



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:57 pm GMT

PDB ID : 1FCB
Title : MOLECULAR STRUCTURE OF FLAVOCYTOCHROME B2 AT 2.4
ANGSTROMS RESOLUTION
Authors : Mathews, F.S.; Xia, Z.-X.
Deposited on : 1990-01-16
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

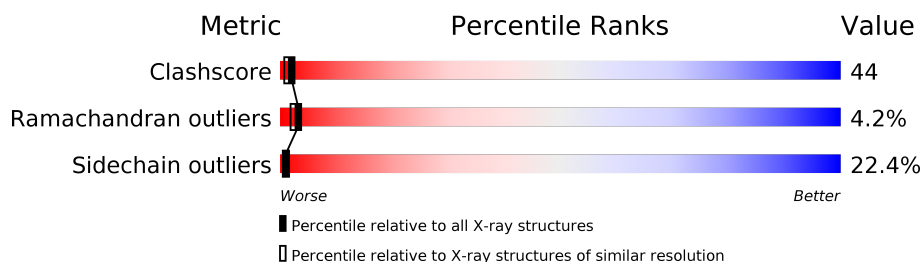
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	
1	B	511	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMN	A	570	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7342 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 FLAVOCYTOCHROME B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3841	2446	652	728	15			
1	B	400	Total	C	N	O	S	0	0	0
			3107	1968	529	599	11			

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



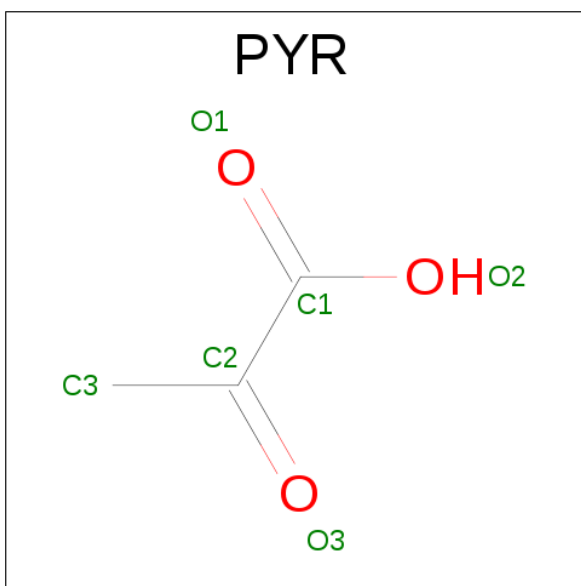
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

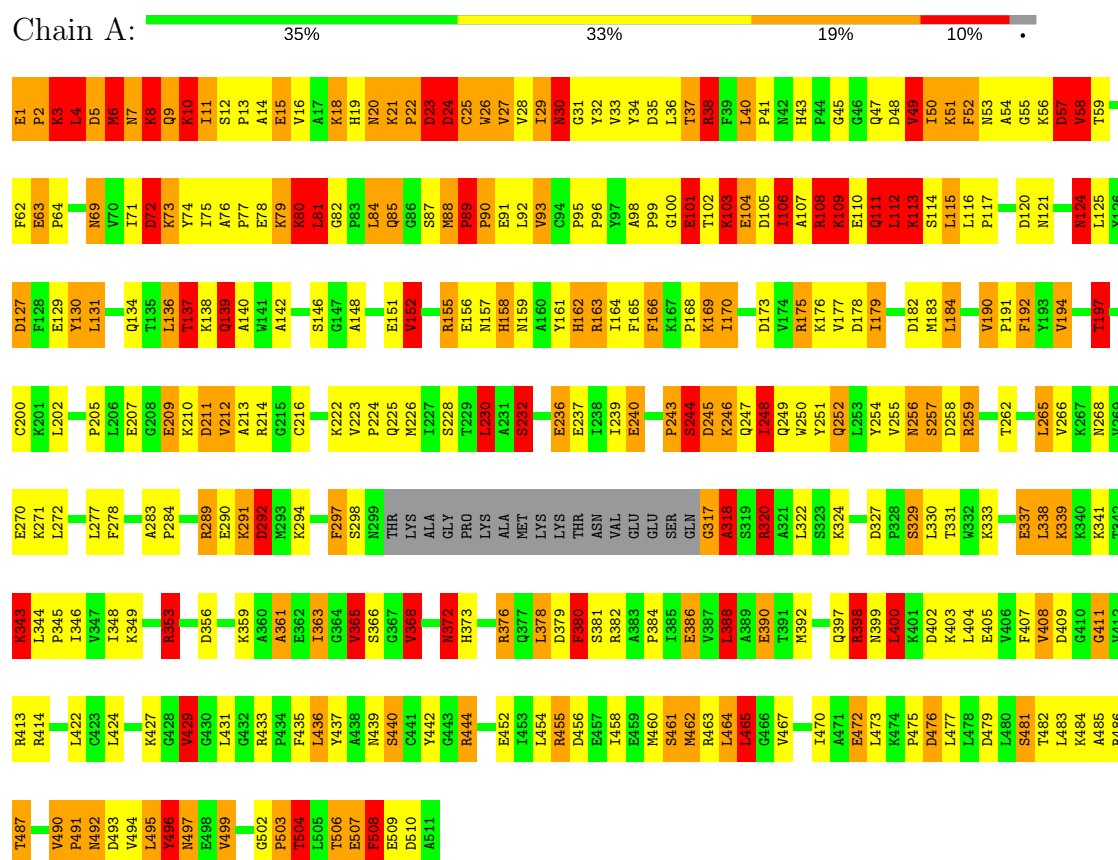
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total 182	O 182	0	0
5	B	101	Total 101	O 101	0	0

3 Residue-property plots

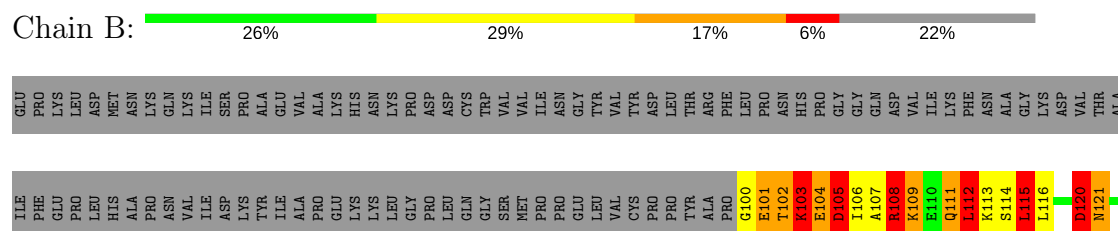
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: FLAVOCYTOCHROME B2



• Molecule 1: FLAVOCYTOCHROME B2



L464	L465	T468	S469	I470	A471	E472	L473	K474	P475	D476	L477	L478	D479	L480	S481	T482	L483	K484	A485	R486	T487	V488	G489	V490	P491	N492	D493	Y496	N497	E498	V499	Y500	E501	G502	P503	T504	L505	T506	E507	F508	E509	D510	A511															
Y254	V255	N256	D258	R259	K260	T261	D263	V266	K267	L268	V269	E270	L272	G273	V274	K275	A276	L277	F278	V281	D282	S285	L286	G287	Q288	R289	E290	K291	D292	N293	K294	L295	K296	F297	S298	N299	THR	LYS	ALA	GLY	PRO	LYS	ALA	MET	LYS	THR	ASN	V312	E313	E314	S315	Q316						
G317	A318	S319	S323	K324	F325	L326	D327	P328	L330	S329	T331	W332	K333	D334	I335	G336	E337	L338	K339	K343	I346	V347	I348	K349	G350	V351	Q352	R353	T354	E355	V363	V369	L370	H373	R376	Q377	L378	D379	F380	S381	R382	A383	P384	I385	E386	V387	L388	A389	E390	T391	M392	P393						
D189	V190	P191	F192	Y193	V194	S195	A196	T197	C200	K201	L202	G203	N204	E207	G208	E209	K210	D211	V212	A213	G147	R214	G217	Q218	G219	V220	T221	K222	V223	P224	Q225	M226	I227	H162	S228	T229	L230	A231	S232	C233	S234	P235	E236	E237	I238	I239	P243	S244	K245	K246	Q247	I248	Q249	W250	Y251	Q252	H187	L253
N124	L125	Y126	D127	F128	E129	Y130	L131	A132	S133	Q134	T135	L136	T137	K138	Q139	A140	Y143	Y144	S145	S146	G147	N149	D150	E151	V152	R155	E156	N159	A160	Y161	H162	R163	T164	F165	F166	K167	P168	K169	L170	L171	V172	D173	V174	R175	K176	V177	D178	D182	N183	L184	G185	S186	H187	V188				

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.51Å 165.51Å 113.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7342	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, HEM, PYR

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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	2/3916 (0.1%)	2.80	286/5303 (5.4%)
1	B	0.97	0/3156	2.83	233/4263 (5.5%)
All	All	0.99	2/7072 (0.0%)	2.81	519/9566 (5.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	GLU	CD-OE1	-5.64	1.19	1.25
1	A	232	SER	CB-OG	-5.27	1.35	1.42

The worst 5 of 519 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH1	41.59	141.09	120.30
1	B	259	ARG	NE-CZ-NH2	32.94	136.77	120.30
1	A	155	ARG	NE-CZ-NH2	32.52	136.56	120.30
1	A	376	ARG	NE-CZ-NH1	30.93	135.76	120.30
1	A	353	ARG	NE-CZ-NH2	-26.04	107.28	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ARG	Sidechain
1	A	353	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	38	ARG	Sidechain
1	B	163	ARG	Sidechain

5.2 Too-close contacts

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	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3841	0	3899	403	2
1	B	3107	0	3156	259	0
2	A	43	0	30	9	0
3	A	31	0	17	0	0
3	B	31	0	18	2	0
4	B	6	0	3	0	0
5	A	182	0	0	9	0
5	B	101	0	0	11	0
All	All	7342	0	7123	628	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 44.

The worst 5 of 628 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:O	1:A:10:LYS:HD3	1.18	1.33
1:A:24:ASP:HA	1:A:37:THR:CG2	1.60	1.27
1:A:1:GLU:N	1:A:71:ILE:HD12	1.49	1.27
1:A:1:GLU:H3	1:A:2:PRO:CD	1.50	1.25
1:A:24:ASP:CA	1:A:37:THR:HG21	1.66	1.25

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:NH2	1:A:245:ASP:OD1[3_665]	2.09	0.11
1:A:38:ARG:CZ	1:A:245:ASP:OD1[3_665]	2.12	0.08

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	Percentiles	
1	A	490/511 (96%)	438 (89%)	27 (6%)	25 (5%)	2	1
1	B	396/511 (78%)	353 (89%)	31 (8%)	12 (3%)	5	4
All	All	886/1022 (87%)	791 (89%)	58 (6%)	37 (4%)	3	2

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	ASP
1	A	7	ASN
1	A	10	LYS
1	A	22	PRO

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	423/440 (96%)	330 (78%)	93 (22%)	1	1
1	B	342/440 (78%)	264 (77%)	78 (23%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	765/880 (87%)	594 (78%)	171 (22%)	1 1

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	B	105	ASP
1	B	463	ARG
1	A	399	ASN
1	A	472	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	A	439	ASN
1	B	377	GLN
1	A	372	ASN
1	B	121	ASN

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](#)

4 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	HEM	A	560	1	28,50,50	2.06	7 (25%)	17,82,82	2.98	7 (41%)
3	FMN	A	570	-	31,33,33	1.07	1 (3%)	38,50,50	3.99	18 (47%)
3	FMN	B	570	-	31,33,33	1.46	3 (9%)	38,50,50	3.83	22 (57%)
4	PYR	B	580	-	2,5,5	5.44	2 (100%)	2,6,6	6.01	2 (100%)

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	A	560	1	-	0/6/54/54	0/0/8/8
3	FMN	A	570	-	1/1/4/4	0/16/18/18	0/3/3/3
3	FMN	B	570	-	-	0/16/18/18	0/3/3/3
4	PYR	B	580	-	-	0/0/4/4	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	560	HEM	C3B-C2B	-5.49	1.33	1.40
2	A	560	HEM	C3C-C2C	-3.97	1.35	1.40
3	B	570	FMN	P-O5'	-2.05	1.53	1.60
2	A	560	HEM	CMD-C2D	2.32	1.56	1.51
2	A	560	HEM	C1B-NB	2.54	1.39	1.36

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	FMN	C4A-C10-N10	-9.73	113.76	120.52
3	A	570	FMN	C4A-C10-N10	-8.22	114.81	120.52
4	B	580	PYR	O3-C2-C3	-7.74	102.50	120.16
3	A	570	FMN	C4A-C4-N3	-6.32	114.49	123.48
3	A	570	FMN	C4-C4A-C10	-6.10	115.03	119.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	570	FMN	C2'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	560	HEM	9	0
3	B	570	FMN	2	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.