

wwPDB X-ray Structure Validation Summary Report (i)

Apr 6, 2022 – 12:04 PM EDT

PDB ID : 7S5O

Title : Crystal structure of Cytochrome c' beta from Nitrosomonas europaea ATCC

19718

Authors: Seattle Structural Genomics Center for Infectious Disease (SSGCID)

Deposited on : 2021-09-11

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

MolProbity : FAILED

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

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 (i)

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

The reported resolution of this entry is 1.80 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 4461 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 Cytochrome_P460 domain-containing protein.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	Λ	156	Total	С	N	О	S	0	4	0
1	A	190	1221	774	206	236	5	0	4	
1	D	156	Total	С	N	О	S	0	4	0
1	I B	156	1228	783	203	238	4	0		
1	C	160	Total	С	N	О	S	0	1	0
1	C	C 160	1229	783	207	235	4	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	_	initiating methionine	UNP Q82W71
A	175	LYS	-	expression tag	UNP Q82W71
A	176	LEU	-	expression tag	UNP Q82W71
A	177	ALA	-	expression tag	UNP Q82W71
A	178	ALA	-	expression tag	UNP Q82W71
A	179	ALA	-	expression tag	UNP Q82W71
A	180	LEU	-	expression tag	UNP Q82W71
A	181	GLU	-	expression tag	UNP Q82W71
A	182	LEU	-	expression tag	UNP Q82W71
A	183	GLU	-	expression tag	UNP Q82W71
A	184	HIS	-	expression tag	UNP Q82W71
A	185	HIS	-	expression tag	UNP Q82W71
A	186	HIS	-	expression tag	UNP Q82W71
A	187	HIS	-	expression tag	UNP Q82W71
A	188	HIS	-	expression tag	UNP Q82W71
A	189	HIS	-	expression tag	UNP Q82W71
В	0	MET	-	initiating methionine	UNP Q82W71
В	175	LYS	-	expression tag	UNP Q82W71
В	176	LEU	-	expression tag	UNP Q82W71
В	177	ALA	-	expression tag	UNP Q82W71
В	178	ALA	-	expression tag	UNP Q82W71
В	179	ALA	-	expression tag	UNP Q82W71
В	180	LEU	-	expression tag	UNP Q82W71

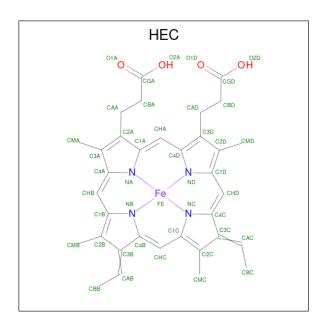


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Chain	Residue	Modelled	Actual	Comment	Reference
В	181	GLU	-	expression tag	UNP Q82W71
В	182	LEU	-	expression tag	UNP Q82W71
В	183	GLU	=	expression tag	UNP Q82W71
В	184	HIS	=	expression tag	UNP Q82W71
В	185	HIS	-	expression tag	UNP Q82W71
В	186	HIS	-	expression tag	UNP Q82W71
В	187	HIS	-	expression tag	UNP Q82W71
В	188	HIS	-	expression tag	UNP Q82W71
В	189	HIS	-	expression tag	UNP Q82W71
С	0	MET	-	initiating methionine	UNP Q82W71
С	175	LYS	ı	expression tag	UNP Q82W71
С	176	LEU	-	expression tag	UNP Q82W71
С	177	ALA	-	expression tag	UNP Q82W71
С	178	ALA	-	expression tag	UNP Q82W71
С	179	ALA	-	expression tag	UNP Q82W71
С	180	LEU	-	expression tag	UNP Q82W71
С	181	GLU	-	expression tag	UNP Q82W71
С	182	LEU	-	expression tag	UNP Q82W71
С	183	GLU	-	expression tag	UNP Q82W71
С	184	HIS	=	expression tag	UNP Q82W71
С	185	HIS	=	expression tag	UNP Q82W71
С	186	HIS	-	expression tag	UNP Q82W71
С	187	HIS	=	expression tag	UNP Q82W71
С	188	HIS	-	expression tag	UNP Q82W71
С	189	HIS	-	expression tag	UNP Q82W71

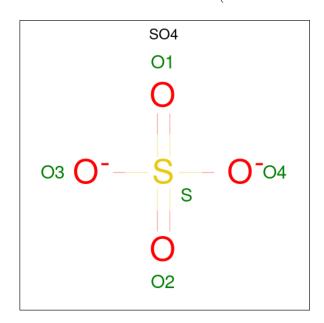
• Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	Λ	1	Total	С	Fe	N	О	0	0	
	Λ		43	34	1	4	4			
2	D	1	Total	С	Fe	N	О	0	0	
	Б	1	43	34	1	4	4	0	U	
9	С	1	Total	С	Fe	N	О	0	0	
		1	43	34	1	4	4	0	U	

 \bullet Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



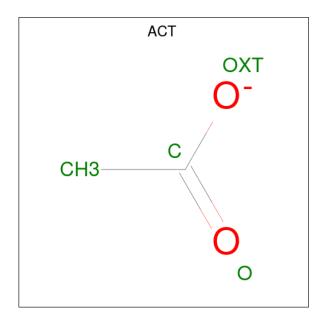
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0



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

 \bullet Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	В	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	210	Total O 216 216	0	6



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	196	Total O 202 202	0	5
5	С	191	Total O 194 194	0	3

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 1 21 1	Depositor
Cell constants	41.79Å 88.17Å 75.85Å	Depositor
a, b, c, α , β , γ	90.00° 101.62° 90.00°	Depositor
Resolution (Å)	35.94 - 1.80	Depositor
% Data completeness	97.5 (35.94-1.80)	Depositor
(in resolution range)	31.9 (30.34-1.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.38 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.155 , 0.190	Depositor
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.585	Xtriage
L-test for twinning ²	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4461	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.98% 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)

12 ligands are modelled in this entry.

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	Tuna	Chain	Res	Link	В	ond leng	gths	В	ond ang	cles
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	С	202	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	A	204	_	4,4,4	0.14	0	6,6,6	0.23	0
2	HEC	A	201	1	26,50,50	2.09	6 (23%)	18,82,82	2.17	5 (27%)
3	SO4	A	202	-	4,4,4	0.13	0	6,6,6	0.09	0
4	ACT	A	203	-	1,3,3	3.91	1 (100%)	0,3,3	-	-
4	ACT	В	203	-	1,3,3	2.49	1 (100%)	0,3,3	_	-
3	SO4	С	205	-	4,4,4	0.13	0	6,6,6	0.08	0
4	ACT	С	203	-	1,3,3	5.87	1 (100%)	0,3,3	-	-
3	SO4	С	204	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	В	202	_	4,4,4	0.13	0	6,6,6	0.14	0
2	HEC	В	201	1	26,50,50	2.26	3 (11%)	18,82,82	1.85	4 (22%)
2	HEC	С	201	1	26,50,50	2.30	5 (19%)	18,82,82	1.70	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	В	201	1	-	0/6/54/54	-
2	HEC	A	201	1	-	0/6/54/54	-
2	HEC	С	201	1	-	0/6/54/54	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	201	HEC	C2B-C3B	-5.90	1.34	1.40
4	С	203	ACT	СН3-С	5.87	1.56	1.48
2	С	201	HEC	C3C-C2C	-5.79	1.34	1.40
2	С	201	HEC	C2B-C3B	-5.59	1.34	1.40
2	В	201	HEC	C3C-C2C	-5.53	1.35	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	${f Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	A	201	HEC	CMC-C2C-C1C	-5.95	119.33	128.46
2	С	201	HEC	CMC-C2C-C1C	-4.62	121.36	128.46



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
2	В	201	HEC	CBA-CAA-C2A	-3.97	105.16	112.48
2	В	201	HEC	CMC-C2C-C1C	-3.80	122.62	128.46
2	A	201	HEC	CMB-C2B-C1B	-3.58	122.95	128.46

There are no chirality outliers.

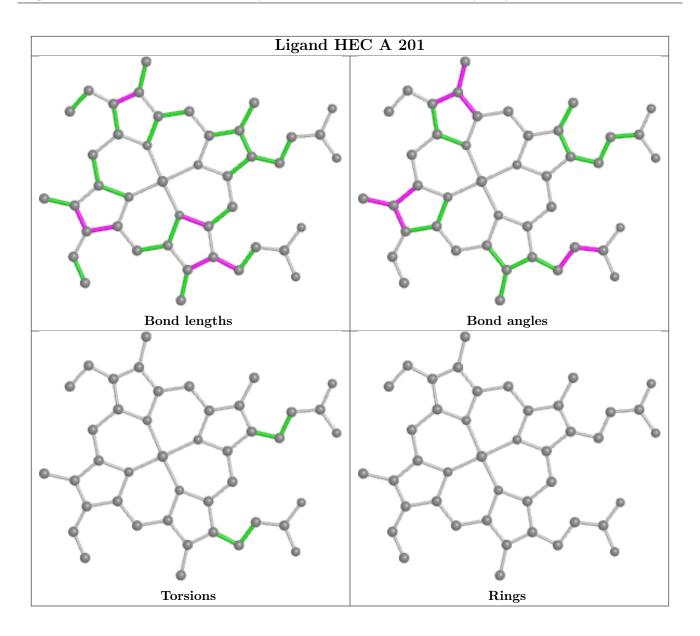
There are no torsion outliers.

There are no ring outliers.

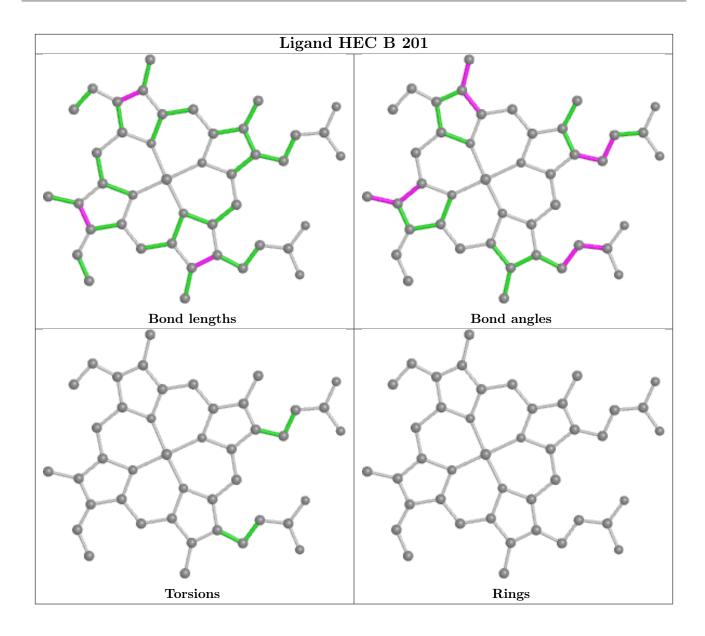
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

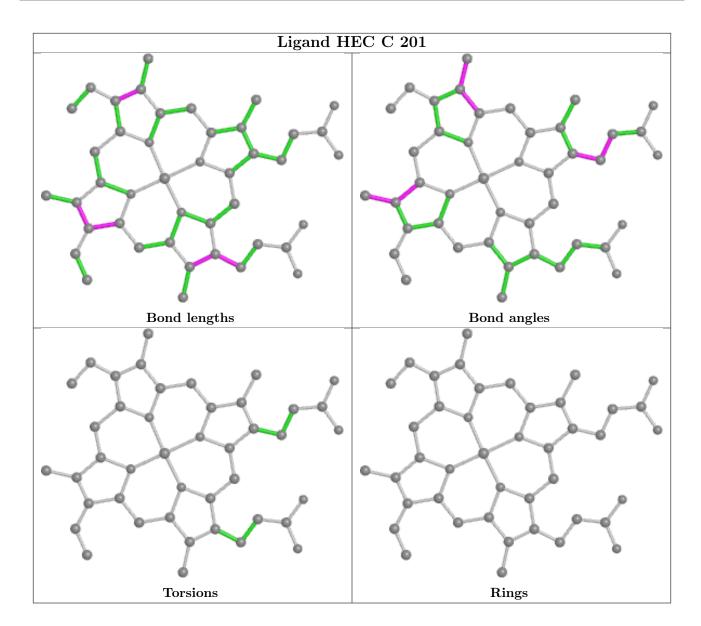












4.7 Other polymers (i)

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.

