



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:36 PM GMT

PDB ID : 1GED  
Title : A positive charge route for the access of nadh to heme formed in the distal heme pocket of cytochrome p450nor  
Authors : Kudo, T.; Takaya, N.; Park, S.-Y.; Shiro, Y.; Shoun, H.  
Deposited on : 2000-11-02  
Resolution : 2.00 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

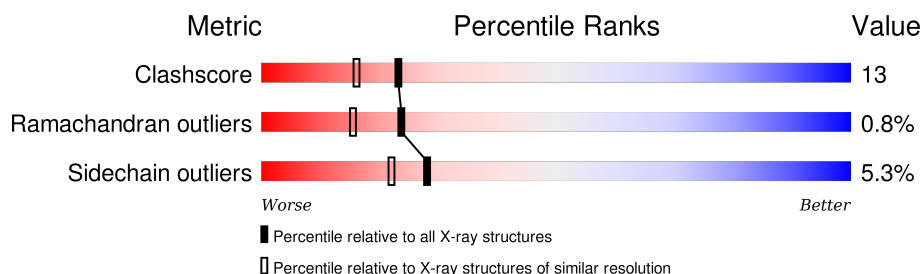
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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  $\geq 3$ , 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	403	

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
2	BR	A	404	-	-	X	-
2	BR	A	405	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3250 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 55A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3099	1971	529	586	13			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Br	0	0
			2	2		

- 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	0	0
			43	34	1	4	4		

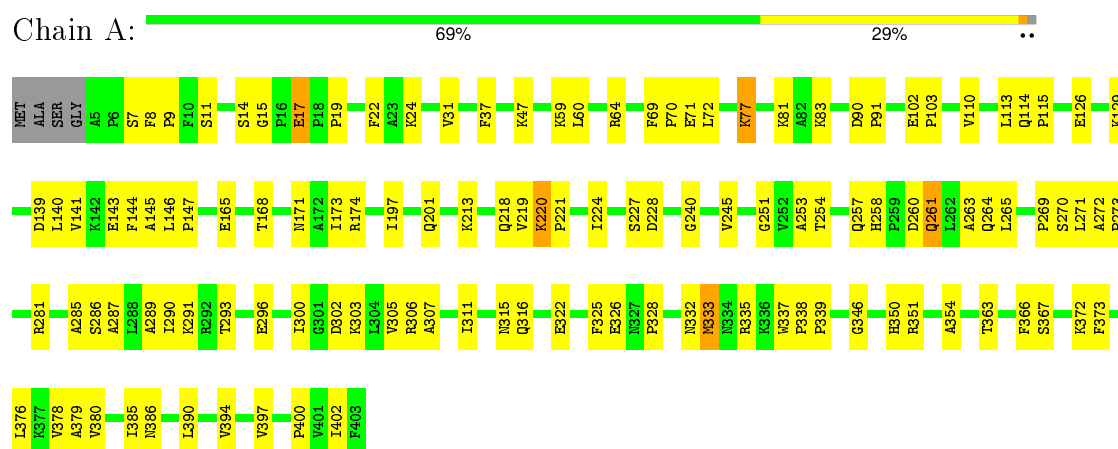
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0



Note EDS was not executed.

- Molecule 1: CYTOCHROME P450 55A1



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.32Å 78.05Å 86.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.9 (30.00-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.214 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 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, BR

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	0.34	0/3166	0.55	0/4303

There are no bond length outliers.

There are no bond angle outliers.

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	3099	0	3115	82	0
2	A	2	0	0	7	0
3	A	43	0	30	5	0
4	A	106	0	0	8	0
All	All	3250	0	3145	84	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 13.

All (84) 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:171:ASN:HB3	2:A:404:BR:BR	2.15	1.01
1:A:141:VAL:HA	1:A:145:ALA:HB3	1.66	0.78
1:A:286:SER:O	2:A:405:BR:BR	2.64	0.71
1:A:289:ALA:HB3	2:A:405:BR:BR	2.46	0.71
1:A:354:ALA:HB2	3:A:501:HEM:HBC2	1.73	0.71
1:A:305:VAL:HG11	1:A:311:ILE:HD11	1.75	0.69
1:A:69:PHE:HA	1:A:293:THR:HG22	1.74	0.69
1:A:220:LYS:HB2	1:A:221:PRO:HD3	1.77	0.67
1:A:197:ILE:O	1:A:201:GLN:HG3	1.95	0.67
1:A:165:GLU:HG2	4:A:607:HOH:O	1.93	0.66
1:A:272:ALA:HB3	1:A:273:PRO:HD3	1.79	0.64
1:A:168:THR:O	2:A:404:BR:BR	2.71	0.64
1:A:83:LYS:HE2	1:A:228:ASP:OD1	1.98	0.63
1:A:335:ARG:HD3	4:A:571:HOH:O	1.98	0.62
1:A:114:GLN:HB3	1:A:115:PRO:HD3	1.79	0.62
1:A:261:GLN:HA	1:A:264:GLN:HG3	1.81	0.61
1:A:372:LYS:HG3	1:A:372:LYS:O	2.03	0.58
1:A:146:LEU:HA	1:A:245:VAL:HG22	1.87	0.57
1:A:261:GLN:OE1	1:A:333:MET:HB3	2.05	0.56
1:A:338:PRO:HB2	1:A:339:PRO:CD	2.35	0.56
1:A:31:VAL:HG21	1:A:300:ILE:HG22	1.89	0.54
1:A:373:PHE:HB3	1:A:376:LEU:HB2	1.89	0.54
1:A:69:PHE:HA	1:A:293:THR:CG2	2.37	0.54
1:A:338:PRO:HB2	1:A:339:PRO:HD2	1.90	0.53
1:A:218:GLN:HB3	1:A:224:ILE:HG12	1.90	0.53
1:A:296:GLU:HA	1:A:307:ALA:HB2	1.90	0.53
1:A:322:GLU:H	1:A:322:GLU:CD	2.12	0.53
1:A:325:PHE:O	1:A:328:PRO:HD3	2.09	0.52
1:A:269:PRO:C	1:A:271:LEU:H	2.12	0.52
1:A:146:LEU:HB3	1:A:147:PRO:HD3	1.93	0.51
1:A:271:LEU:HB3	1:A:333:MET:CE	2.41	0.51
1:A:376:LEU:HA	1:A:402:ILE:O	2.11	0.51
1:A:271:LEU:HB3	1:A:333:MET:HE2	1.92	0.51
1:A:291:LYS:HE2	4:A:594:HOH:O	2.11	0.50
1:A:70:PRO:HG2	1:A:291:LYS:HB3	1.93	0.50
1:A:363:THR:O	1:A:367:SER:HB3	2.12	0.49
1:A:8:PHE:CG	1:A:9:PRO:HA	2.48	0.49
1:A:102:GLU:N	1:A:103:PRO:CD	2.75	0.49
1:A:385:ILE:N	4:A:603:HOH:O	2.46	0.49
1:A:102:GLU:N	1:A:103:PRO:HD2	2.28	0.48
1:A:315:ASN:OD1	2:A:405:BR:BR	2.86	0.48
1:A:64:ARG:HG2	1:A:69:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LYS:O	1:A:81:LYS:HE2	2.13	0.48
1:A:285:ALA:HB1	4:A:530:HOH:O	2.14	0.48
1:A:287:ALA:HB2	1:A:316:GLN:HB2	1.96	0.47
1:A:379:ALA:HB2	1:A:402:ILE:HG23	1.95	0.47
1:A:332:ASN:O	1:A:335:ARG:HB2	2.13	0.47
1:A:72:LEU:HD12	4:A:594:HOH:O	2.14	0.47
1:A:8:PHE:CD1	1:A:9:PRO:HA	2.50	0.47
1:A:285:ALA:HA	1:A:394:VAL:HG12	1.96	0.47
1:A:254:THR:O	1:A:258:HIS:CD2	2.68	0.47
1:A:14:SER:OG	1:A:17:GLU:HG3	2.15	0.47
1:A:380:VAL:CG1	1:A:400:PRO:HG2	2.44	0.47
1:A:219:VAL:HA	1:A:224:ILE:O	2.16	0.45
1:A:144:PHE:C	1:A:147:PRO:HD2	2.37	0.45
1:A:139:ASP:O	1:A:143:GLU:HG2	2.17	0.45
3:A:501:HEM:HAC	4:A:502:HOH:O	2.16	0.45
1:A:281:ARG:HD3	1:A:337:TRP:CZ3	2.52	0.45
1:A:240:GLY:HA3	3:A:501:HEM:C1C	2.51	0.44
1:A:350:HIS:O	1:A:351:ARG:C	2.55	0.44
1:A:19:PRO:HD2	1:A:22:PHE:CE1	2.53	0.44
1:A:302:ASP:OD1	1:A:303:LYS:HG2	2.18	0.44
1:A:265:LEU:HD13	1:A:333:MET:HE3	1.98	0.44
1:A:261:GLN:H	1:A:261:GLN:HG2	1.59	0.43
1:A:144:PHE:O	1:A:147:PRO:HD2	2.18	0.43
1:A:47:LYS:HE3	1:A:47:LYS:HB3	1.68	0.43
1:A:290:ILE:HD11	1:A:346:GLY:HA2	2.00	0.43
1:A:269:PRO:C	1:A:271:LEU:N	2.72	0.42
1:A:386:ASN:ND2	1:A:397:VAL:HB	2.34	0.42
2:A:405:BR:BR	3:A:501:HEM:HMA3	2.74	0.42
1:A:59:LYS:O	1:A:60:LEU:HD23	2.19	0.41
1:A:90:ASP:HB3	1:A:91:PRO:CD	2.50	0.41
1:A:260:ASP:O	1:A:263:ALA:HB3	2.20	0.41
1:A:272:ALA:HB3	1:A:273:PRO:CD	2.49	0.41
1:A:269:PRO:O	1:A:271:LEU:N	2.54	0.41
1:A:332:ASN:O	1:A:335:ARG:CB	2.69	0.41
1:A:354:ALA:CB	3:A:501:HEM:HBC2	2.46	0.41
1:A:251:GLY:HA3	1:A:366:PHE:CZ	2.56	0.41
1:A:253:ALA:O	1:A:257:GLN:HG3	2.21	0.40
1:A:110:VAL:HA	1:A:113:LEU:HD12	2.03	0.40
1:A:126:GLU:OE1	1:A:372:LYS:NZ	2.53	0.40
1:A:71:GLU:HA	4:A:537:HOH:O	2.21	0.40
1:A:289:ALA:N	2:A:405:BR:BR	3.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PHE:HA	1:A:9:PRO:C	2.42	0.40

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	397/403 (98%)	366 (92%)	28 (7%)	3 (1%)	24 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	PHE
1	A	270	SER
1	A	15	GLY

### 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	340/342 (99%)	322 (95%)	18 (5%)	28 22

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	11	SER
1	A	17	GLU
1	A	24	LYS
1	A	77	LYS
1	A	129	LYS
1	A	140	LEU
1	A	173	ILE
1	A	174	ARG
1	A	213	LYS
1	A	220	LYS
1	A	227	SER
1	A	261	GLN
1	A	306	ARG
1	A	326	GLU
1	A	333	MET
1	A	378	VAL
1	A	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	223	ASN
1	A	258	HIS
1	A	334	ASN

### 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

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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 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	HEM	A	501	1	30,50,50	2.95	11 (36%)	24,82,82	2.13	7 (29%)

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	HEM	A	501	1	-	0/10/54/54	0/0/8/8

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HEM	C3C-CAC	-6.75	1.38	1.51
3	A	501	HEM	C3B-C4B	-6.25	1.46	1.51
3	A	501	HEM	C2D-C3D	-5.68	1.37	1.54
3	A	501	HEM	C3D-C4D	-5.63	1.44	1.51
3	A	501	HEM	C2C-C1C	-5.56	1.42	1.52
3	A	501	HEM	C3B-CAB	-5.38	1.41	1.51
3	A	501	HEM	C2D-C1D	-2.54	1.43	1.51
3	A	501	HEM	CHD-C4C	2.29	1.41	1.36
3	A	501	HEM	CBB-CAB	2.31	1.42	1.29
3	A	501	HEM	C1C-NC	3.18	1.39	1.36
3	A	501	HEM	C4C-NC	3.28	1.40	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HEM	C3C-CAC-CBC	-2.35	120.85	124.46
3	A	501	HEM	CMD-C2D-C3D	2.85	126.97	114.35
3	A	501	HEM	C2D-C3D-C4D	3.44	107.34	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	HEM	CAD-C3D-C4D	3.53	124.90	112.47
3	A	501	HEM	CMB-C2B-C3B	3.57	125.45	116.53
3	A	501	HEM	CMC-C2C-C3C	4.30	127.25	116.53
3	A	501	HEM	CAD-C3D-C2D	5.04	127.71	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.