL	-	expression tag	UNP Q92VL2
С	-11	ASP	-	expression tag	UNP Q92VL2
С	-10	LEU	-	expression tag	UNP Q92VL2
С	-9	GLY	-	expression tag	UNP Q92VL2
С	-8	THR	-	expression tag	UNP Q92VL2
С	-7	GLU	-	expression tag	UNP Q92VL2
С	-6	ASN	-	expression tag	UNP Q92VL2
С	-5	LEU	-	expression tag	UNP Q92VL2
С	-4	TYR	-	expression tag	UNP Q92VL2
С	-3	PHE	-	expression tag	UNP Q92VL2
С	-2	GLN	-	expression tag	UNP Q92VL2
С	-1	SER	-	expression tag	UNP Q92VL2
С	0	MSE	-	expression tag	UNP Q92VL2
D	-22	MSE	-	expression tag	UNP Q92VL2
D	-21	HIS	-	expression tag	UNP Q92VL2
D	-20	HIS	-	expression tag	UNP Q92VL2
D	-19	HIS	-	expression tag	UNP Q92VL2
D	-18	HIS	-	expression tag	UNP Q92VL2
D	-17	HIS	-	expression tag	UNP Q92VL2
D	-16	HIS	-	expression tag	UNP Q92VL2
D	-15	SER	-	expression tag	UNP Q92VL2
D	-14	SER	-	expression tag	UNP Q92VL2
D	-13	GLY	-	expression tag	UNP Q92VL2
D	-12	VAL	-	expression tag	UNP Q92VL2
D	-11	ASP	-	expression tag	UNP Q92VL2
D	-10	LEU	-	expression tag	UNP Q92VL2
D	-9	GLY	-	expression tag	UNP Q92VL2
D	-8	THR	-	expression tag	UNP Q92VL2
D	-7	GLU	-	expression tag	UNP Q92VL2
D	-6	ASN	-	expression tag	UNP Q92VL2
D	-5	LEU	-	expression tag	UNP Q92VL2
D	-4	TYR	-	expression tag	UNP Q92VL2
D	-3	PHE	-	expression tag	UNP Q92VL2



Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLN	-	expression tag	UNP Q92VL2
D	-1	SER	-	expression tag	UNP Q92VL2
D	0	MSE	-	expression tag	UNP Q92VL2
Е	-22	MSE	-	expression tag	UNP Q92VL2
Е	-21	HIS	-	expression tag	UNP Q92VL2
Е	-20	HIS	-	expression tag	UNP Q92VL2
Е	-19	HIS	-	expression tag	UNP Q92VL2
Е	-18	HIS	-	expression tag	UNP Q92VL2
Е	-17	HIS	-	expression tag	UNP Q92VL2
Е	-16	HIS	-	expression tag	UNP Q92VL2
Е	-15	SER	-	expression tag	UNP Q92VL2
Е	-14	SER	-	expression tag	UNP Q92VL2
Е	-13	GLY	-	expression tag	UNP Q92VL2
Е	-12	VAL	-	expression tag	UNP Q92VL2
Е	-11	ASP	-	expression tag	UNP Q92VL2
Е	-10	LEU	-	expression tag	UNP Q92VL2
Е	-9	GLY	-	expression tag	UNP Q92VL2
Е	-8	THR	-	expression tag	UNP Q92VL2
Е	-7	GLU	-	expression tag	UNP Q92VL2
Е	-6	ASN	-	expression tag	UNP Q92VL2
Е	-5	LEU	-	expression tag	UNP Q92VL2
Е	-4	TYR	-	expression tag	UNP Q92VL2
Е	-3	PHE	-	expression tag	UNP Q92VL2
Е	-2	GLN	-	expression tag	UNP Q92VL2
Е	-1	SER	-	expression tag	UNP Q92VL2
Е	0	MSE	-	expression tag	UNP Q92VL2
F	-22	MSE	-	expression tag	UNP Q92VL2
F	-21	HIS	-	expression tag	UNP Q92VL2
F	-20	HIS	-	expression tag	UNP Q92VL2
F	-19	HIS	-	expression tag	UNP Q92VL2
F	-18	HIS	-	expression tag	UNP Q92VL2
F	-17	HIS	-	expression tag	UNP Q92VL2
F	-16	HIS	-	expression tag	UNP Q92VL2
F	-15	SER	-	expression tag	UNP Q92VL2
F	-14	SER	-	expression tag	UNP Q92VL2
F	-13	GLY	-	expression tag	UNP Q92VL2
F	-12	VAL	-	expression tag	UNP Q92VL2
F	-11	ASP	-	expression tag	UNP Q92VL2
F	-10	LEU	-	expression tag	UNP Q92VL2
F	-9	GLY	-	expression tag	UNP Q92VL2
F	-8	THR	-	expression tag	UNP Q92VL2
F	-7	GLU	-	expression tag	UNP $Q92VL2$



					DC
Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	ASN	-	expression tag	UNP Q92VL2
F	-5	LEU	-	expression tag	UNP Q92VL2
F	-4	TYR	-	expression tag	UNP Q92VL2
F	-3	PHE	-	expression tag	UNP Q92VL2
F	-2	GLN	-	expression tag	UNP Q92VL2
\mathbf{F}	-1	SER	-	expression tag	UNP Q92VL2
F	0	MSE	-	expression tag	UNP Q92VL2
G	-22	MSE	-	expression tag	UNP Q92VL2
G	-21	HIS	-	expression tag	UNP Q92VL2
G	-20	HIS	-	expression tag	UNP Q92VL2
G	-19	HIS	-	expression tag	UNP Q92VL2
G	-18	HIS	-	expression tag	UNP Q92VL2
G	-17	HIS	-	expression tag	UNP Q92VL2
G	-16	HIS	-	expression tag	UNP Q92VL2
G	-15	SER	-	expression tag	UNP Q92VL2
G	-14	SER	-	expression tag	UNP Q92VL2
G	-13	GLY	-	expression tag	UNP Q92VL2
G	-12	VAL	-	expression tag	UNP Q92VL2
G	-11	ASP	-	expression tag	UNP Q92VL2
G	-10	LEU	-	expression tag	UNP Q92VL2
G	-9	GLY	-	expression tag	UNP Q92VL2
G	-8	THR	-	expression tag	UNP Q92VL2
G	-7	GLU	-	expression tag	UNP Q92VL2
G	-6	ASN	-	expression tag	UNP Q92VL2
G	-5	LEU	-	expression tag	UNP Q92VL2
G	-4	TYR	_	expression tag	UNP Q92VL2
G	-3	PHE	_	expression tag	UNP Q92VL2
G	-2	GLN	_	expression tag	UNP Q92VL2
G	-1	SER	_	expression tag	UNP Q92VL2
G	0	MSE	_	expression tag	UNP Q92VL2
Н	-22	MSE	-	expression tag	UNP Q92VL2
Н	-21	HIS	-	expression tag	UNP Q92VL2
Н	-20	HIS	-	expression tag	UNP Q92VL2
Н	-19	HIS	-	expression tag	UNP Q92VL2
Н	-18	HIS	-	expression tag	UNP Q92VL2
Н	-17	HIS	_	expression tag	UNP Q92VL2
Н	-16	HIS	-	expression tag	UNP Q92VL2
Н	-15	SER	_	expression tag	UNP 092VL2
Н	-14	SER	-	expression tag	UNP Q92VL2
Н	-13	GLY	_	expression tag	UNP 092VL2
H	-12	VAL	_	expression tag	UNP Q92VL2
H	-11	ASP	-	expression tag	UNP Q92VL2
			1	I I	



Chain	Residue	Modelled	Actual	Comment	Reference
Н	-10	LEU	-	expression tag	UNP Q92VL2
Н	-9	GLY	-	expression tag	UNP Q92VL2
Н	-8	THR	-	expression tag	UNP Q92VL2
Н	-7	GLU	-	expression tag	UNP Q92VL2
Н	-6	ASN	-	expression tag	UNP Q92VL2
Н	-5	LEU	-	expression tag	UNP Q92VL2
Н	-4	TYR	-	expression tag	UNP Q92VL2
Н	-3	PHE	-	expression tag	UNP Q92VL2
Н	-2	GLN	-	expression tag	UNP Q92VL2
Н	-1	SER	-	expression tag	UNP Q92VL2
Н	0	MSE	-	expression tag	UNP Q92VL2
Ι	-22	MSE	-	expression tag	UNP Q92VL2
Ι	-21	HIS	-	expression tag	UNP Q92VL2
Ι	-20	HIS	-	expression tag	UNP Q92VL2
Ι	-19	HIS	-	expression tag	UNP Q92VL2
Ι	-18	HIS	-	expression tag	UNP Q92VL2
Ι	-17	HIS	-	expression tag	UNP Q92VL2
Ι	-16	HIS	-	expression tag	UNP Q92VL2
Ι	-15	SER	-	expression tag	UNP Q92VL2
Ι	-14	SER	-	expression tag	UNP Q92VL2
Ι	-13	GLY	-	expression tag	UNP Q92VL2
Ι	-12	VAL	-	expression tag	UNP Q92VL2
Ι	-11	ASP	-	expression tag	UNP Q92VL2
Ι	-10	LEU	-	expression tag	UNP Q92VL2
Ι	-9	GLY	-	expression tag	UNP Q92VL2
Ι	-8	THR	-	expression tag	UNP Q92VL2
Ι	-7	GLU	-	expression tag	UNP Q92VL2
Ι	-6	ASN	-	expression tag	UNP Q92VL2
Ι	-5	LEU	-	expression tag	UNP Q92VL2
Ι	-4	TYR	-	expression tag	UNP Q92VL2
Ι	-3	PHE	-	expression tag	UNP Q92VL2
Ι	-2	GLN	-	expression tag	UNP Q92VL2
Ι	-1	SER	-	expression tag	UNP Q92VL2
Ι	0	MSE	-	expression tag	UNP Q92VL2
J	-22	MSE	-	expression tag	UNP Q92VL2
J	-21	HIS	-	expression tag	UNP Q92VL2
J	-20	HIS	-	expression tag	UNP Q92VL2
J	-19	HIS	-	expression tag	UNP Q92VL2
J	-18	HIS	-	expression tag	UNP Q92VL2
J	-17	HIS	-	expression tag	UNP Q92VL2
J	-16	HIS	-	expression tag	UNP Q92VL2
J	-15	SER	-	expression tag	UNP Q92VL2



				0	
Chain	Residue	Modelled	Actual	Comment	Reference
J	-14	SER	-	expression tag	UNP Q92VL2
J	-13	GLY	-	expression tag	UNP Q92VL2
J	-12	VAL	-	expression tag	UNP Q92VL2
J	-11	ASP	-	expression tag	UNP Q92VL2
J	-10	LEU	-	expression tag	UNP Q92VL2
J	-9	GLY	-	expression tag	UNP Q92VL2
J	-8	THR	-	expression tag	UNP Q92VL2
J	-7	GLU	-	expression tag	UNP Q92VL2
J	-6	ASN	-	expression tag	UNP Q92VL2
J	-5	LEU	-	expression tag	UNP Q92VL2
J	-4	TYR	-	expression tag	UNP Q92VL2
J	-3	PHE	-	expression tag	UNP Q92VL2
J	-2	GLN	-	expression tag	UNP Q92VL2
J	-1	SER	-	expression tag	UNP Q92VL2
J	0	MSE	-	expression tag	UNP Q92VL2
K	-22	MSE	-	expression tag	UNP Q92VL2
K	-21	HIS	-	expression tag	UNP Q92VL2
K	-20	HIS	-	expression tag	UNP Q92VL2
K	-19	HIS	-	expression tag	UNP Q92VL2
K	-18	HIS	-	expression tag	UNP Q92VL2
K	-17	HIS	-	expression tag	UNP Q92VL2
K	-16	HIS	-	expression tag	UNP Q92VL2
K	-15	SER	-	expression tag	UNP Q92VL2
K	-14	SER	-	expression tag	UNP Q92VL2
K	-13	GLY	-	expression tag	UNP Q92VL2
К	-12	VAL	-	expression tag	UNP Q92VL2
K	-11	ASP	-	expression tag	UNP Q92VL2
K	-10	LEU	-	expression tag	UNP Q92VL2
K	-9	GLY	-	expression tag	UNP Q92VL2
К	-8	THR	-	expression tag	UNP Q92VL2
K	-7	GLU	-	expression tag	UNP Q92VL2
K	-6	ASN	-	expression tag	UNP Q92VL2
К	-5	LEU	-	expression tag	UNP Q92VL2
K	-4	TYR	-	expression tag	UNP Q92VL2
К	-3	PHE	-	expression tag	UNP Q92VL2
K	-2	GLN	-	expression tag	UNP Q92VL2
K	-1	SER	-	expression tag	UNP Q92VL2
K	0	MSE	-	expression tag	UNP Q92VL2
L	-22	MSE	-	expression tag	UNP Q92VL2
L	-21	HIS	-	expression tag	UNP Q92VL2
L	-20	HIS	-	expression tag	UNP Q92VL2
L	-19	HIS	-	expression tag	UNP Q92VL2



Chain	Residue	Modelled	Actual	Comment	Reference
L	-18	HIS	-	expression tag	UNP Q92VL2
L	-17	HIS	-	expression tag	UNP Q92VL2
L	-16	HIS	-	expression tag	UNP Q92VL2
L	-15	SER	-	expression tag	UNP Q92VL2
L	-14	SER	-	expression tag	UNP Q92VL2
L	-13	GLY	-	expression tag	UNP Q92VL2
L	-12	VAL	-	expression tag	UNP Q92VL2
L	-11	ASP	-	expression tag	UNP Q92VL2
L	-10	LEU	-	expression tag	UNP Q92VL2
L	-9	GLY	-	expression tag	UNP Q92VL2
L	-8	THR	-	expression tag	UNP Q92VL2
L	-7	GLU	-	expression tag	UNP Q92VL2
L	-6	ASN	-	expression tag	UNP Q92VL2
L	-5	LEU	-	expression tag	UNP Q92VL2
L	-4	TYR	-	expression tag	UNP Q92VL2
L	-3	PHE	-	expression tag	UNP Q92VL2
L	-2	GLN	-	expression tag	UNP Q92VL2
L	-1	SER	-	expression tag	UNP Q92VL2
L	0	MSE	-	expression tag	UNP Q92VL2

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Н	1	Total Cl 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	203	Total O 203 203	0	0
3	В	195	Total O 195 195	0	0
3	С	147	Total O 149 149	0	2
3	D	165	Total O 165 165	0	0
3	Е	146	Total O 147 147	0	1
3	F	124	Total O 124 124	0	0
3	G	105	Total O 106 106	0	1

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	188	Total O 188 188	0	0
3	Ι	166	Total O 167 167	0	1
3	J	133	Total O 134 134	0	1
3	K	117	Total O 118 118	0	1
3	L	140	Total O 140 140	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: oxidase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	116.49Å 122.94Å 147.69Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	20.00 - 1.80	Depositor
Resolution (A)	45.73 - 1.80	EDS
% Data completeness	99.7 (20.00-1.80)	Depositor
(in resolution range)	99.8 (45.73-1.80)	EDS
R_{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.07 (at 1.81 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
P. P.	0.167 , 0.197	Depositor
n, n_{free}	0.169 , 0.198	DCC
R_{free} test set	9819 reflections (5.04%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 53.1	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16207	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 62.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0947e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL

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| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bo	nd lengths	Bond angles		
1VIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.58	0/1282	0.71	0/1729	
1	В	0.64	2/1229~(0.2%)	0.81	5/1657~(0.3%)	
1	С	0.67	0/1276	0.74	1/1722~(0.1%)	
1	D	0.67	2/1238~(0.2%)	0.71	0/1673	
1	Е	0.51	0/1223	0.70	0/1652	
1	F	0.65	2/1197~(0.2%)	0.70	0/1616	
1	G	0.54	0/1205	0.80	4/1628~(0.2%)	
1	Н	0.54	0/1279	0.76	2/1724~(0.1%)	
1	Ι	0.53	0/1329	0.67	0/1789	
1	J	0.63	2/1175~(0.2%)	0.71	2/1589~(0.1%)	
1	Κ	0.54	0/1111	0.66	0/1500	
1	L	0.49	0/1231	0.69	1/1662~(0.1%)	
All	All	0.59	8/14775~(0.1%)	0.72	$15/\overline{19941}~(0.1\%)$	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
1	В	0	1
1	С	0	1
1	D	0	1
1	F	0	1
1	G	0	1
1	Ι	0	1
1	J	0	1
All	All	0	8

The worst 5 of 8 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	F	101[A]	ARG	CA-C	6.79	1.70	1.52
1	F	101[B]	ARG	CA-C	6.79	1.70	1.52
1	D	56[A]	GLN	CA-C	5.82	1.68	1.52
1	D	56[B]	GLN	CA-C	5.82	1.68	1.52
1	J	56[A]	GLN	CA-C	5.56	1.67	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Н	17	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	L	63	MSE	CG-SE-CE	-8.10	81.08	98.90
1	Н	17	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	G	42[A]	HIS	CA-C-N	-6.70	102.46	117.20
1	G	42[B]	HIS	CA-C-N	-6.70	102.46	117.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	54[B]	GLY	Mainchain
1	В	54[A]	GLY	Mainchain
1	С	54[B]	GLY	Mainchain
1	D	54[B]	GLY	Mainchain
1	F	54[B]	GLY	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1248	0	1236	16	0
1	В	1199	0	1184	6	0
1	С	1232	0	1235	10	0
1	D	1197	0	1184	7	0
1	Ε	1196	0	1180	10	0
1	F	1167	0	1156	12	0
1	G	1171	0	1161	15	0
1	H	1246	0	1231	7	0
1	Ι	1286	0	1277	8	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1145	0	1128	16	0
1	K	1082	0	1076	10	0
1	L	1201	0	1189	15	0
2	Н	1	0	0	0	0
3	А	203	0	0	1	0
3	В	195	0	0	0	0
3	С	149	0	0	4	0
3	D	165	0	0	1	0
3	Е	147	0	0	1	0
3	F	124	0	0	2	0
3	G	106	0	0	3	0
3	Н	188	0	0	0	0
3	Ι	167	0	0	3	0
3	J	134	0	0	4	0
3	K	118	0	0	1	0
3	L	140	0	0	1	0
All	All	16207	0	14237	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 114 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance} \ (\text{\AA}) \end{array}$	Clash overlap (Å)
1:F:101[A]:ARG:HG2	1:F:101[A]:ARG:HH11	1.28	0.98
1:A:40:PHE:CZ	1:E:73:ALA:O	2.27	0.87
1:G:6:ILE:HG23	1:G:10:ASP:HB2	1.57	0.84
1:B:40:PHE:CZ	1:L:73:ALA:O	2.32	0.83
1:C:73:ALA:O	1:H:40:PHE:HZ	1.65	0.80

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



Mol	Chain	Analysed	Favoured Allowed Outliers		Percentiles		
1	А	158/176~(90%)	158 (100%)	0	0	100	100
1	В	152/176~(86%)	151 (99%)	1 (1%)	0	100	100
1	С	156/176~(89%)	155 (99%)	0	1 (1%)	25	12
1	D	152/176~(86%)	151 (99%)	1 (1%)	0	100	100
1	Е	150/176~(85%)	148 (99%)	2(1%)	0	100	100
1	F	147/176~(84%)	147 (100%)	0	0	100	100
1	G	148/176~(84%)	146 (99%)	2(1%)	0	100	100
1	Н	157/176~(89%)	155~(99%)	2(1%)	0	100	100
1	Ι	163/176~(93%)	163 (100%)	0	0	100	100
1	J	145/176~(82%)	141 (97%)	4 (3%)	0	100	100
1	Κ	134/176~(76%)	132 (98%)	2(2%)	0	100	100
1	L	151/176~(86%)	150 (99%)	1 (1%)	0	100	100
All	All	1813/2112~(86%)	1797 (99%)	15 (1%)	1 (0%)	51	36

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	74	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	134/143~(94%)	133~(99%)	1 (1%)	84 81
1	В	128/143~(90%)	128 (100%)	0	100 100
1	С	131/143~(92%)	129 (98%)	2(2%)	65 56
1	D	128/143~(90%)	126 (98%)	2(2%)	62 54
1	Е	126/143~(88%)	125~(99%)	1 (1%)	81 78





Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	F	123/143~(86%)	118~(96%)	5(4%)	30	16
1	G	124/143~(87%)	120~(97%)	4(3%)	39	25
1	Н	134/143~(94%)	134 (100%)	0	100	100
1	Ι	139/143~(97%)	137~(99%)	2(1%)	67	59
1	J	121/143~(85%)	119~(98%)	2(2%)	60	51
1	Κ	115/143~(80%)	114 (99%)	1 (1%)	78	75
1	L	127/143~(89%)	$127 \ (100\%)$	0	100	100
All	All	1530/1716~(89%)	1510 (99%)	20 (1%)	73	62

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	53[B]	PRO
1	J	77	ASN
1	Κ	76	ILE
1	J	120	ARG
1	F	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	15	HIS
1	J	77	ASN
1	Κ	140	HIS
1	Κ	13	GLN
1	F	35	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	151/176~(85%)	-0.04	8 (5%) 26 21	9, 17, 36, 56	0
1	В	146/176~(82%)	-0.08	5 (3%) 45 39	11, 18, 31, 65	0
1	С	148/176~(84%)	0.25	10 (6%) 17 13	9, 16, 51, 76	0
1	D	145/176~(82%)	0.24	12 (8%) 11 8	9, 15, 55, 85	0
1	Ε	149/176~(84%)	0.15	9 (6%) 21 17	10, 20, 49, 69	0
1	F	143/176~(81%)	0.45	17 (11%) 4 3	9, 20, 57, 77	0
1	G	143/176~(81%)	0.71	24 (16%) 1 1	10, 23, 73, 93	0
1	Н	152/176~(86%)	-0.10	3 (1%) 65 61	9, 17, 46, 57	0
1	Ι	153/176~(86%)	0.08	10 (6%) 18 15	9, 19, 48, 74	0
1	J	141/176~(80%)	0.79	27~(19%) 1 0	10, 19, 72, 114	0
1	Κ	133/176~(75%)	0.55	23~(17%) 1 1	10, 21, 64, 71	0
1	L	149/176~(84%)	0.32	15 (10%) 7 5	11, 21, 56, 88	0
All	All	1753/2112 (83%)	0.27	163 (9%) 8 6	9, 19, 57, 114	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	76	ILE	11.4
1	G	113	PRO	10.4
1	J	118	ALA	9.3
1	J	116	PRO	8.4
1	А	-5	LEU	8.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CL	Н	201	1/1	0.97	0.07	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.

