

wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2021 – 04:48 AM EDT

PDB ID : 2PO5

Title : Crystal structure of human ferrochelatase mutant with His 263 replaced by

Cys

Authors: Dailey, H.A.; Wu, C.-K.; Horanyi, P.; Medlock, A.E.; Najahi-Missaoui,

A.E.W.; Burden, A.; Dailey, T.A.; Rose, J.P.

Deposited on : 2007-04-25

Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

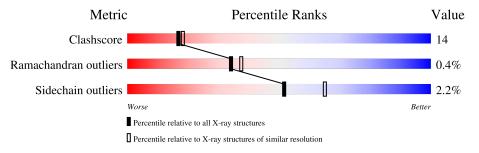
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	359	72%	26%	.
1	В	359	75%	24%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6192 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.

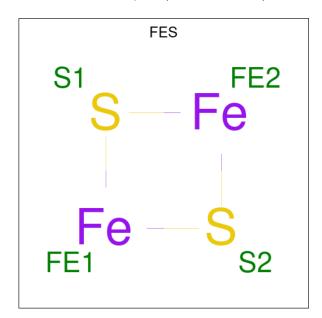
• Molecule 1 is a protein called Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	359	Total	С	N	О	S	0	0	0
1	11	303	2851	1817	488	527	19			
1	D	359	Total	С	N	О	S	0	0	0
1	Б	339	2851	1817	488	527	19	0	U	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	engineered mutation	UNP P22830
A	263	CYS	HIS	engineered mutation	UNP P22830
В	115	LEU	ARG	engineered mutation	UNP P22830
В	263	CYS	HIS	engineered mutation	UNP P22830

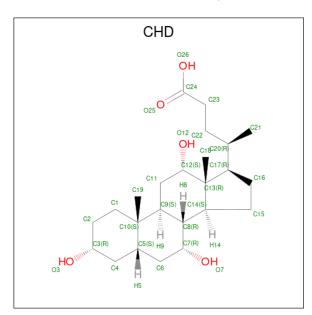
• Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	Fe 2	S 2	0	0
2	В	1	Total 4	Fe 2	S 2	0	0

 \bullet Molecule 3 is CHOLIC ACID (three-letter code: CHD) (formula: $\mathrm{C}_{24}\mathrm{H}_{40}\mathrm{O}_5).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	A	1	Total C O 29 24 5	0	0
3	В	1	Total C O 29 24 5	0	0
3	В	1	Total C O 29 24 5	0	0
3	В	1	Total C O 29 24 5	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	157	Total O 157 157	0	0
4	В	151	Total O 151 151	0	0

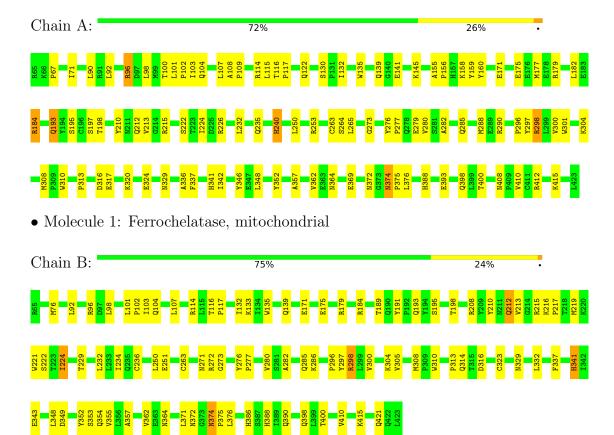


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: Ferrochelatase, mitochondrial





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	93.42Å 87.73Å 109.58Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	19.90 - 2.20	Depositor	
% Data completeness	96.3 (19.90-2.20)	Depositor	
(in resolution range)	30.9 (13.30 2.20)	Depositor	
R_{merge}	0.07	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	CNS 1.0	Depositor	
R, R_{free}	0.209 , 0.240	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	6192	wwPDB-VP	
Average B, all atoms (Å ²)	26.0	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: FES, CHD

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		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.74	1/2920 (0.0%)	0.57	1/3965 (0.0%)	
1	В	0.35	1/2920 (0.0%)	0.57	1/3965 (0.0%)	
All	All	0.58	$2/5840 \ (0.0\%)$	0.57	2/7930 (0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
1	A	96	ARG	CD-NE	36.23	2.08	1.46
1	В	96	ARG	CD-NE	-7.75	1.33	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
1	В	224	ILE	N-CA-C	-5.62	95.84	111.00
1	A	224	ILE	N-CA-C	-5.41	96.41	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	2851	0	2820	88	0
1	В	2851	0	2820	77	0

Continued on next page...



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	В	4	0	0	0	0
3	A	87	0	117	12	0
3	В	87	0	117	10	0
4	A	157	0	0	2	0
4	В	151	0	0	1	0
All	All	6192	0	5874	166	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 14.

The worst 5 of 166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\begin{subarray}{c} \begin{subarray}{c} \begi$
1:A:96:ARG:CD	1:A:96:ARG:NE	2.08	1.16
1:A:297:TYR:H	1:B:398:GLN:HE22	1.13	0.97
1:B:250:LEU:HD12	1:B:250:LEU:H	1.30	0.94
1:B:337:PHE:CE2	1:B:341:HIS:HE1	1.86	0.92
1:A:398:GLN:HE22	1:B:297:TYR:H	1.19	0.90

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	Perce	ntiles	
1	A	357/359 (99%)	345 (97%)	11 (3%)	1 (0%)	41	46
1	В	357/359 (99%)	347 (97%)	8 (2%)	2 (1%)	25	26
All	All	714/718 (99%)	692 (97%)	19 (3%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	372	ASN
1	A	372	ASN
1	В	355	VAL

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	Percent	iles
1	A	316/324 (98%)	310 (98%)	6 (2%)	57	71
1	В	316/324 (98%)	308 (98%)	8 (2%)	47	60
All	All	632/648 (98%)	618 (98%)	14 (2%)	52	35

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	184	ARG
1	В	212	GLN
1	В	374	ASN
1	В	298	ARG
1	В	341	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	341	HIS
1	В	388	HIS
1	В	421	GLN
1	В	398	GLN
1	A	374	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	Trino	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CHD	A	502	-	29,32,32	0.83	1 (3%)	48,51,51	1.18	4 (8%)
3	CHD	A	503	-	29,32,32	0.82	2 (6%)	48,51,51	1.13	3 (6%)
2	FES	В	999	1	0,4,4	-	-	-		
3	CHD	A	501	-	29,32,32	0.85	2 (6%)	48,51,51	1.36	6 (12%)
3	CHD	В	501	-	29,32,32	0.82	2 (6%)	48,51,51	1.33	5 (10%)
3	CHD	В	503	-	29,32,32	0.80	1 (3%)	48,51,51	1.16	5 (10%)
3	CHD	В	502	-	29,32,32	0.86	2 (6%)	48,51,51	1.23	6 (12%)
2	FES	A	499	1	0,4,4	-	=	-		

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	CHD	A	502	-	-	0/7/74/74	0/4/4/4
3	CHD	A	503	-	-	0/7/74/74	0/4/4/4
2	FES	В	999	1	-	-	0/1/1/1
3	CHD	В	501	_	-	0/7/74/74	0/4/4/4
3	CHD	A	501	-	-	0/7/74/74	0/4/4/4
3	CHD	В	503	-	-	0/7/74/74	0/4/4/4

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CHD	В	502	-	-	0/7/74/74	0/4/4/4
2	FES	A	499	1	-	-	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
3	В	502	CHD	C11-C12	2.65	1.57	1.53
3	A	502	CHD	C11-C12	2.47	1.57	1.53
3	В	501	CHD	C11-C12	2.21	1.57	1.53
3	A	501	CHD	C11-C12	2.20	1.57	1.53
3	В	503	CHD	C11-C12	2.19	1.56	1.53

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	501	CHD	C13-C17-C20	-3.84	114.91	119.50
3	В	501	CHD	C13-C17-C20	-3.68	115.10	119.50
3	A	503	CHD	C4-C5-C10	-3.20	109.26	112.66
3	В	503	CHD	C4-C5-C10	-2.99	109.48	112.66
3	A	501	CHD	C23-C22-C20	-2.96	110.74	114.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

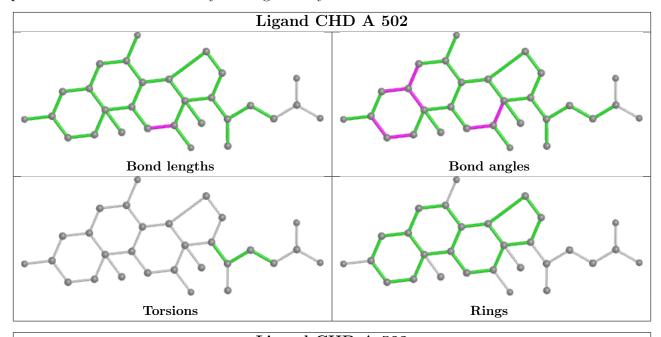
6 monomers are involved in 22 short contacts:

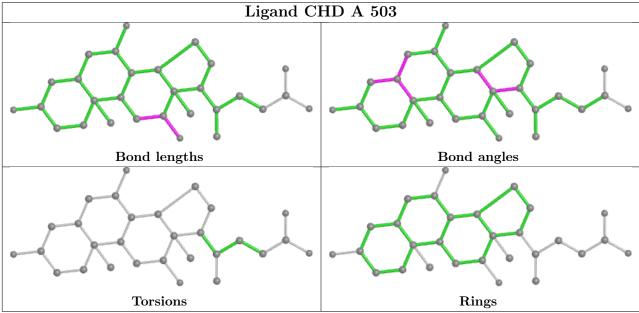
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	CHD	5	0
3	A	503	CHD	1	0
3	A	501	CHD	8	0
3	В	501	CHD	7	0
3	В	503	CHD	2	0
3	В	502	CHD	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

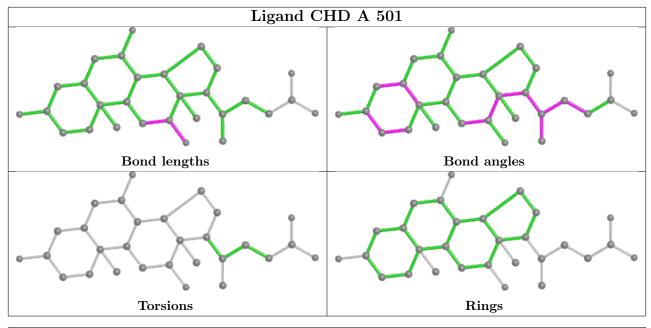


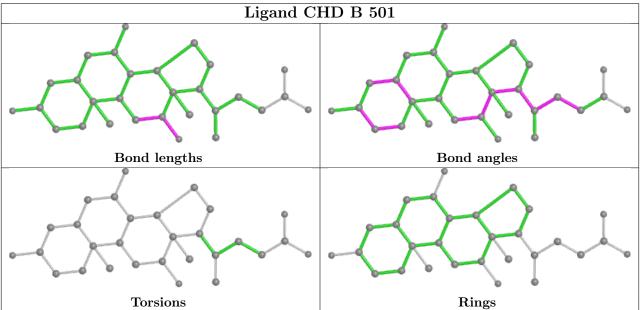
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



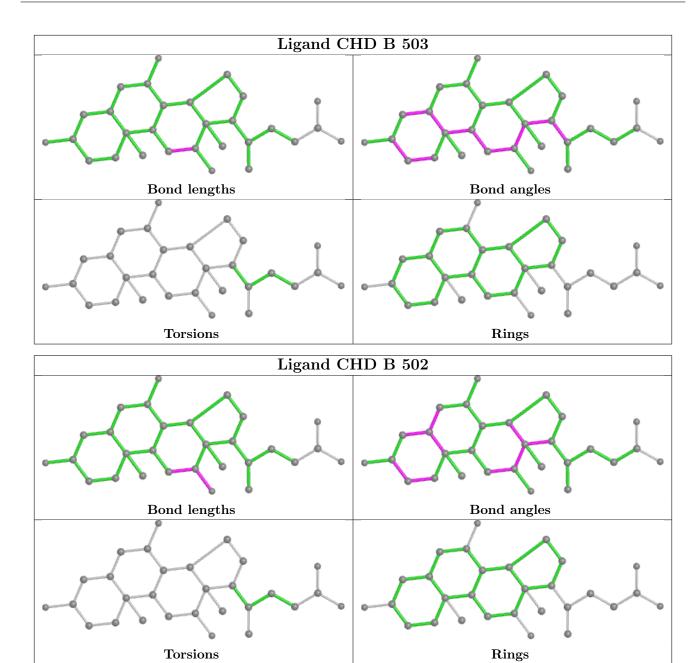












5.7 Other polymers (i)

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

