



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:15 am BST

PDB ID : 2XDQ  
Title : Dark Operative Protochlorophyllide Oxidoreductase (ChlN-ChlB)<sub>2</sub> Complex  
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Deposited on : 2010-05-06  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

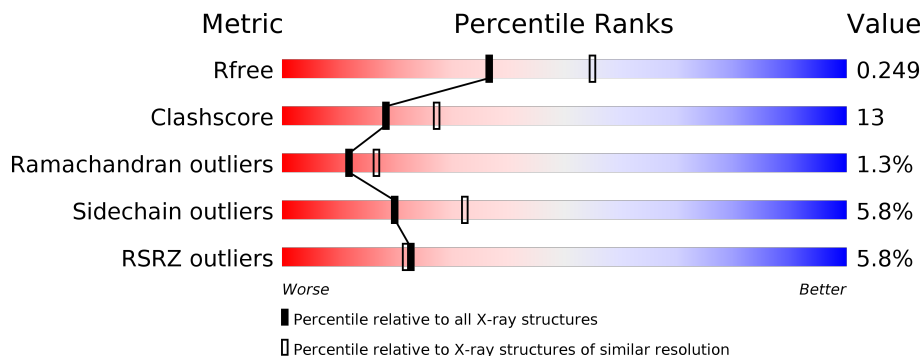
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	460	
2	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
5	SO4	B	1503	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7097 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 LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3401	2186	579	613	23	0	9	0

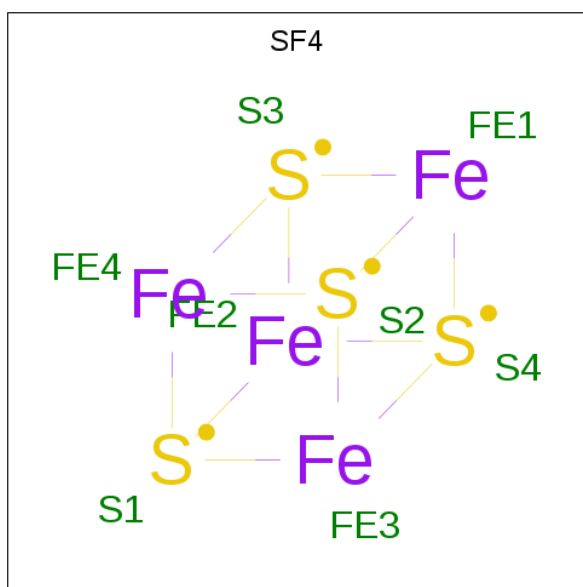
- Molecule 2 is a protein called LIGHT-INDEPENDENT PROTOCHLOROPHYLLIDE REDUCTASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	440	3533	2237	635	640	21	0	12	0

There are 3 discrepancies between the modelled and reference sequences:

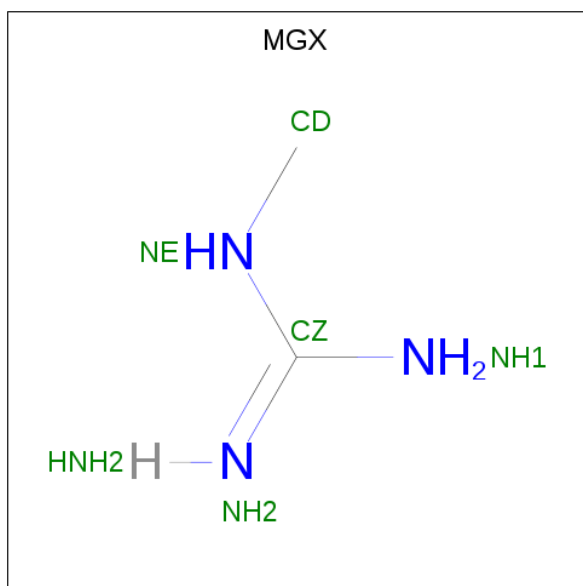
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ALA	-	expression tag	UNP Q8DGC6
B	-1	ALA	-	expression tag	UNP Q8DGC6
B	0	ALA	-	expression tag	UNP Q8DGC6

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is 1-METHYLGUANIDINE (three-letter code: MGX) (formula:  $C_2H_7N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	2	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).

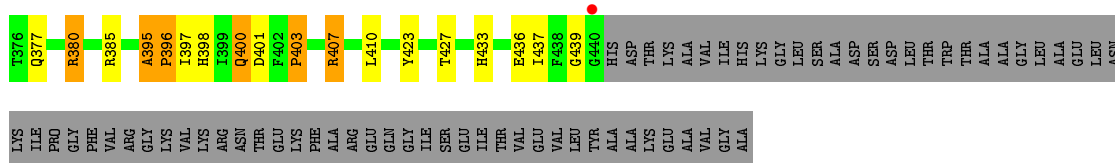


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	103	Total	O	0	0
			103	103		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.09Å 192.09Å 132.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	103.65 – 2.40 24.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (103.65-2.40) 98.7 (24.75-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.41Å)	Xtrriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.201 , 0.257 0.198 , 0.249	Depositor DCC
$R_{free}$ test set	2817 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtrriage
Anisotropy	0.523	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: SF4, MGX, SO4

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	0.94	3/3504 (0.1%)	0.88	2/4755 (0.0%)
2	B	0.90	2/3642 (0.1%)	0.90	9/4938 (0.2%)
All	All	0.92	5/7146 (0.1%)	0.89	11/9693 (0.1%)

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
2	B	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	CB-CG	7.06	1.65	1.52
2	B	203	ALA	CA-CB	6.90	1.67	1.52
1	A	417	TRP	CB-CG	-6.52	1.38	1.50
2	B	403	PRO	CB-CG	5.02	1.75	1.50
1	A	22	CYS	CB-SG	5.00	1.90	1.82

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	LEU	C-N-CD	-20.43	75.66	120.60
2	B	395	ALA	C-N-CD	-18.84	79.15	120.60
2	B	200	ILE	C-N-CD	-15.04	87.50	120.60
1	A	228	LEU	C-N-CA	13.65	179.32	122.00
2	B	396	PRO	CA-N-CD	-6.46	102.45	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	200	ILE	Mainchain,Peptide
2	B	395	ALA	Mainchain,Peptide

## 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	3401	0	3456	89	0
2	B	3533	0	3553	104	0
3	A	8	0	0	0	0
4	A	5	0	6	0	0
5	B	10	0	0	0	0
6	A	37	0	0	0	0
6	B	103	0	0	5	0
All	All	7097	0	7015	186	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.

The worst 5 of 186 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)
2:B:403:PRO:CG	2:B:403:PRO:CB	1.75	1.39
2:B:128[A]:ARG:HH11	2:B:128[A]:ARG:HG3	1.09	1.15
2:B:64:VAL:HG13	2:B:69:SER:OG	1.51	1.10
2:B:64:VAL:HA	2:B:68:GLY:HA3	1.37	1.06
2:B:128[A]:ARG:HH11	2:B:128[A]:ARG:CG	1.67	1.06

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	430/460 (94%)	410 (95%)	14 (3%)	6 (1%)	11	15
2	B	450/511 (88%)	423 (94%)	22 (5%)	5 (1%)	14	20
All	All	880/971 (91%)	833 (95%)	36 (4%)	11 (1%)	12	17

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	357	ALA
2	B	201	PRO
2	B	396	PRO
1	A	453	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	367/389 (94%)	343 (94%)	24 (6%)	17	27
2	B	380/420 (90%)	356 (94%)	24 (6%)	18	28
All	All	747/809 (92%)	699 (94%)	48 (6%)	20	28

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	ARG

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Mol	Chain	Res	Type
2	B	46	LEU
2	B	385[B]	ARG
1	A	454	TRP
2	B	29	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	76	ASN
2	B	433	HIS
2	B	210	GLN
2	B	13	HIS
2	B	180	HIS

### 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
3	SF4	A	602	1,2	0,12,12	0.00	-	-	-	-
5	SO4	B	1504	-	4,4,4	0.18	0	6,6,6	0.47	0
4	MGX	A	1463	-	4,4,4	0.38	0	4,4,4	1.62	1 (25%)
5	SO4	B	1503	-	4,4,4	0.31	0	6,6,6	0.40	0

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	SF4	A	602	1,2	-	-	0/6/5/5
4	MGX	A	1463	-	-	0/2/2/2	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1463	MGX	CD-NE-CZ	3.19	127.27	121.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	425/460 (92%)	0.28	44 (10%) 6 6	45, 68, 102, 130	0
2	B	440/511 (86%)	-0.25	6 (1%) 75 73	34, 55, 128, 276	0
All	All	865/971 (89%)	0.01	50 (5%) 23 22	34, 62, 114, 276	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	GLY	7.0
1	A	6	PRO	5.7
1	A	162	THR	5.0
1	A	459	ALA	5.0
1	A	455	GLN	4.7

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	1503	5/5	0.77	0.49	61,61,117,500	0
5	SO4	B	1504	5/5	0.90	0.23	61,64,179,500	0
4	MGX	A	1463	5/5	0.93	0.20	81,84,89,108	0
3	SF4	A	602	8/8	0.99	0.05	42,46,47,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.