



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:53 PM GMT

PDB ID : 1VPR  
Title : Crystal structure of a luciferase domain from the dinoflagellate *Lingulodinium polyedrum*  
Authors : Schultz, L.W.; Liu, L.; Cegielski, M.; Hastings, J.W.  
Deposited on : 2004-11-15  
Resolution : 1.80 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.

---

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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

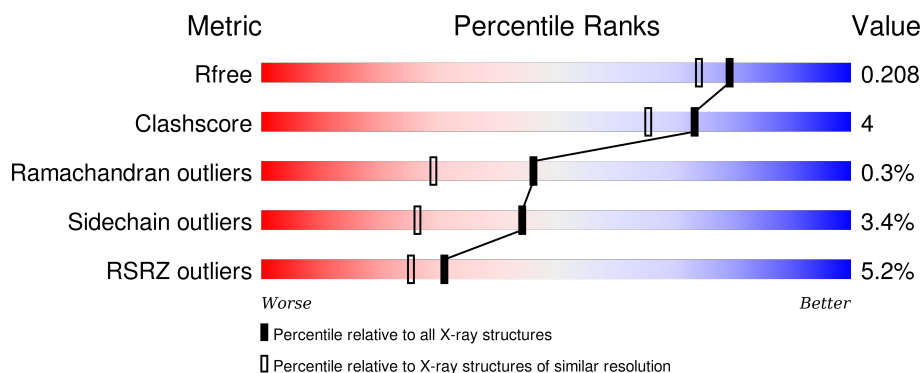
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	374	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2912 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 luciferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	351	2660	1694	458	493	8	7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	898	MSE	MET	MODIFIED RESIDUE	UNP O77206
A	912	MSE	MET	MODIFIED RESIDUE	UNP O77206
A	957	MSE	MET	MODIFIED RESIDUE	UNP O77206
A	990	MSE	MET	MODIFIED RESIDUE	UNP O77206
A	1070	MSE	MET	MODIFIED RESIDUE	UNP O77206
A	1132	MSE	MET	MODIFIED RESIDUE	UNP O77206
A	1153	MSE	MET	MODIFIED RESIDUE	UNP O77206

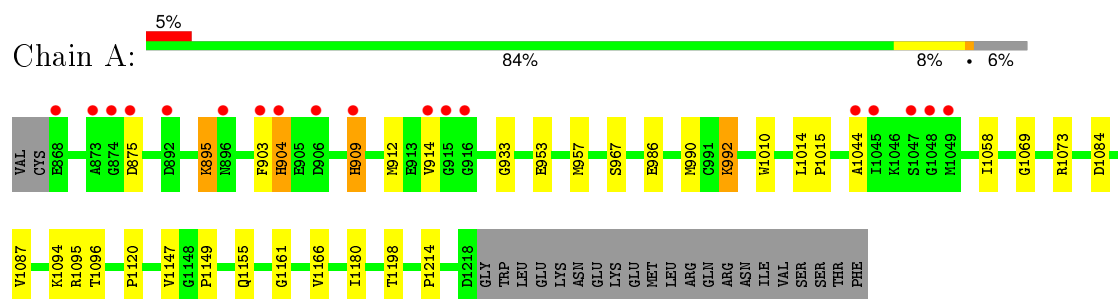
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	252	Total	O	0	0
			252	252		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: luciferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.99Å 63.95Å 96.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.60 – 1.80 28.85 – 1.70	Depositor EDS
% Data completeness (in resolution range)	88.0 (28.60-1.80) 83.6 (28.85-1.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.230 0.209 , 0.208	Depositor DCC
$R_{free}$ test set	2569 reflections (8.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.7	Xtriage
Anisotropy	1.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35879 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.49	0/2730	0.72	2/3695 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	933	GLY	N-CA-C	5.85	127.72	113.10
1	A	1069	GLY	N-CA-C	-5.58	99.16	113.10

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	2660	0	2489	21	0
2	A	252	0	0	4	0
All	All	2912	0	2489	21	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 4.

All (21) 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:957:MSE:HE2	1:A:1147:VAL:HG12	1.55	0.87
1:A:1084:ASP:OD1	1:A:1094:LYS:HG2	1.75	0.86
1:A:895:LYS:N	1:A:895:LYS:HD3	2.15	0.62
1:A:912:MSE:HE2	1:A:914:VAL:CG2	2.30	0.61
1:A:1073:ARG:HB2	1:A:1084:ASP:HB2	1.87	0.57
1:A:967:SER:HB2	2:A:240:HOH:O	2.09	0.51
1:A:909:HIS:H	1:A:909:HIS:CD2	2.27	0.51
1:A:992:LYS:HD2	2:A:23:HOH:O	2.11	0.50
1:A:912:MSE:HE2	1:A:914:VAL:HG22	1.92	0.50
1:A:903:PHE:O	1:A:904:HIS:C	2.51	0.49
1:A:1161:GLY:HA2	2:A:235:HOH:O	2.13	0.49
1:A:986:GLU:O	1:A:990:MSE:HG3	2.12	0.48
1:A:1010:TRP:O	1:A:1198:THR:HA	2.13	0.48
1:A:895:LYS:H	1:A:895:LYS:HD3	1.79	0.47
1:A:1155:GLN:HB3	1:A:1166:VAL:HB	1.97	0.46
1:A:1096:THR:OG1	1:A:1180:ILE:HG13	2.15	0.46
1:A:1044:ALA:CB	1:A:1058:ILE:HD13	2.45	0.46
1:A:1014:LEU:HD12	1:A:1015:PRO:HD2	1.99	0.43
1:A:1044:ALA:HB2	1:A:1058:ILE:HD13	2.00	0.42
1:A:1087:VAL:HG22	2:A:221:HOH:O	2.18	0.42
1:A:909:HIS:H	1:A:909:HIS:HD2	1.69	0.41

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	349/374 (93%)	340 (97%)	8 (2%)	1 (0%)	46 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	904	HIS

### 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	264/300 (88%)	255 (97%)	9 (3%)	44 26

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	875	ASP
1	A	895	LYS
1	A	909	HIS
1	A	953	GLU
1	A	992	LYS
1	A	1095	ARG
1	A	1120	PRO
1	A	1149	PRO
1	A	1214	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	896	ASN
1	A	909	HIS
1	A	1056	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	344/374 (91%)	-0.02	18 (5%) 31 25	12, 20, 43, 53	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1049	MET	9.8
1	A	873	ALA	3.9
1	A	1048	GLY	3.6
1	A	892	ASP	3.5
1	A	916	GLY	3.4
1	A	914	VAL	3.3
1	A	909	HIS	3.2
1	A	1047	SER	3.1
1	A	915	GLY	3.1
1	A	904	HIS	3.0
1	A	1044	ALA	2.9
1	A	1045	ILE	2.9
1	A	874	GLY	2.7
1	A	868	GLU	2.6
1	A	896	ASN	2.6
1	A	906	ASP	2.5
1	A	875	ASP	2.1
1	A	903	PHE	2.0

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.