WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 02:10 AM EDT

PDB ID	:	2PSF
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	:	1.40 Å(reported)

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	:	2.23.2
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)	:	2.23.2

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 1.40 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.
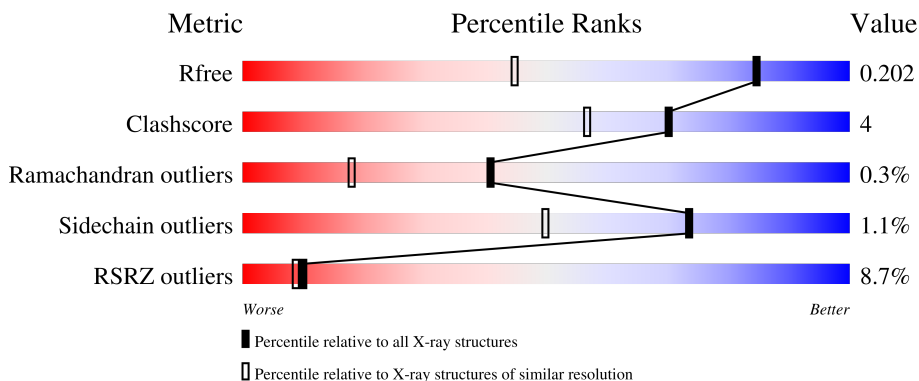
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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 <=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	310	6% / 94% / 5% ·
1	B	310	11% / 87% / 9% · ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 5773 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
1	A	307	Total	C	N	O	S	0	0	0
			2516	1631	422	454	9			
1	B	301	Total	C	N	O	S	0	0	0
			2467	1599	415	444	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	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	287	LEU	SER	engineered mutation	UNP P27652
B	2	GLY	-	expression tag	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
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	287	LEU	SER	engineered mutation	UNP P27652

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	425	Total	O	0	0
			425	425		

Continued on next page...

Continued from previous page...

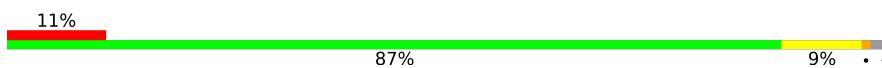| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	365	Total 365	O 365	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
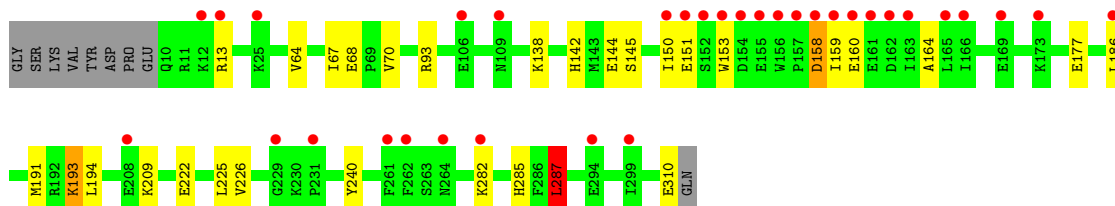
• Molecule 1: Renilla-luciferin 2-monooxygenase

Chain A:
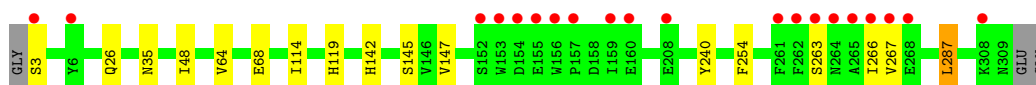
• Molecule 1: Renilla-luciferin 2-monooxygenase

Chain B:

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.18Å 82.28Å 90.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.40 48.69 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-1.40) 98.2 (48.69-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.194 0.181 , 0.202	Depositor DCC
R_{free} test set	5880 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5773	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/2588	0.59	0/3504
1	B	0.36	0/2537	0.59	1/3434 (0.0%)
All	All	0.36	0/5125	0.59	1/6938 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2516	0	2481	16	0
1	B	2467	0	2434	20	0
2	A	425	0	0	2	0
2	B	365	0	0	4	0
All	All	5773	0	4915	36	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.

The worst 5 of 36 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:263:SER:O	1:A:267:VAL:HG23	1.54	1.05
1:A:147:VAL:HG21	1:A:266:ILE:HG23	1.49	0.92
1:A:147:VAL:CG2	1:A:266:ILE:HG23	2.00	0.91
1:B:193:LYS:CE	2:B:667:HOH:O	2.34	0.75
1:B:67:ILE:O	1:B:70:VAL:HG22	1.92	0.70

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	305/310 (98%)	296 (97%)	9 (3%)	0	100	100
1	B	299/310 (96%)	285 (95%)	12 (4%)	2 (1%)	22	5
All	All	604/620 (97%)	581 (96%)	21 (4%)	2 (0%)	41	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	ASP
1	B	159	ILE

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/273 (99%)	269 (99%)	2 (1%)	84	66
1	B	265/273 (97%)	261 (98%)	4 (2%)	65	37
All	All	536/546 (98%)	530 (99%)	6 (1%)	73	50

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	240	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	142	HIS
1	B	178	ASN
1	B	285	HIS
1	A	142	HIS
1	A	264	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	307/310 (99%)	1.06	20 (6%)	18	17	15, 18, 26, 36	0
1	B	301/310 (97%)	1.23	33 (10%)	5	5	15, 18, 29, 38	0
All	All	608/620 (98%)	1.14	53 (8%)	10	9	15, 18, 28, 38	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	TRP	12.2
1	A	262	PHE	12.1
1	B	153	TRP	11.8
1	A	156	TRP	11.0
1	B	158	ASP	10.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.