wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 01:17 pm GMT

PDB ID	:	2VKU
Title	:	4,4'-Dihydroxybenzophenone Mimics Sterol Substrate in the Binding Site of Sterol 14alpha-Demethylase (CYP51) in the X-ray Structure of the Complex
Authors	:	Eddine, A.N.; von Kries, J.P.; Podust, M.V.; Podust, L.M.
Deposited on	:	2007-12-29
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.

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

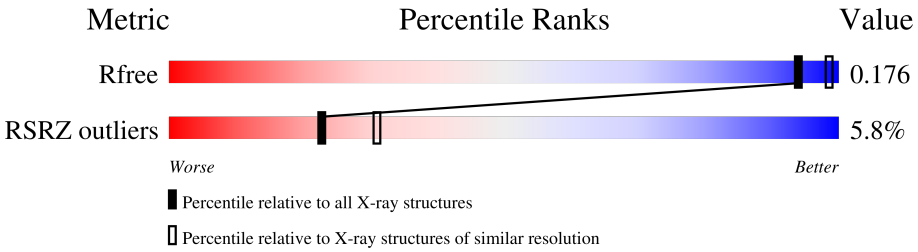
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

MolProbity 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 4217 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.

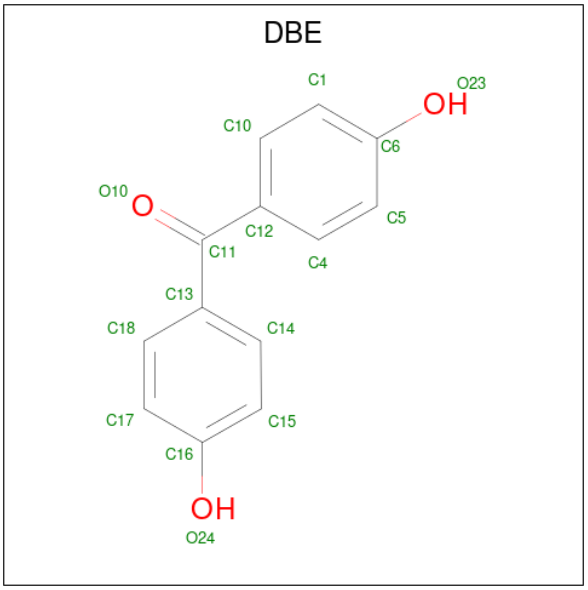
- Molecule 1 is a protein called CYTOCHROME P450 51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3546	2233	639	657	17	0	3	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	LEU	CYS	engineered mutation	UNP P0A512
A	442	ALA	CYS	engineered mutation	UNP P0A512

- Molecule 2 is bis(4-hydroxyphenyl)methanone (three-letter code: DBE) (formula: $C_{13}H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	16	13	3		0	0
2	A	1	Total	C	O		0	1
			32	26	6			

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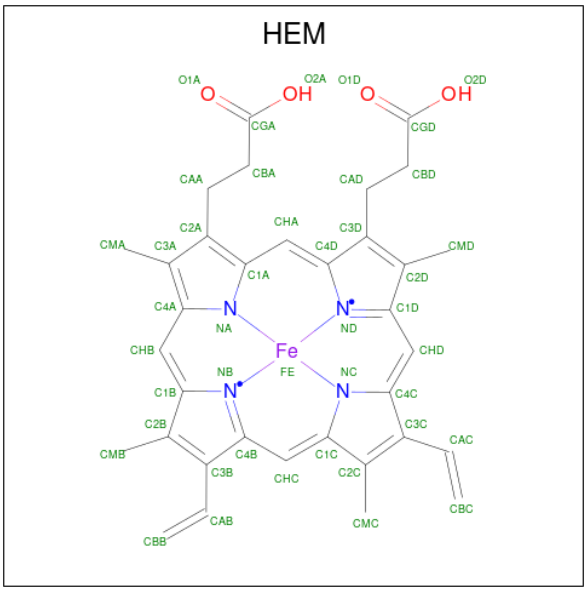
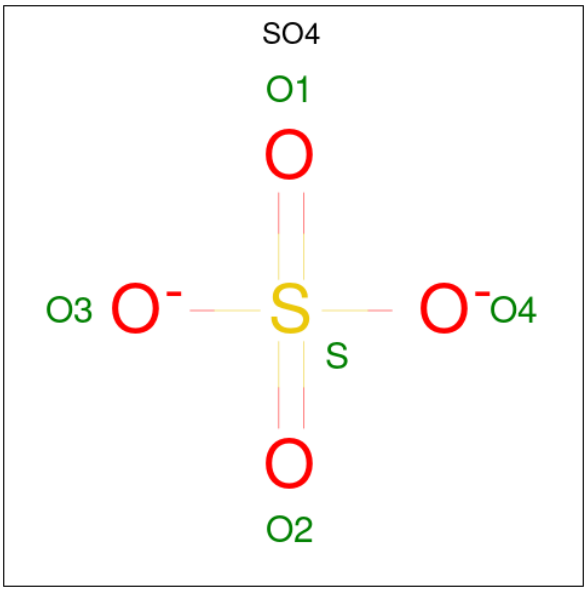
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 13 3	0	0
2	A	1	Total C O 16 13 3	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	518	Total O 518 518	0	0

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

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.73Å 82.09Å 85.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 1.95 47.17 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.17-1.95) 99.6 (47.17-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.41 (at 1.95Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.177 , 0.212 0.174 , 0.176	Depositor DCC
R_{free} test set	4033 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4217	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DBE	A	1447[A]	-	17,17,17	2.03	6 (35%)	23,23,23	0.91	1 (4%)
4	SO4	A	1456	-	4,4,4	0.70	0	6,6,6	0.42	0
3	HEM	A	1450	1	41,50,50	1.31	5 (12%)	45,82,82	1.10	2 (4%)
4	SO4	A	1454	-	4,4,4	0.60	0	6,6,6	0.40	0
4	SO4	A	1455	-	4,4,4	0.68	0	6,6,6	0.38	0
4	SO4	A	1452	-	4,4,4	0.49	0	6,6,6	0.39	0
2	DBE	A	1448	-	17,17,17	1.86	5 (29%)	23,23,23	1.09	1 (4%)
4	SO4	A	1457	-	4,4,4	0.65	0	6,6,6	0.41	0
2	DBE	A	1447[B]	-	17,17,17	1.90	8 (47%)	23,23,23	0.88	1 (4%)
2	DBE	A	1446	-	17,17,17	2.05	8 (47%)	23,23,23	1.12	1 (4%)
2	DBE	A	1449	-	17,17,17	1.88	7 (41%)	23,23,23	0.93	1 (4%)
4	SO4	A	1453	-	4,4,4	0.61	0	6,6,6	0.45	0

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	DBE	A	1447[A]	-	-	4/8/8/8	0/2/2/2
3	HEM	A	1450	1	-	3/12/54/54	-
2	DBE	A	1448	-	-	4/8/8/8	0/2/2/2
2	DBE	A	1447[B]	-	-	2/8/8/8	0/2/2/2
2	DBE	A	1446	-	-	0/8/8/8	0/2/2/2
2	DBE	A	1449	-	-	0/8/8/8	0/2/2/2

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1450	HEM	C3C-CAC	-3.35	1.40	1.47
2	A	1447[A]	DBE	C12-C11	3.02	1.54	1.49
2	A	1446	DBE	C14-C13	3.00	1.44	1.39
2	A	1446	DBE	C12-C11	2.92	1.54	1.49
2	A	1448	DBE	C18-C13	2.92	1.44	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1446	DBE	C13-C11-C12	3.40	125.87	120.28
2	A	1448	DBE	C13-C11-C12	2.78	124.86	120.28
3	A	1450	HEM	C4B-C3B-C2B	-2.70	104.97	107.11
2	A	1447[A]	DBE	C13-C11-C12	2.57	124.51	120.28
2	A	1449	DBE	C13-C11-C12	2.56	124.49	120.28

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

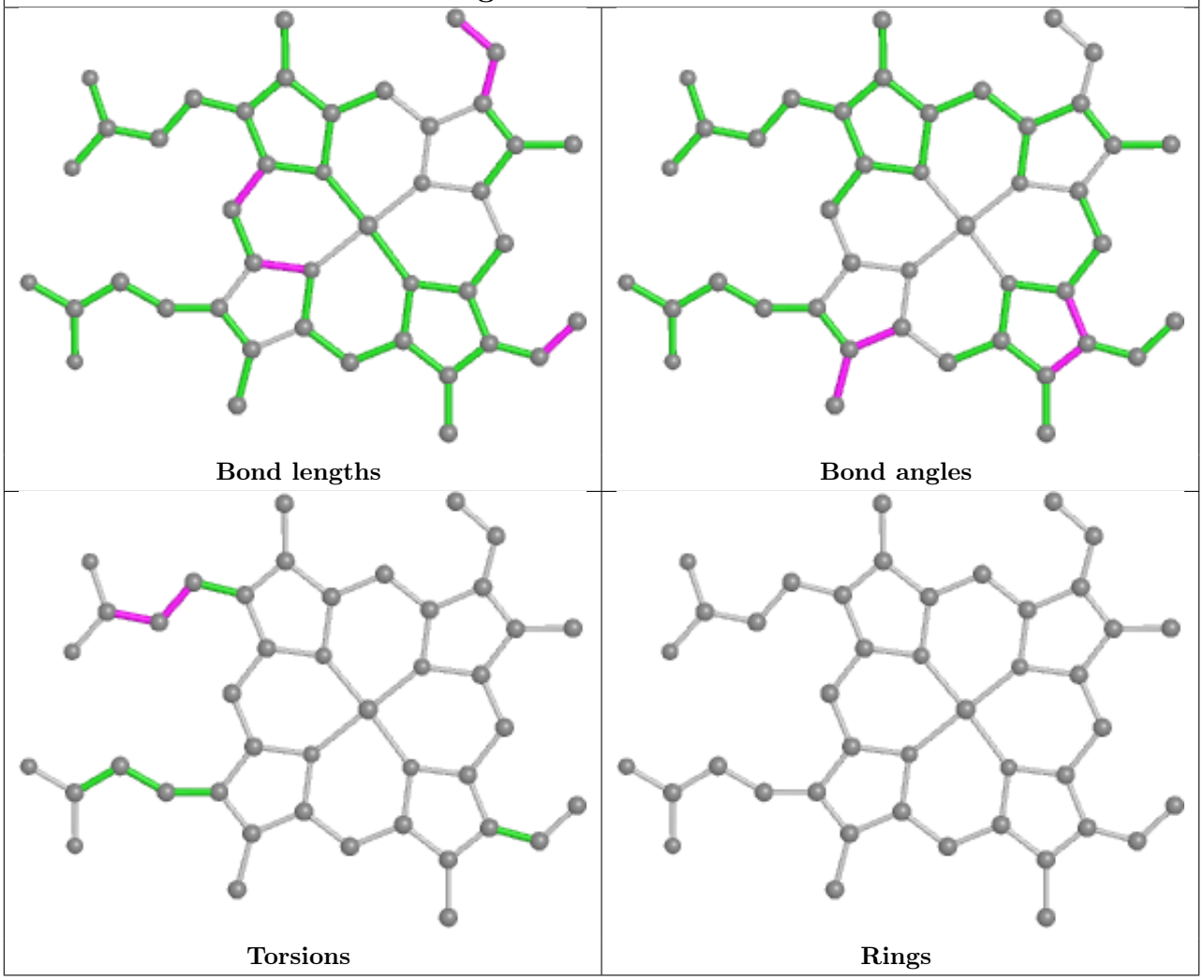
Mol	Chain	Res	Type	Atoms
2	A	1447[A]	DBE	O10-C11-C13-C18
2	A	1447[A]	DBE	C12-C11-C13-C18
2	A	1447[A]	DBE	C12-C11-C13-C14
2	A	1447[A]	DBE	O10-C11-C13-C14
3	A	1450	HEM	C3D-CAD-CBD-CGD

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.

Ligand HEM A 1450



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

5.1 Protein, DNA and RNA chains

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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	445/455 (97%)	0.09	26 (5%)	23	31	11, 20, 49, 65	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	THR	7.2
1	A	219	ASP	5.9
1	A	217	PRO	5.4
1	A	216	PRO	5.0
1	A	7	PRO	4.3

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

There are no monosaccharides in this entry.

5.4 Ligands

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	B-factors(Å^2)	Q<0.9
2	DBE	A	1447[A]	16/16	0.70	0.35	37,40,41,42	16
2	DBE	A	1447[B]	16/16	0.70	0.35	35,36,37,38	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1457	5/5	0.81	0.23	98,98,99,99	0
4	SO4	A	1456	5/5	0.84	0.26	64,64,66,66	0
2	DBE	A	1448	16/16	0.86	0.18	24,27,30,32	0
2	DBE	A	1446	16/16	0.90	0.15	29,31,34,35	0
4	SO4	A	1455	5/5	0.93	0.17	63,63,64,64	0
2	DBE	A	1449	16/16	0.95	0.14	14,21,24,25	0
4	SO4	A	1454	5/5	0.97	0.10	32,33,34,38	0
3	HEM	A	1450	43/43	0.97	0.13	10,13,27,37	0
4	SO4	A	1453	5/5	0.98	0.10	31,31,34,35	0
4	SO4	A	1452	5/5	0.99	0.12	23,25,27,27	0

5.5 Other polymers (i)

There are no such residues in this entry.