



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 06:52 PM EDT

PDB ID : 8CAT
Title : The NADPH binding site on beef liver catalase
Authors : Murthy, M.R.N.; Reid III, T.J.; Sicignano, A.; Tanaka, N.; Fita, I.; Rossmann, M.G.
Deposited on : unknown
Resolution : 2.50 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) : rb-20030345

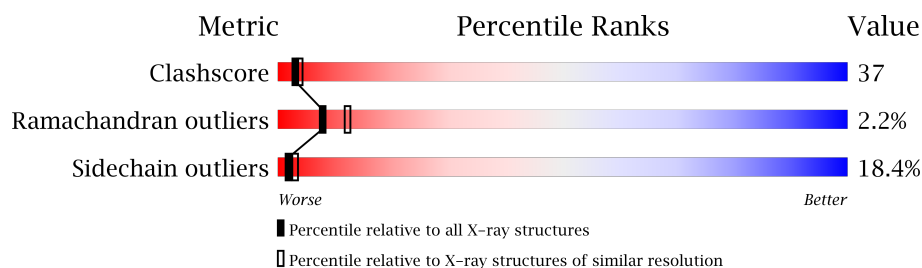
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

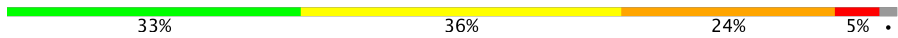
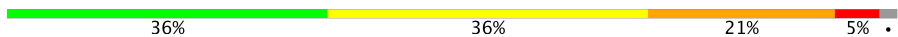
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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	506	
1	B	506	

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	NDP	A	508	X	-	-	-
3	NDP	B	508	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8296 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 CATALASE.

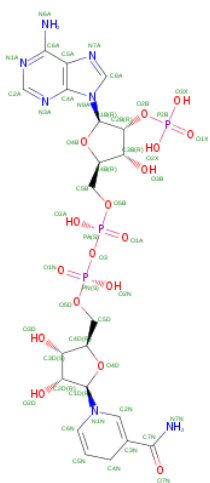
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			
1	B	498	Total	C	N	O	S	0	0	0
			4008	2543	714	737	14			

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	48	Total O 48 48	0	0
4	B	50	Total O 50 50	0	0

LYS	D437	L365	F293	F219	V145
PRO	M438		R294	K220	G146
LYS	V439	L370	F295	L221	M147
ASN	T440	Q371	F296	V222	M148
	Q441	I372	D297	R223	T149
	V442	P373	L298	A224	P150
	R443	V374	T299	D225	I151
	T444	M375	K300		F152
	F445		V301	A228	F153
	V446	Y378	M302	V229	I154
	L447	R379	P303	C231	D156
	V448	A380	H304		A157
	V449	R381	G305	Y235	L158
	L450	V382	D306	K236	L159
	M451	A383	P307	T237	F160
	E452	M384	P308	D238	P161
	E453	Y385	L309	Q239	S162
	Q454	Q386	T310		F163
	R455	R387	P311	K242	
	K456	D388	V312	M243	K168
	R457		G313	L244	R169
	L458	C392	K314	S245	M170
	Q459	M393	L315	V246	P171
	E460	M394	V316	E247	O172
	V461	D395	L317	D248	T173
	T462	M396	R318		H174
			R319	R251	L175
	L466	A400	M320	L252	K176
	K467	P401	P321	A253	D177
	D468	M402	V322	H254	P178
	A469	Y403		E255	D179
	Q470	Y404	L331	D256	M180
	L471	P405	A332	L261	W181
	F472	M406	D333	D262	D183
		S407	P334	L264	
	K475	F408	P335		L187
	K476	S409	S336	D263	R188
	A477	A410	R337	L264	P189
	V478	P411	M338		E190
	K479	E412	P339	A267	S191
		H413			L192
	D483	Q414	E343	N272	H193
	V484	P415		Y273	Q194
	H485	S416	D347	P274	V195
	P486	A417	K348	S275	
	E487		M349	W276	L198
	Y488	H420	L350		
		R421	Q351	Y279	
	R491		G352		D201
	T492	S425	R353	V282	R202
	Q493	G426	L354	M283	
	A494	D427	F355	T284	D206
	L495	V428	A356	F285	
	L496	Q429		S286	R209
	D497	R430	D359	E287	
	K498	P431	T360	A288	D212
	Y499	M432	H361	E289	G213
			R362	L290	F291
	H500	M435	H363	P292	
	GLU	D436	R364		T218

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.00 Å 142.00 Å 103.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.50 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.50-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8296	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: HEM, NDP

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	1.53	22/4128 (0.5%)	2.37	195/5607 (3.5%)
1	B	1.57	20/4128 (0.5%)	2.42	229/5607 (4.1%)
All	All	1.55	42/8256 (0.5%)	2.39	424/11214 (3.8%)

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

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	CD-NE	-6.86	1.34	1.46
1	A	343	GLU	N-CA	6.53	1.59	1.46
1	A	166	SER	CB-OG	6.43	1.50	1.42
1	B	100	GLU	CD-OE2	-6.36	1.18	1.25
1	B	119	SER	CB-OG	-6.30	1.34	1.42

The worst 5 of 424 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	CD-NE-CZ	25.86	159.81	123.60
1	B	92	ARG	NE-CZ-NH1	23.28	131.94	120.30
1	B	126	ARG	NE-CZ-NH2	21.12	130.86	120.30
1	B	261	LEU	CA-CB-CG	20.39	162.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ARG	NE-CZ-NH2	-20.36	110.12	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	430	ARG	Sidechain
1	A	71	ARG	Sidechain
1	B	105	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	4008	0	3830	329	3
1	B	4008	0	3825	293	2
2	A	43	0	30	15	0
2	B	43	0	30	9	0
3	A	48	0	24	0	0
3	B	48	0	24	3	0
4	A	48	0	0	4	1
4	B	50	0	0	5	0
All	All	8296	0	7763	596	3

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 37.

The worst 5 of 596 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:155:ARG:NH2	1:A:438:ASN:HD21	1.19	1.40
1:B:155:ARG:HH22	1:B:438:ASN:ND2	1.28	1.30
1:A:155:ARG:HH22	1:A:438:ASN:ND2	1.28	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NH2	1:B:438:ASN:HD21	1.34	1.24
1:A:367:PRO:HG2	1:A:390:PRO:HG2	1.19	1.14

All (3) 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:419:GLU:OE2	1:B:430:ARG:NH1[6_556]	1.78	0.42
1:A:10:GLN:NE2	4:A:541:HOH:O[6_556]	1.86	0.34
1:A:183:ASP:OD1	1:B:407:SER:OG[6_556]	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	496/506 (98%)	418 (84%)	64 (13%)	14 (3%)	6	8
1	B	496/506 (98%)	425 (86%)	63 (13%)	8 (2%)	11	19
All	All	992/1012 (98%)	843 (85%)	127 (13%)	22 (2%)	8	12

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	LYS
1	A	267	ALA
1	A	373	PRO
1	A	440	THR
1	A	451	ASN

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	430/437 (98%)	351 (82%)	79 (18%)	2	3
1	B	430/437 (98%)	351 (82%)	79 (18%)	2	3
All	All	860/874 (98%)	702 (82%)	158 (18%)	2	3

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	LEU
1	B	51	VAL
1	B	414	GLN
1	A	475	LYS
1	B	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	GLN
1	B	21	GLN
1	B	420	HIS
1	A	438	ASN
1	A	485	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 [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	507	1	28,50,50	3.14	11 (39%)	17,82,82	3.12	8 (47%)
3	NDP	A	508	-	43,52,52	2.50	7 (16%)	49,80,80	2.18	12 (24%)
2	HEM	B	507	1	28,50,50	2.73	9 (32%)	17,82,82	2.29	7 (41%)
3	NDP	B	508	-	43,52,52	2.51	6 (13%)	49,80,80	2.19	12 (24%)

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	507	1	-	0/6/54/54	0/0/8/8
3	NDP	A	508	-	1/1/14/17	0/30/77/77	0/5/5/5
2	HEM	B	507	1	-	0/6/54/54	0/0/8/8
3	NDP	B	508	-	1/1/14/17	0/30/77/77	0/5/5/5

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	507	HEM	C1C-NC	-5.88	1.29	1.36
3	B	508	NDP	O3B-C3B	-5.21	1.31	1.43
3	A	508	NDP	O3B-C3B	-5.16	1.31	1.43
2	B	507	HEM	C1C-NC	-5.14	1.30	1.36
3	B	508	NDP	C4N-C5N	-4.69	1.38	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	NDP	O4B-C1B-C2B	-6.31	95.55	106.59
3	B	508	NDP	O4B-C1B-C2B	-6.29	95.59	106.59
3	A	508	NDP	O3X-P2B-O2B	-3.44	90.35	106.00
3	B	508	NDP	O3X-P2B-O2B	-3.43	90.40	106.00
2	B	507	HEM	CMD-C2D-C1D	-3.26	123.45	128.46

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	508	NDP	C3B
3	A	508	NDP	C3B

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	HEM	15	0
2	B	507	HEM	9	0
3	B	508	NDP	3	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.