



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2PSH / pdb_00002psh
Title : Crystal Structures of the Luciferase and Green Fluorescent Protein from Renilla Reniformis
Authors : Loening, A.M.; Fenn, T.D.; Gambhir, S.S.
Deposited on : 2007-05-06
Resolution : 1.79 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

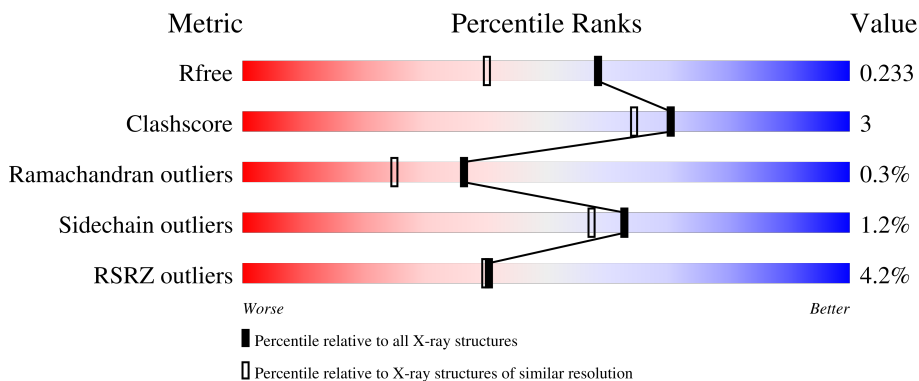
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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 $\leq 5\%$. 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	319	 3% 89% 5% 7%
1	B	319	 4% 83% 9% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5336 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 Renilla-luciferin 2-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2429	1576	411	433	9	0	0	0
1	B	299	2431	1575	411	436	9	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	engineered mutation	UNP P27652
A	25	ALA	LYS	engineered mutation	UNP P27652
A	55	THR	ALA	engineered mutation	UNP P27652
A	124	ALA	CYS	engineered mutation	UNP P27652
A	130	ALA	SER	engineered mutation	UNP P27652
A	136	ARG	LYS	engineered mutation	UNP P27652
A	143	MET	ALA	engineered mutation	UNP P27652
A	185	VAL	MET	engineered mutation	UNP P27652
A	253	LEU	MET	engineered mutation	UNP P27652
A	277	ALA	GLU	engineered mutation	UNP P27652
A	287	LEU	SER	engineered mutation	UNP P27652
A	312	VAL	-	expression tag	UNP P27652
A	313	ASP	-	expression tag	UNP P27652
A	314	HIS	-	expression tag	UNP P27652
A	315	HIS	-	expression tag	UNP P27652
A	316	HIS	-	expression tag	UNP P27652
A	317	HIS	-	expression tag	UNP P27652
A	318	HIS	-	expression tag	UNP P27652
A	319	HIS	-	expression tag	UNP P27652
B	2	ALA	THR	engineered mutation	UNP P27652
B	25	ALA	LYS	engineered mutation	UNP P27652
B	55	THR	ALA	engineered mutation	UNP P27652
B	124	ALA	CYS	engineered mutation	UNP P27652
B	130	ALA	SER	engineered mutation	UNP P27652
B	136	ARG	LYS	engineered mutation	UNP P27652

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Chain	Residue	Modelled	Actual	Comment	Reference
B	143	MET	ALA	engineered mutation	UNP P27652
B	185	VAL	MET	engineered mutation	UNP P27652
B	253	LEU	MET	engineered mutation	UNP P27652
B	277	ALA	GLU	engineered mutation	UNP P27652
B	287	LEU	SER	engineered mutation	UNP P27652
B	312	VAL	-	expression tag	UNP P27652
B	313	ASP	-	expression tag	UNP P27652
B	314	HIS	-	expression tag	UNP P27652
B	315	HIS	-	expression tag	UNP P27652
B	316	HIS	-	expression tag	UNP P27652
B	317	HIS	-	expression tag	UNP P27652
B	318	HIS	-	expression tag	UNP P27652
B	319	HIS	-	expression tag	UNP P27652

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	237	Total O 237 237	0	0
2	B	239	Total O 239 239	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.78Å 75.65Å 89.19Å 90.00° 76.48° 90.00°	Depositor
Resolution (Å)	86.71 – 1.79 86.71 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.5 (86.71-1.79) 97.5 (86.71-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.229 0.199 , 0.233	Depositor DCC
R_{free} test set	3119 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtrriage
Anisotropy	0.417	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5336	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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 [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	0.58	0/2497	0.74	0/3378
1	B	0.55	0/2497	0.75	0/3377
All	All	0.57	0/4994	0.75	0/6755

There are no bond length outliers.

There are no bond angle outliers.

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	2429	0	2408	8	0
1	B	2431	0	2413	25	0
2	A	237	0	0	0	0
2	B	239	0	0	1	0
All	All	5336	0	4821	33	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 3.

The worst 5 of 33 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:14:MET:HE3	1:B:198:GLU:HG3	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:MET:CE	1:B:197:GLU:HB2	1.90	1.02
1:B:14:MET:HE2	1:B:197:GLU:HB2	1.55	0.89
1:B:14:MET:HE1	1:B:197:GLU:HB2	1.57	0.86
1:B:27:MET:HE1	1:B:107:LEU:CB	2.11	0.81

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	294/319 (92%)	286 (97%)	8 (3%)	0	100	100
1	B	295/319 (92%)	285 (97%)	8 (3%)	2 (1%)	18	8
All	All	589/638 (92%)	571 (97%)	16 (3%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	GLU
1	B	179	ASN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/280 (93%)	258 (99%)	2 (1%)	73	70
1	B	261/280 (93%)	257 (98%)	4 (2%)	57	49
All	All	521/560 (93%)	515 (99%)	6 (1%)	63	57

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	LYS
1	B	240	TYR
1	B	287	LEU
1	A	287	LEU
1	A	261	PHE

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

Mol	Chain	Res	Type
1	B	128	HIS
1	B	142	HIS
1	B	26	GLN
1	B	42	HIS
1	B	97	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 oligosaccharides 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	298/319 (93%)	0.18	11 (3%) 45 45	13, 21, 35, 47	0
1	B	299/319 (93%)	0.18	14 (4%) 36 35	13, 21, 37, 45	0
All	All	597/638 (93%)	0.18	25 (4%) 40 40	13, 21, 36, 47	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	TRP	6.4
1	B	163	ILE	5.3
1	A	261	PHE	4.8
1	A	262	PHE	4.6
1	B	261	PHE	3.1

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 oligosaccharides 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.