



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1GFL / pdb_00001gfl
Title : STRUCTURE OF GREEN FLUORESCENT PROTEIN
Authors : Yang, F.; Moss, L.G.; Phillips Jr., G.N.
Deposited on : 1996-08-23
Resolution : 1.90 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
Xtriage (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

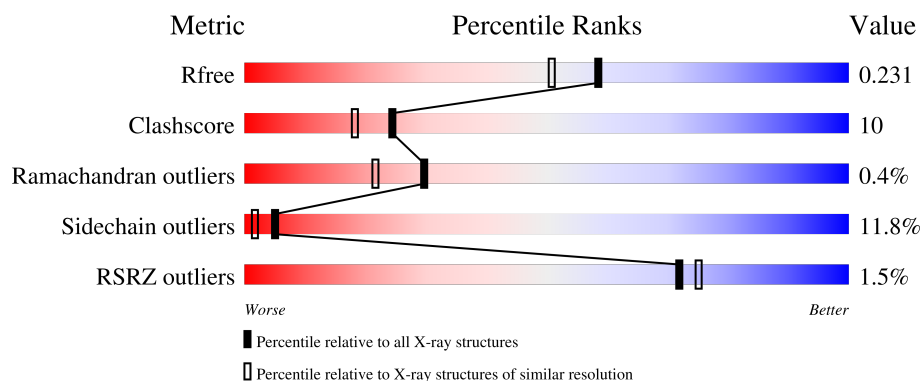
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	238	
1	B	238	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3950 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 GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1825	1161	309	349	6			
1	B	230	Total	C	N	O	S	0	0	0
			1825	1161	309	349	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total	O	0	0
			142	142		
2	B	158	Total	O	0	0
			158	158		

• Molecule 1: GREEN FLUORESCENT PROTEIN

LYS	L137	A1	E6	M153	P13	M164	H169	N23	Q177	V29	R181	L195	T203	L207	K209	E213	M218	L221	V224	T230	HIS	GLY	MET	ASP	GLU	LEU	TYR
	H138	S2		K158	I14		L15	N170		G24		L178		Y39		G40		Y66		P196							
	H148	K3		K158	I15		N171	H25				P197	Q204	S208	K214	E213	M218	L221	V224	T230	HIS	GLY	MET	ASP	GLU	LEU	TYR

• Molecule 1: GREEN FLUORESCENT PROTEIN

Lys	K126	K127	K128	D129	F130	L137	G138	H139	Q157	K158	M164	H169	E172	L178	H181	Y182	Q183	Q184	M185	I188	G189	D190	L195	P196	D197	N198	H199	Q204	L207	E213	K214	R215	D216	D217	L221	V224	I229	T230	H1S	GLY	MET	ASP	GLU	LEU	TRP
	A1	S2	K3	G4	E5	E6	P13	I14	L15	L18	N23	G24	H25	V29	G33	K41	L42	T43	L44	K45	F46	I47	K52	L53	P54	V55	V61	V66	P75	D76	H77	M78	H81	E95	R96	K107	T108	R109	A110	E111	T118	L119	V120	N121	R122

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.23Å 89.23Å 119.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.8 (10.00-1.90) 96.0 (10.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.91Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.262 0.192 , 0.231	Depositor DCC
R_{free} test set	3906 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3950	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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	0.99	8/1868 (0.4%)	1.13	21/2524 (0.8%)
1	B	1.00	13/1868 (0.7%)	1.16	27/2524 (1.1%)
All	All	0.99	21/3736 (0.6%)	1.15	48/5048 (1.0%)

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	A	1	3
1	B	1	1
All	All	2	4

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	TYR	CA-CB	-8.89	1.38	1.53
1	A	25	HIS	CG-CD2	7.35	1.44	1.35
1	B	66	TYR	CA-CB	-7.34	1.41	1.53
1	B	77	HIS	CG-CD2	7.16	1.43	1.35
1	B	25	HIS	CD2-NE2	6.32	1.44	1.37

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	TYR	N-CA-CB	13.39	133.13	110.49
1	A	66	TYR	N-CA-CB	11.88	130.57	110.49
1	B	199	HIS	ND1-CG-CD2	8.84	114.94	106.10
1	A	66	TYR	CA-CB-CG	8.57	129.32	113.90
1	A	81	HIS	CB-CG-CD2	-8.35	120.34	131.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	66	TYR	CA
1	B	66	TYR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	TYR	Sidechain
1	A	73	ARG	Sidechain
1	A	96	ARG	Peptide
1	B	96	ARG	Peptide

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	1825	0	1778	38	0
1	B	1825	0	1778	37	0
2	A	142	0	0	10	0
2	B	158	0	0	16	0
All	All	3950	0	3556	71	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 10.

The worst 5 of 71 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:183:GLN:HE21	1:A:185:ASN:HD21	1.10	0.97
1:B:183:GLN:HE21	1:B:185:ASN:HD21	1.09	0.92
1:B:2:SER:HB3	2:B:355:HOH:O	1.82	0.78
1:A:221:LEU:HB3	2:A:340:HOH:O	1.84	0.76
1:A:130:PHE:HB3	1:A:137:LEU:HD23	1.69	0.73

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	228/238 (96%)	223 (98%)	4 (2%)	1 (0%)	30	22
1	B	228/238 (96%)	223 (98%)	4 (2%)	1 (0%)	30	22
All	All	456/476 (96%)	446 (98%)	8 (2%)	2 (0%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	TYR
1	B	66	TYR

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	200/207 (97%)	176 (88%)	24 (12%)	5	2
1	B	200/207 (97%)	177 (88%)	23 (12%)	5	2
All	All	400/414 (97%)	353 (88%)	47 (12%)	5	2

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	VAL
1	B	120	VAL
1	B	41	LYS
1	B	66	TYR

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Mol	Chain	Res	Type
1	B	128	ILE

Sometimes 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	81	HIS
1	B	139	HIS
1	B	185	ASN
1	B	135	ASN
1	B	149	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 oligosaccharides 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 [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	230/238 (96%)	-0.20	1 (0%) 88 90	12, 24, 46, 62	0
1	B	230/238 (96%)	-0.19	6 (2%) 57 61	11, 23, 46, 64	2 (0%)
All	All	460/476 (96%)	-0.19	7 (1%) 72 75	11, 23, 47, 64	2 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	3.5
1	B	3	LYS	3.2
1	B	2	SER	3.1
1	B	230	THR	2.8
1	A	39	TYR	2.6

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.