



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2017 – 09:33 pm GMT

PDB ID : 1VCR  
Title : An icosahedral assembly of light-harvesting chlorophyll a/b protein complex from pea thylakoid membranes  
Authors : Hino, T.; Kanamori, E.; Shen, J.-R.; Kouyama, T.  
Deposited on : 2004-03-10  
Resolution : 9.50 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](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

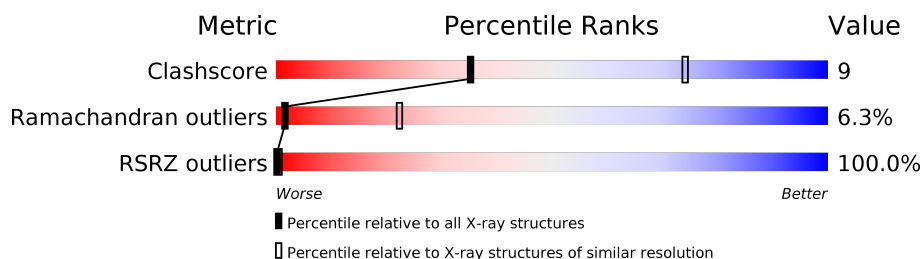
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 9.50 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	1037 (15.00-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
RSRZ outliers	101464	1004 (11.50-3.72)

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.

Mol	Chain	Length	Quality of chain
1	A	232	

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	CLA	A	251	X	-	-	X
2	CLA	A	252	X	-	-	-
2	CLA	A	253	X	-	-	-
2	CLA	A	254	X	-	-	X
2	CLA	A	255	X	-	-	-
2	CLA	A	256	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CLA	A	257	X	-	-	-
3	CHL	A	265	-	-	-	X

## 2 Entry composition [i](#)

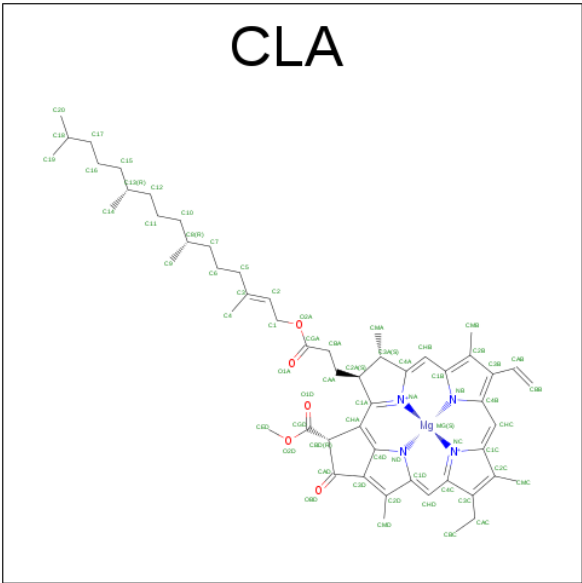
There are 3 unique types of molecules in this entry. The entry contains 796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chlorophyll a-b binding protein AB80.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	101	496	294	101	101	0	0	0

- Molecule 2 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



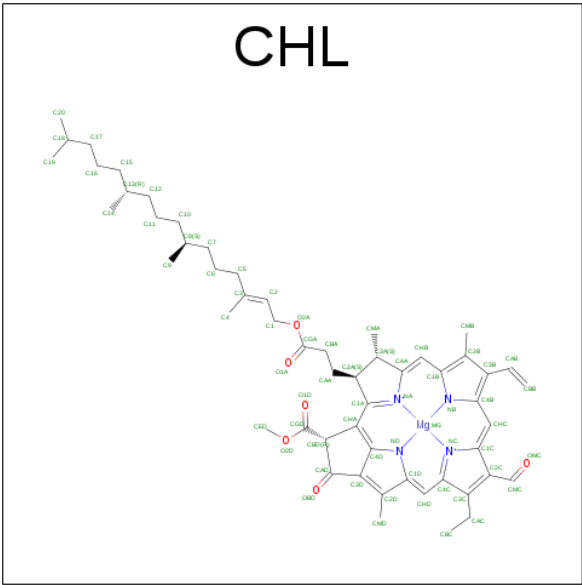
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Mg	N		
2	A	1	25	20	1	4	0	0
2	A	1	25	20	1	4	0	0
2	A	1	25	20	1	4	0	0
2	A	1	25	20	1	4	0	0
2	A	1	25	20	1	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
2	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 3 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).

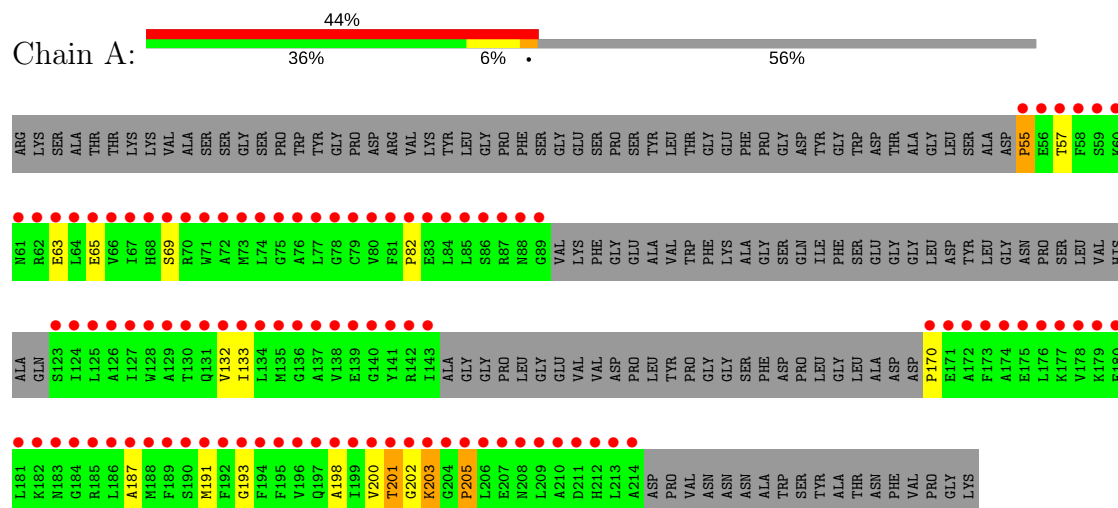


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
3	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
3	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
3	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
3	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Chlorophyll a-b binding protein AB80



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	360.65Å 360.65Å 360.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 9.50 208.22 – 9.50	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-9.50) 99.7 (208.22-9.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.26 (at 9.99Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.379 , 0.353 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	272.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , -110.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.15$ , $\langle L^2 \rangle = 0.04$	Xtriage
Estimated twinning fraction	0.460 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.45	EDS
Total number of atoms	796	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	296.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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: CHL, CLA

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	0/493	0.63	4/680 (0.6%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	PRO	N-CA-CB	5.58	109.99	103.30
1	A	205	PRO	N-CA-CB	5.56	109.98	103.30
1	A	170	PRO	N-CA-CB	5.49	109.89	103.30
1	A	82	PRO	N-CA-CB	5.46	109.85	103.30

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	496	0	239	10	0
2	A	175	0	21	0	0
3	A	125	0	15	0	0
All	All	796	0	275	10	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 9.



The worst 5 of 10 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:63:GLU:C	1:A:65:GLU:H	1.97	0.66
1:A:55:PRO:C	1:A:57:THR:H	2.03	0.62
1:A:200:VAL:O	1:A:201:THR:CB	2.50	0.58
1:A:198:ALA:HA	1:A:203:LYS:O	2.10	0.52
1:A:63:GLU:C	1:A:65:GLU:N	2.63	0.51

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	95/232 (41%)	79 (83%)	10 (10%)	6 (6%)	<b>1</b> <b>22</b>

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	THR
1	A	203	LYS
1	A	205	PRO
1	A	132	VAL
1	A	202	GLY

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

12 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	CLA	A	251	-	17,32,73	2.93	7 (41%)	24,54,113	1.91	5 (20%)
2	CLA	A	252	-	17,32,73	2.98	7 (41%)	24,54,113	1.91	6 (25%)
2	CLA	A	253	-	17,32,73	2.99	7 (41%)	24,54,113	1.93	5 (20%)
2	CLA	A	254	-	17,32,73	2.99	7 (41%)	24,54,113	1.93	6 (25%)
2	CLA	A	255	-	17,32,73	2.98	7 (41%)	24,54,113	1.89	5 (20%)
2	CLA	A	256	-	17,32,73	2.95	7 (41%)	24,54,113	1.89	5 (20%)
2	CLA	A	257	-	17,32,73	2.89	7 (41%)	24,54,113	1.96	5 (20%)
3	CHL	A	261	-	24,32,74	5.35	18 (75%)	18,54,114	6.08	14 (77%)
3	CHL	A	262	-	24,32,74	5.30	18 (75%)	18,54,114	6.08	14 (77%)
3	CHL	A	263	-	24,32,74	5.30	18 (75%)	18,54,114	6.08	14 (77%)
3	CHL	A	265	-	24,32,74	5.32	18 (75%)	18,54,114	6.08	14 (77%)
3	CHL	A	266	-	24,32,74	5.40	18 (75%)	18,54,114	6.08	14 (77%)

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	CLA	A	251	-	3/3/7/25	0/0/66/135	0/0/8/9
2	CLA	A	252	-	3/3/7/25	0/0/66/135	0/0/8/9
2	CLA	A	253	-	3/3/7/25	0/0/66/135	0/0/8/9
2	CLA	A	254	-	3/3/7/25	0/0/66/135	0/0/8/9
2	CLA	A	255	-	3/3/7/25	0/0/66/135	0/0/8/9
2	CLA	A	256	-	3/3/7/25	0/0/66/135	0/0/8/9
2	CLA	A	257	-	3/3/7/25	0/0/66/135	0/0/8/9
3	CHL	A	261	-	-	0/0/92/177	0/0/8/9
3	CHL	A	262	-	-	0/0/92/177	0/0/8/9
3	CHL	A	263	-	-	0/0/92/177	0/0/8/9
3	CHL	A	265	-	-	0/0/92/177	0/0/8/9
3	CHL	A	266	-	-	0/0/92/177	0/0/8/9

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	265	CHL	CHD-C4C	-8.38	1.38	1.53
3	A	266	CHL	CHD-C4C	-8.33	1.38	1.53
3	A	263	CHL	CHD-C4C	-8.29	1.38	1.53
3	A	262	CHL	CHD-C4C	-8.25	1.38	1.53
3	A	261	CHL	CHD-C4C	-8.21	1.38	1.53

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	253	CLA	C3C-C2C-C1C	-4.72	101.76	107.19
2	A	257	CLA	C3C-C2C-C1C	-4.66	101.84	107.19
2	A	251	CLA	C3C-C2C-C1C	-4.63	101.87	107.19
2	A	256	CLA	C3C-C2C-C1C	-4.58	101.93	107.19
2	A	254	CLA	C3C-C2C-C1C	-4.56	101.95	107.19

5 of 21 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	257	CLA	NC
2	A	257	CLA	ND
2	A	257	CLA	NA
2	A	256	CLA	NC
2	A	256	CLA	ND

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	101/232 (43%)	10.97	101 (100%) 0 0	295, 297, 297, 297	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	SER	25.2
1	A	87	ARG	22.9
1	A	175	GLU	22.9
1	A	171	GLU	21.5
1	A	135	MET	21.4

### 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CLA	A	251	25/65	-0.32	2.67	0.70	293,296,296,296	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CHL	A	265	25/66	-0.31	2.98	0.26	296,296,296,296	0
2	CLA	A	254	25/65	-0.07	1.30	-0.12	294,296,296,296	0
3	CHL	A	263	25/66	-0.59	2.96	-	294,296,296,296	0
2	CLA	A	252	25/65	-0.55	2.68	-	295,296,296,296	0
2	CLA	A	255	25/65	-0.69	2.07	-	296,296,296,296	0
3	CHL	A	266	25/66	-0.64	3.56	-	295,296,296,296	0
2	CLA	A	257	25/65	-0.64	2.57	-	296,296,296,296	0
3	CHL	A	262	25/66	-0.23	2.43	-	295,296,296,296	0
2	CLA	A	256	25/65	-0.68	3.14	-	294,296,296,296	0
2	CLA	A	253	25/65	-0.45	2.67	-	295,296,296,296	0
3	CHL	A	261	25/66	-0.53	3.75	-	295,296,296,296	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.