

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 08:16 AM EDT

PDB ID	:	6W0S
Title	:	Crystal structure of substrate free cytochrome P450 NasF5053 from Strepto-
		myces sp. NRRL F-5053
Authors	:	Luo, Z.; Jia, X.; Sun, C.; Qu, X.; Kobe, B.
Deposited on		
Resolution	:	1.70 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
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)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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.



6W0S

2 Entry composition (i)

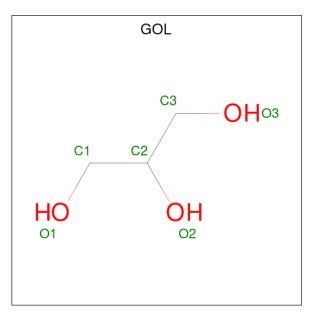
There are 7 unique types of molecules in this entry. The entry contains 12933 atoms, of which 5953 are hydrogens and 0 are deuteriums.

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 P450-F5053.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	397	Total 6047	C 1926		N 558	O 571	S 12	0	1	0
1	В	396	Total 6013	C 1923		N 557	O 569	S 12	0	1	0

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C H O 14 3 8 3	0	0

• Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

[Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	А	2	Total Br 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	2	Total Br 2 2	0	0

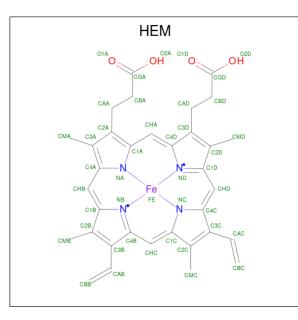
• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	4	Total Cl 4 4	0	0
4	В	2	Total Cl 2 2	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

\mathbf{M}	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
5		А	1	Total Na 1 1	0	0
5		В	1	Total Na 1 1	0	0

• Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		A	tom	s			ZeroOcc	AltConf
6	А	1	Total 49	C 34	Fe 1	Н 6	N 4	0 4	0	0

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Mol	Chain	Residues		A	tom	IS			ZeroOcc	AltConf
6	В	1	Total	C 24	Fe	H 7	N 4	0	0	0
			06	34	T	(4	4		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	378	Total O 378 378	0	0
7	В	370	Total O 370 370	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	42.21Å 91.33Å 98.28Å	Depositor
a, b, c, α , β , γ	90.00° 96.41° 90.00°	Depositor
Resolution (Å)	43.06 - 1.70	Depositor
% Data completeness	99.7 (43.06-1.70)	Depositor
(in resolution range)	55.1 (45.00 1.10)	-
R _{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.91 (at 1.70 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.186 , 0.220	Depositor
Wilson B-factor $(Å^2)$	17.1	Xtriage
Anisotropy	0.410	Xtriage
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12933	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 51.93 % 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 5.2301e-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.

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 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 for Mogul analysis.

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



N/-1	T 0	Chain	Dag	T : 1-	Bond lengths			Bond angles		
Mol	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	HEM	А	409	1,7	41,50,50	1.59	7 (17%)	45,82,82	1.41	6 (13%)
2	GOL	А	401	-	$5,\!5,\!5$	0.53	0	$5,\!5,\!5$	0.97	0
6	HEM	В	406	1,7	41,50,50	1.47	7 (17%)	45,82,82	1.47	6 (13%)

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).

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
6	HEM	А	409	1,7	-	0/12/54/54	-
2	GOL	А	401	-	-	2/4/4/4	-
6	HEM	В	406	1,7	-	3/12/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	А	409	HEM	C3C-C2C	-4.91	1.33	1.40
6	В	406	HEM	C3C-C2C	-4.53	1.34	1.40
6	А	409	HEM	CAA-C2A	3.89	1.57	1.52
6	В	406	HEM	CAA-C2A	3.11	1.56	1.52
6	В	406	HEM	C3B-C2B	-2.79	1.31	1.37
6	А	409	HEM	C3C-CAC	2.67	1.53	1.47
6	А	409	HEM	CAB-C3B	2.50	1.54	1.47
6	А	409	HEM	C3B-C2B	-2.38	1.32	1.37
6	А	409	HEM	C1A-NA	2.27	1.40	1.36
6	В	406	HEM	C3C-CAC	2.17	1.52	1.47
6	В	406	HEM	C1A-NA	2.12	1.40	1.36
6	В	406	HEM	CAB-C3B	2.09	1.53	1.47
6	В	406	HEM	CMD-C2D	2.07	1.55	1.50
6	А	409	HEM	CMD-C2D	2.01	1.55	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
6	В	406	HEM	C2C-C3C-C4C	4.81	110.26	106.90
6	А	409	HEM	C2C-C3C-C4C	4.63	110.13	106.90

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	409	HEM	C4A-C3A-C2A	3.26	109.26	107.00
6	В	406	HEM	CMA-C3A-C4A	-3.10	123.70	128.46
6	В	406	HEM	C3C-C4C-NC	-2.94	105.38	110.94
6	А	409	HEM	CMA-C3A-C4A	-2.92	123.98	128.46
6	В	406	HEM	C4A-C3A-C2A	2.68	108.86	107.00
6	А	409	HEM	C3B-C2B-C1B	2.54	108.37	106.49
6	В	406	HEM	C4B-CHC-C1C	2.51	125.86	122.56
6	А	409	HEM	C3C-C4C-NC	-2.49	106.24	110.94
6	А	409	HEM	C4B-CHC-C1C	2.49	125.84	122.56
6	В	406	HEM	CMC-C2C-C3C	2.27	128.93	124.68

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There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	401	GOL	O1-C1-C2-O2
2	А	401	GOL	O1-C1-C2-C3
6	В	406	HEM	CAD-CBD-CGD-O2D
6	В	406	HEM	CAD-CBD-CGD-O1D
6	В	406	HEM	CAA-CBA-CGA-O2A

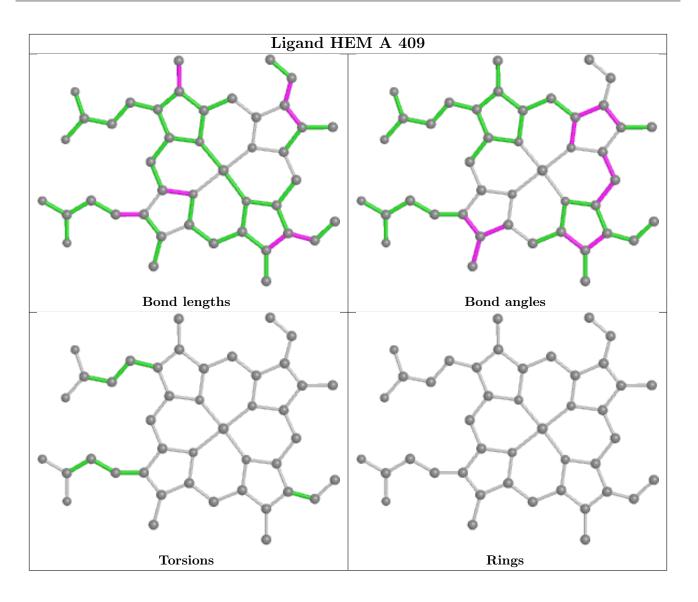
There are no ring outliers.

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.

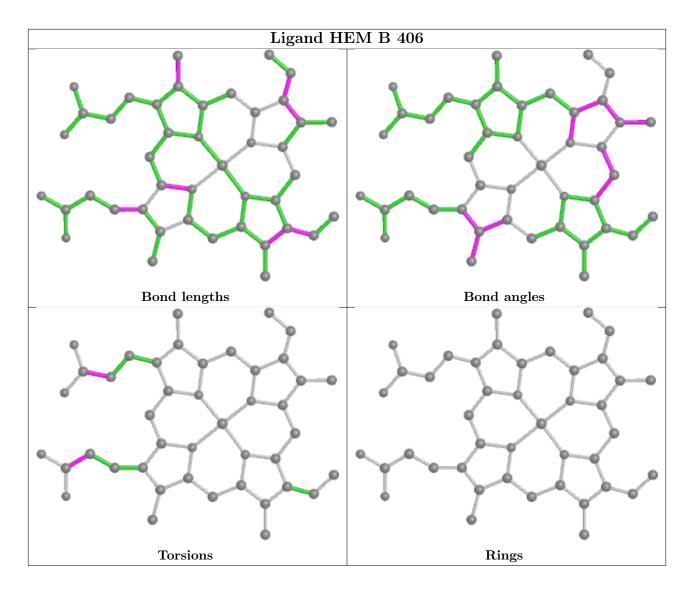












4.7 Other polymers (i)

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.

