



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3K9Y
Title : Crystal structure of rat mitochondrial P450 24A1 S57D in complex with CYMAL-5
Authors : Annalora, A.J.; Goodin, D.B.; Hong, W.; Zhang, Q.; Johnson, E.F.; Stout, C.D.
Deposited on : 2009-10-16
Resolution : 2.80 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

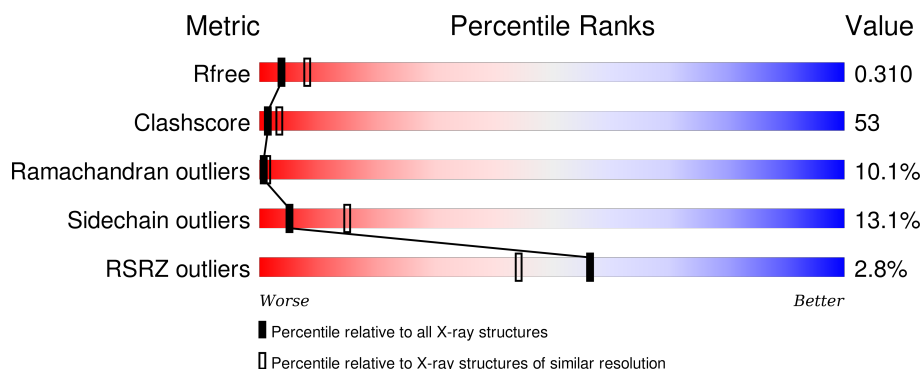
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	482	<div> <div>2%</div> <div>30% 51% 12% . .</div> </div>
1	B	482	<div> <div>3%</div> <div>30% 49% 15% . .</div> </div>

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	CM5	A	516	X	-	-	X
3	CM5	A	517	X	-	X	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7703 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 1,25-dihydroxyvitamin D(3) 24-hydroxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3769	2415	656	677	21			
1	B	462	Total	C	N	O	S	0	0	0
			3780	2421	660	678	21			

There are 4 discrepancies between the modelled and reference sequences:

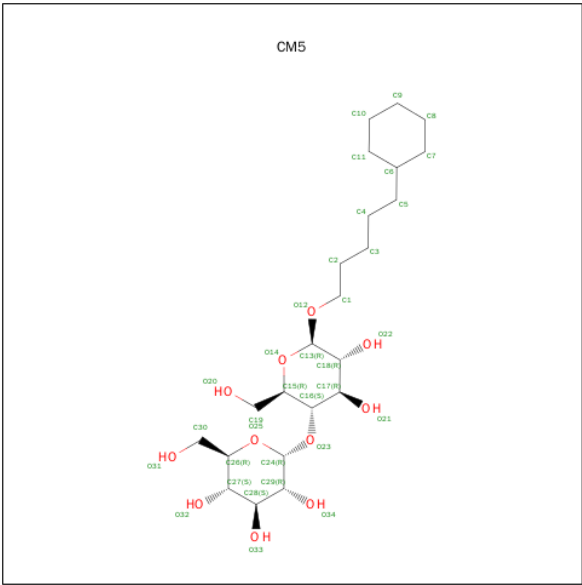
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	EXPRESSION TAG	UNP Q09128
A	57	ASP	SER	ENGINEERED	UNP Q09128
B	33	MET	-	EXPRESSION TAG	UNP Q09128
B	57	ASP	SER	ENGINEERED	UNP Q09128

- 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	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula: C₂₃H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			34	23	11		
3	A	1	Total	C	O	0	0
			34	23	11		

R505	I441	N373	Q308	K174
E506	Q442	M374	D309	L175
L507	R443	P375	R310	D176
P508	E444	Y376	I311	K177
I509	R445	L377	S312	K178
A510	R446	K378	K313	E181
F511	I447	A379	K314	L182
P512	F450	C380	E315	V183
R514	L453	L381	L316	A184
	P454	E383	Y317	
	P455	R386	A318	
	Q456	L387	V319	L187
	I457	T388	T320	E188
	Q458	P389	T321	R189
	R459		E322	M190
	R460	P392	L323	D191
	M461	F393	Q324	E192
	Q462	T394	L325	L193
	I463	T395		C194
	Q464	R396	E328	
	R465	T397	T330	R197
	R466	L398	T331	G198
	I467		A332	R199
	A468		N333	L200
	E469	T402	S334	E201
	L470	V403	M335	D202
	Q471	L404	M336	L203
	L472	G405	W337	S205
	H473	E406	I338	E206
	L474	P410	L339	L207
	A475	K411	Y340	W208
	L476	G412	N341	K209
	C477	T413	L342	W210
	W478	V414	S343	S211
	I479	L415	R344	F212
	L480	T416	N345	
	Q481	L417	A348	I215
	K482	N418	Q349	C216
	Y483	T419	R350	L217
	D484	Q420	R351	V218
	I485	V421	L352	L219
	Y486	L422	L353	Y220
	A487		Q354	E221
	T488	S425	E355	K222
	D489	E426	V356	R223
	W490	D427	Q291	F224
	E491	N428	R292	G225
	P492	F429	Y293	L226
	M495	E430	L360	L227
	L496	D431	S294	Q228
	H497	S432	Q295	K229
	L498	F435	D300	E230
	Q499	R436	F301	T231
	I500	P437	R367	E232
	L501	E438	A368	E233
	S504	L501	E369	E234
		R439	D370	A235
		W440	L371	
			Y306	I239
			Q307	
			R372	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.30Å 81.30Å 108.71Å 90.00° 122.44° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 36.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.80) 97.2 (36.74-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.251 , 0.318 0.257 , 0.310	Depositor DCC
R_{free} test set	1619 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 84.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 32345 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CM5

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	0.41	0/3857	0.72	1/5216 (0.0%)
1	B	0.44	0/3868	0.72	1/5230 (0.0%)
All	All	0.42	0/7725	0.72	2/10446 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	486	VAL	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3769	0	3827	394	0
1	B	3780	0	3840	406	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	68	0	84	31	0
All	All	7703	0	7811	821	0

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 53.

The worst 5 of 821 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)
3:A:517:CM5:H11	3:A:517:CM5:H15	1.29	1.10
1:A:352:LEU:HD12	1:A:480:ILE:HD13	1.37	1.06
3:A:516:CM5:H18	3:A:516:CM5:H22A	1.34	1.05
1:A:165:LYS:HD3	1:A:301:PHE:HB2	1.35	1.05
1:B:118:LEU:HB2	1:B:404:LEU:HD21	1.35	1.04

There are no symmetry-related clashes.

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	459/482 (95%)	341 (74%)	66 (14%)	52 (11%)	0	1
1	B	460/482 (95%)	340 (74%)	79 (17%)	41 (9%)	1	2
All	All	919/964 (95%)	681 (74%)	145 (16%)	93 (10%)	1	1

5 of 93 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	64	TRP
1	A	66	LEU
1	A	92	LYS
1	A	147	LEU

5.3.2 Protein sidechains ⓘ

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	415/433 (96%)	369 (89%)	46 (11%)	8	23
1	B	416/433 (96%)	353 (85%)	63 (15%)	3	10
All	All	831/866 (96%)	722 (87%)	109 (13%)	5	15

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	LEU
1	B	201	PRO
1	B	453	LEU
1	B	101	LEU
1	B	141	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	A	490	ASN
1	B	452	HIS
1	A	354	GLN
1	A	497	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
3	CM5	A	516	-	36,36,36	0.56	1 (2%)	49,49,49	2.40	15 (30%)
3	CM5	A	517	-	36,36,36	0.56	1 (2%)	49,49,49	1.09	4 (8%)
2	HEM	A	520	1	30,50,50	3.64	12 (40%)	24,82,82	2.70	10 (41%)
2	HEM	B	520	1	30,50,50	3.63	12 (40%)	24,82,82	2.58	9 (37%)

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
3	CM5	A	516	-	5/5/11/11	0/17/65/65	0/3/3/3
3	CM5	A	517	-	5/5/11/11	0/17/65/65	0/3/3/3
2	HEM	A	520	1	-	0/10/54/54	0/0/8/8
2	HEM	B	520	1	-	0/10/54/54	0/0/8/8

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	520	HEM	C3B-C4B	-9.85	1.43	1.51
2	B	520	HEM	C3B-C4B	-9.74	1.43	1.51
2	B	520	HEM	C3C-CAC	-8.26	1.35	1.51
2	B	520	HEM	C3D-C4D	-7.96	1.41	1.51
2	A	520	HEM	C3D-C4D	-7.82	1.41	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	516	CM5	C24-O23-C16	-9.00	94.50	118.01
3	A	516	CM5	C13-C18-C17	-5.09	99.94	109.97
3	A	516	CM5	C28-C27-C26	-4.27	102.76	110.20
3	A	516	CM5	C3-C4-C5	-2.79	103.74	113.66
3	A	516	CM5	C5-C6-C11	-2.68	106.43	112.10

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	517	CM5	C15
3	A	517	CM5	C18
3	A	517	CM5	C16
3	A	517	CM5	C29
3	A	517	CM5	C24

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	516	CM5	16	0
3	A	517	CM5	23	0
2	A	520	HEM	3	0
2	B	520	HEM	5	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 [i](#)

6.1 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, 95th 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	461/482 (95%)	0.06	11 (2%) 62 50	29, 73, 117, 182	0
1	B	462/482 (95%)	0.12	15 (3%) 51 39	28, 74, 120, 184	0
All	All	923/964 (95%)	0.09	26 (2%) 56 44	28, 74, 119, 184	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	5.3
1	A	447	ILE	5.2
1	A	230	GLU	3.8
1	B	75	TRP	3.7
1	A	231	THR	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CM5	A	516	34/34	0.74	0.32	3.02	78,92,101,102	0
3	CM5	A	517	34/34	0.75	0.32	2.94	78,89,96,100	0
2	HEM	B	520	43/43	0.96	0.21	-0.54	26,32,39,72	0
2	HEM	A	520	43/43	0.96	0.20	-0.98	25,37,50,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.