

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2CIB
Title	:	High throughput screening and x-ray crystallography assisted evaluation of
		small molecule scaffolds for CYP51 inhibitors
Authors	:	Podust, L.M.; Kim, Y.; Yermalitskaya, L.V.; Von Kries, J.P.; Waterman, M.R.
Deposited on	:	2006-03-17
Resolution	:	1.50 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	:	1.8.4, 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

PERCENTILES INFOmissingINFO



1 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3803 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					AltConf	Trace
1	А	420	Total 3373	C 2132	N 613	0 611	S 17	0	5	1

There are 2 discrepancies between the modelled and reference sequences:

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

• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	А	1	Total 43	С 34	Fe 1	N 4	0 4	0	0

• Molecule 3 is (2S)-2-[(2,1,3-BENZOTHIADIAZOL-4-YLSULFONYL)AMINO]-2-PHENYL-



N-PYRIDIN-4-YLACETAMIDE (three-letter code: CM6) (formula: $C_{19}H_{15}N_5O_3S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	А	1	Total 29	C 19	N 5	O 3	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	358	Total O 358 358	0	0

SEQUENCE-PLOTS INFOmissingINFO



2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	44.94Å 85.89Å 111.01Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	33.97 - 1.50	Depositor
Resolution (A)	33.97 - 1.50	EDS
% Data completeness	93.8 (33.97-1.50)	Depositor
(in resolution range)	93.7 (33.97 - 1.50)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.45 (at 1.50 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.204 , 0.226	Depositor
II, II free	0.199 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	17.7	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.54 , 64.1	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3803	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 5.17% of the height of the origin peak. No significant pseudotranslation is detected.

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.

3 Model quality (i)

3.1 Standard geometry (i)

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

3.2 Too-close contacts (i)

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

3.3 Torsion angles (i)

3.3.1 Protein backbone (i)

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

3.3.2 Protein sidechains (i)

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

3.3.3 RNA (i)

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

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

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

2 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



	Mol	Turne	Chain	Dec	T :1.	Bo	ond leng	$_{\rm ths}$	Bond angles		
		Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	2	HEM	А	1449	3,1	41,50,50	1.36	8 (19%)	45,82,82	1.12	3 (6%)
	3	CM6	А	1450	2	32,32,32	1.74	7 (21%)	36,45,45	1.33	5 (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
2	HEM	А	1449	3,1	-	0/12/54/54	-
3	CM6	А	1450	2	-	0/23/23/23	0/4/4/4

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	1450	CM6	S1-N3	4.47	1.69	1.61
2	А	1449	HEM	C3C-CAC	-3.46	1.40	1.47
3	А	1450	CM6	C8-C13	3.30	1.45	1.42
2	А	1449	HEM	CBB-CAB	3.10	1.45	1.30
3	А	1450	CM6	C7-C1	-2.91	1.47	1.54
3	А	1450	CM6	C2-N1	-2.74	1.36	1.41
2	А	1449	HEM	C3C-C2C	-2.38	1.37	1.40
2	А	1449	HEM	CHB-C1B	2.38	1.41	1.35
2	А	1449	HEM	CBC-CAC	2.36	1.44	1.29
3	А	1450	CM6	S2-N5	-2.34	1.57	1.65
2	А	1449	HEM	CAB-C3B	-2.30	1.41	1.47
3	А	1450	CM6	S2-N4	-2.26	1.57	1.65
3	А	1450	CM6	C6-C5	-2.26	1.34	1.38
2	А	1449	HEM	C4A-NA	2.09	1.40	1.36
2	А	1449	HEM	C2C-C1C	2.01	1.47	1.42

All (15) bond length outliers are listed below:

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	1449	HEM	C3B-C2B-C1B	3.63	109.18	106.49
3	А	1450	CM6	C5-N2-C4	3.45	124.96	116.85
2	А	1449	HEM	CBA-CAA-C2A	-3.13	107.28	112.62
3	А	1450	CM6	C9-C8-S1	2.94	120.46	116.98

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	1450	CM6	C6-C5-N2	-2.64	119.02	123.62
3	А	1450	CM6	C3-C4-N2	-2.63	119.05	123.62
2	А	1449	HEM	C4B-C3B-C2B	-2.44	105.18	107.11
3	А	1450	CM6	O3-S1-O2	2.02	122.03	119.55

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There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



4 Fit of model and data (i)

4.1 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	< RSRZ >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	420/455~(92%)	0.39	25 (5%) 21 23	14, 21, 38, 61	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	449	THR	6.6
1	А	105	LEU	4.7
1	А	106	ARG	4.3
1	А	107	GLY	4.2
1	А	108	GLU	3.9
1	А	67	ASP	3.9
1	А	336	GLY	3.9
1	А	68	ASP	3.7
1	А	222	ASP	3.4
1	А	333	GLU	3.0
1	А	372	GLN	3.0
1	А	84	GLY	2.8
1	А	393	ARG	2.8
1	А	140	PHE	2.8
1	А	315	LEU	2.5
1	А	329	LYS	2.5
1	А	321	LEU	2.4
1	А	322	ILE	2.4
1	А	235	GLU	2.4
1	А	338[A]	ARG	2.3
1	А	66	GLY	2.3
1	А	234	ALA	2.2
1	А	24	THR	2.2
1	А	185	TYR	2.0
1	А	63	PHE	2.0



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

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

4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

4.4 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	${f B}$ -factors(Å ²)	Q < 0.9
3	CM6	А	1450	29/29	0.88	0.14	17,20,29,33	0
2	HEM	А	1449	43/43	0.96	0.11	14,17,28,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









4.5 Other polymers (i)

There are no such residues in this entry.

