



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:25 pm BST

PDB ID : 6AC3
Title : Structure of a natural red emitting luciferase from Phrixothrix hirtus (P3121 crystal form)
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Deposited on : 2018-07-24
Resolution : 3.60 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

<https://www.wwpdb.org/validation/2017/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
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

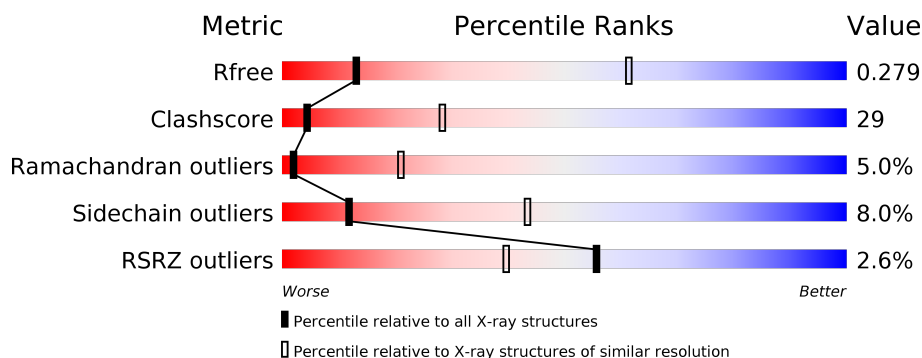
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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	546	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>31%</div> <div>• •</div> <div>23%</div> </div> </div>
1	B	546	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>40%</div> <div>12%</div> <div>• •</div> </div> </div>
1	C	546	<div> <div>%</div> <div> <div></div> <div>43%</div> <div>30%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	546	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>27%</div> <div>•</div> <div>24%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13982 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.

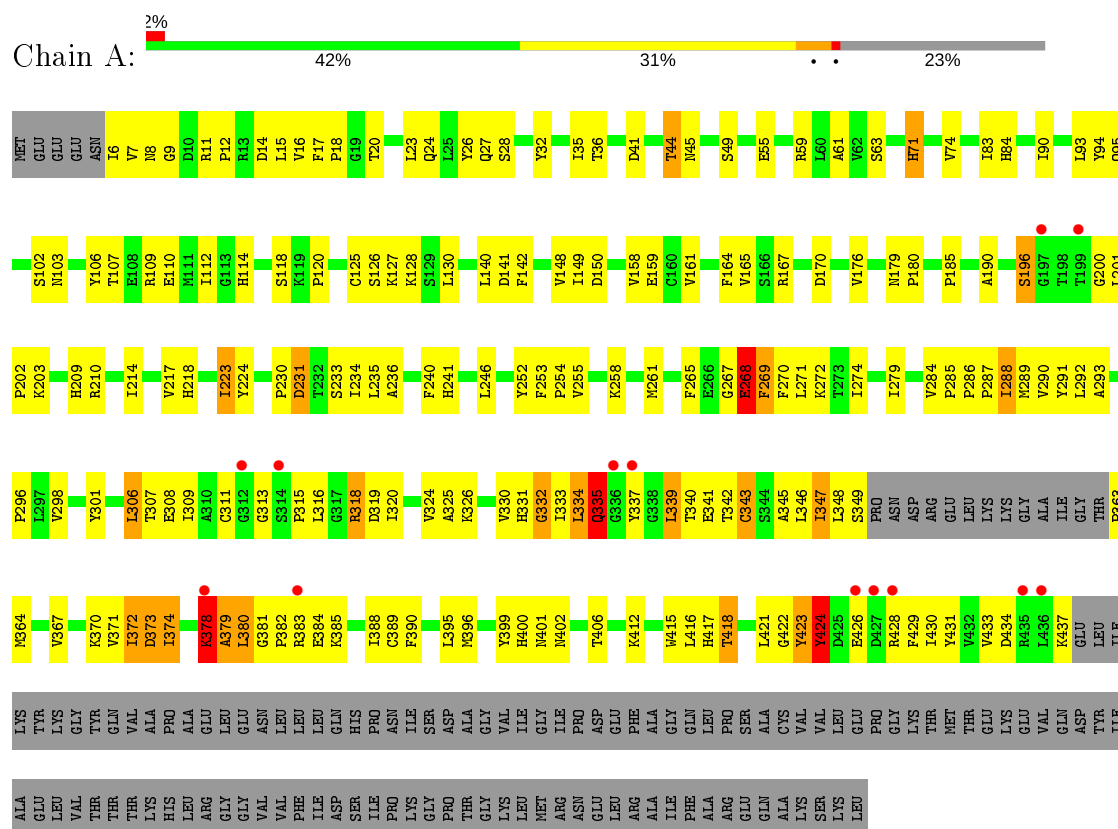
- Molecule 1 is a protein called Red-bioluminescence eliciting luciferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3296	2134	544	599	19			
1	B	528	Total	C	N	O	S	0	0	0
			4135	2667	686	760	22			
1	C	417	Total	C	N	O	S	0	0	0
			3279	2122	541	597	19			
1	D	416	Total	C	N	O	S	0	0	0
			3272	2117	540	596	19			

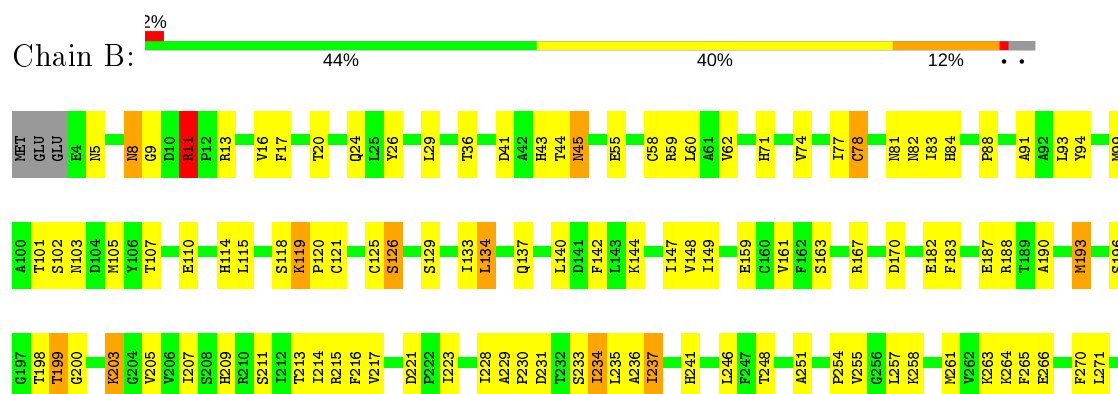
3 Residue-property plots

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: Red-bioluminescence eliciting luciferase



- Molecule 1: Red-bioluminescence eliciting luciferase





LEU	ALA	G377	T307	P222	M103
ARG	GLU	K378	E308	I223	
GLY	LEU	A379	I309		T107
VAL	GLU	L380	A310	I228	E108
VAL	ASN	G381	C311	A229	R109
PHE	LEU	P382	G312	P230	
ILE	LEU	R383	G313	D231	I112
ASP	LEU	E384	S314		G113
SER	GLN	K385	P315	I234	H114
HIS	PRO		L316		
ILE	PRO	I388	G317	I237	S118
ASN	ASN	G389	R318		K119
ILE	ILE	F390	D319	F240	P120
SER	SER			H241	G121
PRO	ASP	Q393	K323		L122
THR	ALA	M394	V324	F249	S126
GLY	ALA	L395	A325		L134
LYS	GLY	M396	K326	L246	L140
LEU	VAL	K397	R327	A251	F142
MET	ILE	G398	L328		K145
ARG	GLY	Y399		P254	I149
ASN	PRO		H331		E159
GLU	ASP	N402	G332	V260	C160
LEU	GLU		I333	M261	V161
ARG	PHE	A405	L334	K263	F162
ALA	ALA	T406	Q335	K264	S163
ILE	GLY	R407	G336	F265	F173
PHE	GLN	D408	Y337	E266	D174
ALA	LEU		G338	G267	
ARG	PRO	T418	L339	E268	K177
GLU	SER			F269	P185
GLN	ALA	L421	T342	L270	L186
ALA	CYS	G422	C343	L271	A190
LYS	VAL	Y423	S344	I274	T194
SER	VAL	Y424	A345		G197
LYS	LEU	D425	L346	I279	T198
LEU	GLU	E426	I347	A280	T199
PRO	PRO	D427	L348	S281	G200
GLY	LYS	R428	S349		K203
LYS	LYS	F429	PRO	V284	G204
THR	MET	I430	ASN	P285	H209
THR	THR	Y431	ASP	P286	R210
GLU	GLU	V432	ARG	P287	S211
LYS	LYS	V433	LEU	I288	
GLU	GLU	D434	LYS	M289	
VAL	VAL	R435	LYS	V290	
GLN	GLN	L436	GLY	Y291	
ASP	ASP		ALA	L292	
LEU	LEU	LYS	ILE	A293	
TYR	TYR	GLU	ILE	K294	
ILE	ILE	LYS	GLY	S295	
ALA	ALA	LYS	THR	P296	
GLU	GLU	TYR	P363	L297	
LEU	LEU	LYS		V298	
VAL	VAL	GLY	V371		
THR	THR	TYR	B372		
THR	THR	GLN	D373	L303	
THR	THR	VAL	I374	S304	
LYS	LYS	ALA	R375	S305	
HIS	HIS	PRO	T376	L306	
					D221

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.10Å 119.10Å 351.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 3.60 19.85 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.85-3.60) 99.1 (19.85-3.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.207 , 0.271 0.226 , 0.279	Depositor DCC
R_{free} test set	1020 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13982	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.58	0/3375	0.83	2/4573 (0.0%)
1	B	0.60	0/4229	0.77	2/5730 (0.0%)
1	C	0.56	0/3358	0.78	0/4551
1	D	0.57	0/3351	0.78	0/4541
All	All	0.58	0/14313	0.79	4/19395 (0.0%)

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	B	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	TYR	CA-CB-CG	7.25	127.18	113.40
1	B	134	LEU	CA-CB-CG	-5.30	103.10	115.30
1	B	328	LEU	CA-CB-CG	-5.17	103.40	115.30
1	A	423	TYR	C-N-CA	-5.17	108.78	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	ARG	Sidechain
1	B	511	ARG	Sidechain
1	B	539	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	3296	0	3330	209	0
1	B	4135	0	4187	291	0
1	C	3279	0	3306	164	0
1	D	3272	0	3297	157	0
All	All	13982	0	14120	808	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 29.

The worst 5 of 808 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:B:336:GLY:CA	1:B:348:LEU:HB3	1.41	1.46
1:A:9:GLY:CA	1:A:363:PRO:HG2	1.57	1.34
1:B:347:ILE:HD12	1:B:390:PHE:CE2	1.68	1.28
1:B:347:ILE:CD1	1:B:390:PHE:HE2	1.48	1.26
1:C:339:LEU:HD23	1:C:344:SER:CB	1.69	1.23

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	415/546 (76%)	342 (82%)	54 (13%)	19 (5%)	2	23
1	B	524/546 (96%)	397 (76%)	88 (17%)	39 (7%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	413/546 (76%)	355 (86%)	43 (10%)	15 (4%)	3	29
1	D	412/546 (76%)	343 (83%)	54 (13%)	15 (4%)	3	29
All	All	1764/2184 (81%)	1437 (82%)	239 (14%)	88 (5%)	2	21

5 of 88 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	231	ASP
1	A	319	ASP
1	A	378	LYS
1	A	379	ALA

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	365/471 (78%)	341 (93%)	24 (7%)	16	51
1	B	456/471 (97%)	389 (85%)	67 (15%)	3	20
1	C	363/471 (77%)	347 (96%)	16 (4%)	28	63
1	D	362/471 (77%)	345 (95%)	17 (5%)	26	61
All	All	1546/1884 (82%)	1422 (92%)	124 (8%)	12	43

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	378	LYS
1	B	456	LEU
1	D	260	VAL
1	B	389	CYS
1	B	434	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	531	ASN
1	C	116	ASN
1	D	275	GLN
1	C	27	GLN
1	B	71	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](#)

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, 95th 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 ²)	Q<0.9
1	A	419/546 (76%)	-0.29	13 (3%) 49 33	30, 84, 159, 208	0
1	B	528/546 (96%)	-0.30	11 (2%) 63 48	46, 85, 145, 200	0
1	C	417/546 (76%)	-0.32	8 (1%) 66 51	49, 92, 160, 207	0
1	D	416/546 (76%)	-0.35	15 (3%) 42 28	51, 87, 160, 191	0
All	All	1780/2184 (81%)	-0.32	47 (2%) 56 40	30, 87, 157, 208	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	427	ASP	5.7
1	D	198	THR	4.7
1	D	331	HIS	4.5
1	A	426	GLU	4.0
1	C	426	GLU	3.9

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.