

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 23, 2020 – 02:59 pm BST

PDB ID : 5N76

Title : Crystal structure of the apo-form of the CO dehydrogenase accessory protein

CooT from Rhodospirillum rubrum

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Deposited on : 2017-02-19

Resolution : 1.90 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 following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} Mol Probity & : & 4.02 \text{b-}467 \\ Xtriage (Phenix) & : & 1.13 \end{array}$ 

EDS: 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

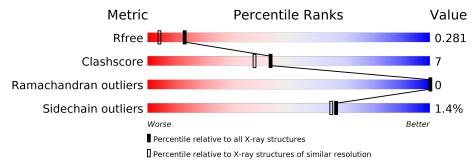
Validation Pipeline (wwPDB-VP) : 2.11

# 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 1.90 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 on 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%

Mol	Chain	Length	Quality of chain		
1	A	66	80%	12%	• 6%
1	В	66	73%	23%	5%
1	С	66	76%	18%	• 5%
1	D	66	77%	14%	• 6%
1	E	66	83%	11%	6%
1	F	66	77%	11% •	11%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3047 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 CooT.

Mol	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$			ZeroOcc	AltConf	Trace
1	A	62	Total 488	C 306	N 84	O 96	S 2	0	5	0
1	D	62	Total 467	C 293	N 82	O 90	S 2	0	1	0
1	В	63	Total 468	C 294	N 83	O 89	S 2	0	1	0
1	С	63	Total 473	C 297	N 83	O 91	S 2	0	1	0
1	Е	62	Total 468	C 294	N 81	O 90	S 3	0	2	0
1	F	59	Total 444	C 279	N 77	O 86	S 2	0	1	0

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	45	Total O 45 45	0	0
2	D	47	Total O 47 47	0	0
2	В	34	Total O 34 34	0	0
2	С	35	Total O 35 35	0	0
2	Е	40	Total O 40 40	0	0
2	F	38	Total O 38 38	0	0



Chain F:

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: CooT Chain A: 80% 12% • Molecule 1: CooT Chain D: 77% • Molecule 1: CooT Chain B: 73% • Molecule 1: CooT Chain C: 76% 18% • Molecule 1: CooT Chain E: 83% • Molecule 1: CooT

77%







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	$108.94 \text{\AA}  108.94 \text{Å}  110.73 \text{Å}$	Donositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.59 - 1.90	Depositor
Resolution (A)	44.60 - 1.90	EDS
% Data completeness	99.2 (44.59-1.90)	Depositor
(in resolution range)	99.3 (44.60-1.90)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.57 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
D D.	(Not available) , (Not available)	Depositor
$R, R_{free}$	0.262 , $0.281$	DCC
$R_{free}$ test set	2631 reflections $(5.00\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37, 55.4	EDS
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.028  for -h,l,k	Xtriage
Estimated twinning fraction	0.027  for -l,-k,-h	Attrage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

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	Boı	nd lengths	Bo	ond angles
WIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5
1	A	1.03	$2/506 \ (0.4\%)$	1.17	6/681 (0.9%)
1	В	0.99	1/474~(0.2%)	1.05	1/638~(0.2%)
1	С	0.90	1/479~(0.2%)	1.02	4/645 (0.6%)
1	D	0.98	0/470	1.04	3/633~(0.5%)
1	Е	1.02	1/477~(0.2%)	1.13	4/642~(0.6%)
1	F	1.10	1/449~(0.2%)	1.10	2/605~(0.3%)
All	All	1.00	6/2855~(0.2%)	1.09	20/3844~(0.5%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain		Type		$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	F	17	GLU	CD-OE1	-9.75	1.15	1.25
1	E	23	GLU	CD-OE2	-9.36	1.15	1.25
1	С	39	GLU	CD-OE1	-6.20	1.18	1.25
1	В	11	ALA	C-O	5.67	1.34	1.23
1	A	39[A]	GLU	CG-CD	5.22	1.59	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	Е	23	GLU	OE1-CD-OE2	-9.92	111.39	123.30
1	A	2	CYS	CA-CB-SG	-6.99	101.41	114.00
1	D	50	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	F	50	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	20	ASP	CB-CG-OD1	6.45	124.10	118.30

There are no chirality outliers.

There are no planarity outliers.



### 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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	Α	488	0	506	10	0
1	В	468	0	484	12	0
1	С	473	0	489	12	1
1	D	467	0	480	13	0
1	Ε	468	0	485	5	1
1	F	444	0	451	6	0
2	A	45	0	0	1	1
2	В	34	0	0	1	0
2	С	35	0	0	2	0
2	D	47	0	0	2	0
2	Ε	40	0	0	1	1
2	F	38	0	0	0	0
All	All	3047	0	2895	37	2

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 7.

The worst 5 of 37 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:A:22:LEU:HD11	1:D:54:ARG:HD2	1.26	1.10
1:B:4:ALA:HB3	1:C:53:LEU:HD21	1.42	0.99
1:A:22:LEU:HD11	1:D:54:ARG:CD	1.95	0.96
1:A:22:LEU:CD1	1:D:54:ARG:HD2	2.02	0.89
1:A:22:LEU:CD1	1:D:54:ARG:CD	2.57	0.81

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	Clash overlap (Å)
2:A:125:HOH:O	2:E:108:HOH:O[2_675]	1.96	0.24
1:C:38:ASP:OD1	1:E:11:ALA:CB[8_666]	2.16	0.04



### 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.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percen	tiles
1	A	65/66~(98%)	65 (100%)	0	0	100	100
1	В	62/66 (94%)	60 (97%)	2 (3%)	0	100	100
1	С	62/66 (94%)	62 (100%)	0	0	100	100
1	D	61/66 (92%)	61 (100%)	0	0	100	100
1	E	62/66 (94%)	61 (98%)	1 (2%)	0	100	100
1	F	56/66 (85%)	56 (100%)	0	0	100	100
All	All	368/396 (93%)	365 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	A	$53/52 \; (102\%)$	53 (100%)	0	100	100
1	В	49/52 (94%)	48 (98%)	1 (2%)	55	51
1	С	50/52~(96%)	49 (98%)	1 (2%)	55	51
1	D	49/52 (94%)	47 (96%)	2 (4%)	30	21
1	E	50/52~(96%)	50 (100%)	0	100	100
1	F	47/52 (90%)	47 (100%)	0	100	100
All	All	298/312 (96%)	294 (99%)	4 (1%)	67	68



All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	CYS
1	D	22	LEU
1	В	63	GLU
1	С	2	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 carbohydrates in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

